ON STEINER TREES OF THE REGULAR SIMPLEX*

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Abstract. In the Euclidean Steiner Tree problem, we are given as input a set of points (called *terminals*) in the ℓ_2-metric space and the goal is to find the minimum-cost tree connecting them. Additional points (called *Steiner points*) from the space can be introduced as nodes in the solution.

The seminal works of Arora [1] and Mitchell [28] provide a Polynomial Time Approximation Scheme (PTAS) for solving the Euclidean Steiner Tree problem in fixed dimensions. However, the problem remains poorly understood in higher dimensions (such as when the dimension is logarithmic in the number of terminals) and ruling out a PTAS for the problem in high dimensions is a notoriously long standing open problem (for example, see Trevisan [38]). Moreover, the explicit construction of optimal Steiner trees remains unknown for almost all well-studied high-dimensional point configurations. Furthermore, a vast majority the state-of-the-art structural results on (high-dimensional) Euclidean Steiner trees were established in the 1960s, with no noteworthy update in over half a century.

In this paper, we revisit high-dimensional Euclidean Steiner trees, proving new structural results. We also establish a link between the computational hardness of the Euclidean Steiner Tree problem and understanding the optimal Steiner trees of regular simplices (and simplicial complexes), proposing several conjectures and showing that some of them suffice to resolve the status of the inapproximability of the Euclidean Steiner Tree problem. Motivated by this connection, we investigate optimal Steiner trees of regular simplices, proving new structural properties of their optimal Steiner trees, revisiting an old conjecture of Smith [34] about their optimal topology, and providing the first explicit, general construction of candidate optimal Steiner trees for that topology.

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1 Introduction

Given a finite set of points in space (called *terminals*), a *Steiner tree* of those points is a tree connecting those points. In addition to the terminals, the tree may contain additional points from the ambient space (called *Steiner points*). Finding the minimum cost Steiner tree is one of the most fundamental problems in Computer Science, Operations Research, and Combinatorial Optimization [26]. For example, Steiner trees arise naturally in network design [3, 29, 20], the design of integrated circuits [25, 3, 20], location problems [3, 20], machine learning [3], computer vision [33], systems biology [21, 39], and bioinformatics [21, 39, 3, 20].

In this work, we focus on the Euclidean Steiner tree problem, perhaps the most fabled setting of the problem, where the terminals lie in the Euclidean metric space. It was first studied in full generality at least as far back as 1811 and has been discussed in letters of Gauss. For three points, the Fermat-Toricelli problem, optimal Steiner trees were characterized completely as early as the 1600s by Toricelli. The interested reader may see [2] for more details on the history of the Euclidean Steiner tree problem.

Jarník and Kössler [23] first derived most of the known fundamental structural properties of Euclidean Steiner trees in 1934. The seminal work of Gilbert and Pollak [16] gave additional proofs of these properties and several others. Their structural results essentially remain the best existing tools for analyzing high-dimensional Euclidean Steiner trees.

Computational Aspects. Building on the work of Garey and Johnson [15] wherein they proved that the Rectilinear Steiner Tree problem (i.e., terminals are in ℓ_1-metric space) is NP-hard, in a joint work with Graham [14], they proved that the Euclidean Steiner Tree problem is also NP-hard by a clever planar gadget construction. In their seminal works, Arora [1] and Mitchell [28] gave a polynomial-time approximation scheme (PTAS) for the Steiner Tree problem in all ℓ_p-metric spaces, albeit in constant dimensions. However, their work left open the hardness of approximation of the Euclidean Steiner Tree problem in high dimensions (such as when the dimension is at least logarithmic in the number of terminals). Trevisan [38] showed that the Rectilinear Steiner Tree problem is APX-hard by a reduction from the Steiner Tree problem in the Hamming metric (which was previously shown to be APX-hard [8]). Trevisan's reduction appeals to the Hamming metric's discrete combinatorial structure. In fact, an even simpler proof can be derived from much earlier known structural results about Hamming and Rectilinear Steiner trees (e.g., Lemma 1 of [8] combined with Theorem 4 of [18]).

Proving the APX-hardness of the Steiner Tree problem in ℓ_p-metrics, for $p > 1$, appears to require engaging with the delicate structure of $\mathbb{R}^d$ directly. Due to the PTAS for the problem in fixed dimensions, any such argument requires dealing with truly high-dimensional hard instances. Recently, Fleischmann et al. [13] showed that the Steiner Tree problem is APX-hard in the ℓ_∞-metric. They also showed that when the set of candidate Steiner points is provided as part of the input (as a special case of the graph Steiner Tree problem), then this discrete variant of the Steiner Tree problem is APX-hard in all ℓ_p-metric spaces. However, the hardness of approximation of the classical Euclidean Steiner Tree problem remains unresolved in arbitrary dimensions.

Open Question 1. *Is the Euclidean Steiner Tree problem* APX*-hard in high dimensions?*

Existing techniques in the area pave the way for a simple approach to prove the APX-hardness of the Euclidean Steiner Tree problem in high dimensions. Trevisan [38] uses a simple gap-preserving reduction from the Vertex Cover problem, and a similar reduction applies in the setting where the candidate Steiner points are provided as input.

As motivation, we sketch a simple reduction framework for proving APX-hardness of the Euclidean Steiner Tree problem. We formalize this in Appendix A. We reduce from the Vertex Cover problem on bounded degree triangle-free graphs. Namely, there exists some $\rho > 0$ such that it is NP-hard to decide whether a triangle-free graph $G = (V, E)$ has a vertex cover of size $r|E|$ or all of its vertex covers are of size at least $(1 + \rho) \cdot r|E|$ (for some $r, \rho > 0$) [5, 24]. Now, we embed G into $\mathbb{R}^{|V|}$ by embedding each edge $\{u, v\} \in E$ as $\mathbf{e}_u + \mathbf{e}_v$, where $\mathbf{e}_u$ is the standard basis vector with 1 in the coordinate indexed by u and 0 elsewhere. Thus, each edge is embedded as its characteristic vector. The embedding of the set of edges incident to a single vertex forms the regular simplex of side length $\sqrt{2}$. The point configuration as a whole composes of the vertices of a regular simplicial complex (where we take the union of the simplices associated with each vertex).

Observe that a vertex cover of G of size $r|E|$ induces a partition of the embedded simplicial complex into $r|E|$ regular simplices. Moreover, any partition of the simplicial complex into regular simplices induces a vertex cover in G of the same size (using that G is triangle-free). Then, it would suffice to show that there exist $s, \beta > 0$ such that the following holds:

1. Any embedded point configuration forming the vertices of a regular simplicial complex partitionable into $r|E|$ regular simplices has a Steiner tree of cost at most $s|E|$.
2. Any embedded point configuration forming the vertices of a regular simplicial complex such that the minimum size of a partition into regular simplices is at least $(1 + \rho)r|E|$ has minimum Steiner tree of cost at least $(1 + \beta)s|E|$.

Namely, this would imply that the Euclidean Steiner Tree problem is NP-hard to approximate within a factor less than $(1 + \beta)$. Why might we expect this reduction to even be gap-preserving? On the one hand, this reduction, interpreted instead in the ℓ_1-metric, *is* used to show APX-hardness of the Rectilinear Steiner Tree problem (e.g., see [38]).

Additionally, heuristically, regular simplices have incredibly efficient Steiner trees, so having a valid Steiner tree composed of few Steiner trees of a regular simplex should result in especially low cost optimal Steiner trees. To understand this, we consider the notion of *Steiner ratios*: the Steiner ratio of a finite point configuration $P \subset \mathbb{R}^d$ is the ratio of the cost of its optimal Steiner tree to the cost of its minimum spanning tree. For example, the Steiner ratio of the vertices of an equilateral triangle is $\sqrt{3}/2$—the optimal Steiner tree is formed by connecting the three vertices to a Steiner point at the center of the triangle. The Steiner ratio of a point configuration measures the efficiency of its Steiner tree relative to trivially connecting the points in a minimum spanning tree. Gilbert and Pollak famously conjectured that the vertices of an equilateral triangle, i.e., the vertices of a 2-dimensional regular simplex, form the most efficient Steiner tree among all planar point configurations.

Conjecture 1 (Gilbert-Pollak Steiner Ratio Conjecture [16])**.** *The minimum Steiner ratio over planar point configurations is* $\sqrt{3}/2$.

This important conjecture remains open after nearly 50 years (despite at least one high-profile incorrect proof [22]). They further conjectured that the vertices of a regular simplex have the minimum Steiner ratio in higher dimensions. This is false: for example, the configuration of many regular simplices overlapping on a common vertex has a smaller Steiner ratio [11]. Nonetheless, the constructions of all known counterexamples require increasing the number of points in the configuration. We conjecture that this is necessary: the vertices of a regular simplex have the minimum Steiner ratio over all point configurations on at most that many terminals.

Conjecture 2 (Simplex is the Best)**.** *The* $d+1$ *vertices of a* d*-dimensional regular simplex have the minimum Steiner ratio over all point configurations of* $d+1$ *points in Euclidean space.*

While this is akin to the generalized Gilbert-Pollak conjecture in that it is about point configurations minimizing the Steiner ratio, the key difference is that we bound the number of terminals, not the number of dimensions. This is much more natural from a computational perspective. The natural dimension bound is then that any $d+1$ points can be embedded into d-dimensional space. Importantly, regular simplices meet this bound.

This conjecture would have structural implications for our efforts to prove APX-hardness of Euclidean Steiner Tree. The following weaker version of Conjecture 2 is also relevant to this reduction strategy.

Conjecture 3 (Simplex is the Best for Graph Embeddings)**.** *Over all graphs with* m *edges, the embedding*[1] *of the star graph on* m *edges has the minimum cost Steiner tree.*

Note that, since the graphs all have the same number of edges, their minimum spanning tree costs are all the same. Hence, Conjecture 3 can also be viewed as a conjecture about the point configuration with the minimum Steiner ratio. In this sense, it is a restricted version of Conjecture 2. We have verified the weaker Conjecture 3 computationally up to $m = 10$ using the exact algorithm of Smith [34].

The aforementioned reduction strategy to Euclidean Steiner tree problem appears deceptively simple to employ and either verify or reject. However, there is a fundamental obstacle: **we do not know how to efficiently construct the optimal Steiner tree for any (non-trivial) high-dimensional Euclidean point configuration.**[2] Perhaps the simplest possible point configuration in $\mathbb{R}^{d+1}$ is the collection of standard basis vectors.

[1] Here we allude to embedding each edge by it's characteristic vector, as detailed in the aforementioned reduction from the Vertex Cover problem.

[2] There are several optimization models permitting, in theory, the computation of optimal solutions to the Euclidean Steiner tree problem [27, 12, 30, 31]. Nonetheless, they are not a sufficient aid to our ignorance of the structure of solutions for even the most basic instances of the problem.

These points are precisely the vertices of a d-dimensional regular simplex. Even the optimal Steiner tree of the (vertices of the) regular simplex is unknown, although Gilbert and Chung [6] constructed candidate optimal trees in the special case of the number of vertices being a sum of up to three powers of two. For almost every other natural high-dimensional point configuration, we are completely ignorant of the structure of the optimal Steiner tree.

The objective of this paper is to revitalize this important line of work in the hope of ultimately resolving Open Question 1. To achieve this, we need to extend our understanding of high-dimensional Euclidean Steiner trees beyond the results of the previous century.

1.1 Organization of the paper

In Section 2, we define the terminology we will use in discussing the Euclidean Steiner tree problem, establish notational conventions, and recall several relevant classical structural properties of Steiner trees. In Section 3, we prove three new structural results about Euclidean Steiner trees: two of them extend previous results of [16] and the third provides a simple condition for restricting the topologies of optimal Steiner trees. In Section 4, we discuss a little-known conjecture of Smith [34] about the topology of optimal Steiner trees of the regular simplex, motivating it from a new viewpoint and describing its interdisciplinary connections to existing work in chemical graph theory and computational biology. In Section 5, we prove several new structural results about the optimal Steiner trees of the regular simplex and show how to explicitly construct Steiner trees of the conjectured optimal topologies. In Section 6, we revisit Conjecture 3 from Section 1, making partial progress toward the conjecture. Finally, in Appendix A, we state an analytic conjecture about the Steiner tree problem on regular simplicial complexes, proving that it implies APX-hardness of the Euclidean Steiner Tree problem (Open Problem 1).

2 Preliminaries

In this paper, we consider the Euclidean Steiner Tree problem. The problem is as follows. Given $P \subset \mathbb{R}^d$ finite, find $S \subset \mathbb{R}^d$ such that the minimum cost spanning tree T of $P \cup S$ has the infimum cost of all trees over all choices of S. The length of each edge in the tree is the Euclidean distance between its endpoints. The elements of P are *terminals*, the additional points in S are *Steiner points*, and any spanning tree of $P \cup S$ for any choice of S is a *Steiner tree*. An *optimal Steiner tree* for P is a Steiner tree of minimum cost for P.

For much of the paper, we will consider Steiner trees of the vertices of *regular simplices*. Regular simplices are polytopes such that all vertices are equidistant. In particular, the vertices of a $(d-1)$-dimensional regular simplex can be embedded in d dimensions as the set of d standard basis vectors in $\mathbb{R}^d$. For $1 \le i \le d$, we denote these vectors by $\mathbf{e_i}$. For clarity with the number of terminals, we use *regular d-simplex* to refer to regular simplices with d vertices. For simplicity, when we consider the Steiner trees of the regular d-simplex, we mean the vertices of the regular simplex expressed as standard basis vectors (unless otherwise specified). Throughout the paper, for a point $\mathbf{p} \in \mathbb{R}^d$, we use p_i to refer to its i^{th} coordinate.

We now recall several useful facts about optimal Steiner trees from [16]. Although it is always possible to trivially add Steiner points without increasing the length of a Steiner tree (by subdividing an edge), we assume that optimal Steiner trees do not contain such Steiner points.

Theorem 1 ([16, §3.2]). *Let* $\mathbf{x}$ *be a vertex in an optimal Steiner tree. Suppose there are two edges incident to* $\mathbf{x}$*. Then the angle included by these edges is at least* $120°$.

Corollary 1 ([16, §3.3]). *In an optimal Steiner tree, there are exactly 3 edges incident to every Steiner point. Moreover, these lines are co-planar.*

The co-planarity property was not explicitly stated in [16], but it is easy to see from Theorem 1 and the first part of Corollary 1.

Theorem 2 ([16, §3.4]). *In an optimal Steiner tree of* n *terminals, there are at most* $n - 2$ *Steiner points.*

In particular, a Steiner tree with n terminals and exactly $n - 2$ Steiner points is a *full* Steiner tree.

Theorem 3 ([16, §3.5]). *Let* P *be the set of terminals of an optimal Steiner tree. Then all Steiner points lie within the convex hull of* P.

Theorem 4 ([16, §4, Uniqueness Theorem]). *For a given topology of a Steiner tree on the set of terminals in any Euclidean space, there always exists a unique Steiner tree with this topology of minimal length.*

By *topology*, we mean the choice of edges in the Steiner tree between (unlabeled) Steiner points and the (labeled) terminals. For a fixed topology, the *relatively minimal tree* refers to the unique tree from Theorem 4.

The easiest case to consider is the equilateral triangle, i.e. 2-dimensional regular simplex. For general triangles, it was solved as early as 17$^{\text{th}}$ century by Torricelli, Cavalieri and others and it was thoroughly analysed from different points of view in the last century—see [7] or [35]. The conclusion is that the optimal Steiner tree contains a Steiner point (also called *Fermat point*) if and only if all of the interior angles are strictly less than $120°$. In [6], they provide a formula for computing all distances to the Steiner point when a suitable triangle is given.

3 New structural properties of Steiner trees

In this section we introduce several structural results about Euclidean Steiner trees that apply even in the high-dimensional setting. Garey, Graham, and Johnson's proof of NP-hardness of Euclidean Steiner Tree proves NP-hardness in the plane using that edges do not cross in an optimal tree [14]. This property is extremely powerful in analyzing planar Steiner trees, but, while still true in higher dimensions, it is no longer useful. We do not know how to prove even NP-hardness of Euclidean Steiner Tree without proving it in the plane, partly for lack of effective higher dimensional tools. The purpose of this section is to begin to ameliorate this deficiency.

3.1 Edge lengths in optimal Steiner trees

In [16, §8.4], the authors presents a bound on the length of edges between Steiner points in any optimal Steiner tree relative to the nearby edges in the tree. The argument only applies to Steiner trees on the plane (e.g., see [25, §9]). In this section we use the local planarity of optimal Steiner trees to prove a similar result which holds in any Euclidean space.

Theorem 5. *Let* $\mathbf{s_1}$ *and* $\mathbf{s_2}$ *be two Steiner points connected by an edge in an optimal Steiner tree* T *in the Euclidean space of dimension* $d \geq 3$*. Let* $N(\mathbf{x})$ *denote the neighbourhood of a vertex* $\mathbf{x} \in T$ *and* $L_0 = \min_{\mathbf{s} \in \{\mathbf{s_1},\mathbf{s_2}\}} \min_{\mathbf{v} \in N(\mathbf{s}) \setminus \{\mathbf{s_1},\mathbf{s_2}\}} ||\mathbf{s}-\mathbf{v}||$*. Then* $||\mathbf{s_1}-\mathbf{s_2}|| \geq \left(\frac{\sqrt{6}}{2}-1\right) L_0$*.*

Proof. The proof is similar to the proof in [16, §8.4]. Without loss of generality, assume there is a point $\mathbf{x_1}$ in T adjacent to $\mathbf{s_1}$ and at distance L_0 and let $\mathbf{y_1}$ be a point at distance L_0 from $\mathbf{s_1}$ in the line incident to $\mathbf{s_1}$ not containing $\mathbf{s_2}$ or $\mathbf{x_1}$. Similarly, let $\mathbf{x_2}, \mathbf{y_2}$ be the two points at distance L_0 from $\mathbf{s_2}$ on the lines of T incident to $\mathbf{s_2}$ but not containing $\mathbf{s_1}$. See Figure 1.

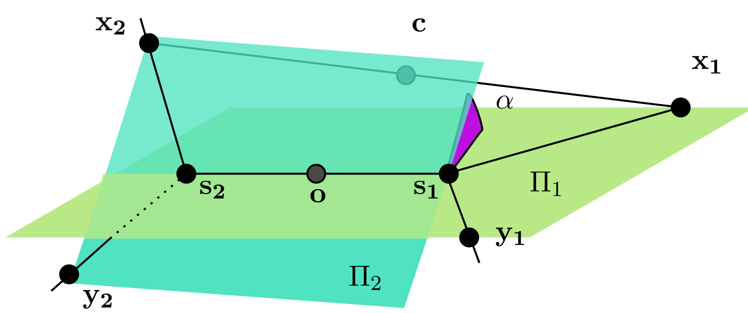

Figure 1: 3-dimensional space defined by the intersecting planes with key points labeled.

From Corollary 1, we have that for the Euclidean space of dimension $d \geq 2$, the lines incident to a given Steiner point are co-planar. Thus, two adjacent Steiner points define two planes that meet at a line, so we only need to consider the 3-dimensional space defined by these two intersecting planes. Let Π_1 and Π_2 denote such planes defined by the points $\mathbf{x_1}, \mathbf{y_1}, \mathbf{s_2}$ and $\mathbf{x_2}, \mathbf{y_2}, \mathbf{s_1}$, respectively. So either Π_1 and Π_2 meets only in the line defined by $\mathbf{s_1}$ and $\mathbf{s_2}$, or $\Pi_1 = \Pi_2$. We only need to consider the former case by [16, §8.4]. For this, let α denote the angle at which Π_1 and Π_2 intersect (α is the acute angle between the lines $\overleftrightarrow{\mathbf{x_1 y_1}}$ and $\overleftrightarrow{\mathbf{x_2 y_2}}$ when both are translated to include the origin).

Let us introduce a coordinate system with unit length L_0 and origin $\mathbf{o}$ placed at the midpoint of the segment $\mathbf{s_1 s_2}$, given by shifting and scaling the original space. If $x = ||\mathbf{x_1}-\mathbf{x_2}||$ and $s = ||\mathbf{s_1}-\mathbf{s_2}||$, then we have the following:

$$
\begin{aligned}
\mathbf{o} &= (0,0,0) \\
\mathbf{s_1} &= \left(\frac{s}{2}, 0, 0\right) \\
\mathbf{s_2} &= \left(-\frac{s}{2}, 0, 0\right) \\
\mathbf{x_1} &= \left(\frac{1+s}{2}, \frac{\sqrt{3}}{2}\cos\left(-\frac{\alpha}{2}\right), \frac{\sqrt{3}}{2}\sin\left(-\frac{\alpha}{2}\right)\right) \\
\mathbf{x_2} &= \left(-\frac{1+s}{2}, \frac{\sqrt{3}}{2}\cos\left(\frac{\alpha}{2}\right), \frac{\sqrt{3}}{2}\sin\left(\frac{\alpha}{2}\right)\right) \\
\mathbf{y_1} &= \left(\frac{1+s}{2}, \frac{-\sqrt{3}}{2}\cos\left(-\frac{\alpha}{2}\right), \frac{-\sqrt{3}}{2}\sin\left(-\frac{\alpha}{2}\right)\right) \\
\mathbf{y_2} &= \left(-\frac{1+s}{2}, \frac{-\sqrt{3}}{2}\cos\left(\frac{\alpha}{2}\right), \frac{-\sqrt{3}}{2}\sin\left(\frac{\alpha}{2}\right)\right) \\
\mathbf{c} &= \left(0, \frac{\sqrt{3}}{2}\cos\left(\frac{\alpha}{2}\right), 0\right)
\end{aligned}
$$

where $\mathbf{c}$ is the midpoint of the line segment $\mathbf{x_1 x_2}$.

Now, we consider a second tree T' derived from T by removing $\mathbf{s_1}, \mathbf{s_2}$ and instead adding $\mathbf{x_1}, \mathbf{x_2}, \mathbf{y_1}$, and $\mathbf{y_2}$ as Steiner points and joining $\mathbf{x_1}, \mathbf{x_2}$ (respectively, $\mathbf{y_1}, \mathbf{y_2}$) to the Fermat point of triangle $\triangle\mathbf{x_1 x_2 o}$ (respectively, $\triangle\mathbf{y_1 y_2 o}$), respectively, and connecting those Fermat points (via a line passing through $\mathbf{o}$). Call these Fermat points $\mathbf{r_1}$ and $\mathbf{r_2}$, respectively. We are interested in finding the coordinates of $\mathbf{r_1}$ and using the optimality of T to obtain a bound on $||\mathbf{s_1} - \mathbf{s_2}||$ (it suffices to consider $\mathbf{r_1}$ by symmetry in this coordinate system).

Consider $\triangle\mathbf{c x_1 r_1}$. By symmetry of $\mathbf{x_1}$ and $\mathbf{x_2}$ about the line $\mathbf{oc}$ and the definition of a Fermat point, $\triangle\mathbf{c x_1 r_1}$ is a 30-60-90 triangle. Then, letting $x = \sqrt{(1+s)^2 + 3\sin^2(\frac{\alpha}{2})}$, we have that $||\mathbf{c} - \mathbf{r_1}|| = \frac{x}{2\sqrt{3}}$, $||\mathbf{c} - \mathbf{x_1}|| = x/2$, and $||\mathbf{x_1} - \mathbf{r_1}|| = x/\sqrt{3}$. Then, the difference in the length of trees T' and T is

$$
\underbrace{4||\mathbf{x_1} - \mathbf{r_1}|| + 2(||\mathbf{o} - \mathbf{c}|| - ||\mathbf{c} - \mathbf{r_1}||)}_{\text{from } T} - \underbrace{(s+4)}_{\text{from } T'} = \sqrt{3}\left(x + \cos\left(\frac{\alpha}{2}\right)\right) - (s+4) \leq 0,
$$

with the ≤ 0 inequality coming from optimality of T. Solving for s, we get the inequality

$$
s \geq \sqrt{3}\cos\left(\frac{\alpha}{2}\right) - 1.
$$

This is minimized for $\alpha = \frac{\pi}{2}$, where we get the inequality

$$||\mathbf{s_1} - \mathbf{s_2}|| \geq \left(\frac{\sqrt{6}}{2} - 1\right) L_0. \qquad \square$$

3.2 Bounds on the coordinates of Steiner points

Throughout this section we assume that our optimal Steiner trees do not contain trivial Steiner points (that is, Steiner points subdividing a line).

We prove that optimal Steiner trees in Euclidean spaces are not only contained in the convex hull of the input terminals, but the value of each coordinate of a Steiner point is also strictly contained in the interval formed by the minimum and maximum value in that coordinate among the terminals. This is formalized in the next lemma.

Lemma 1. *Let $P \subseteq \mathbb{R}^d$ be a finite point-set such that for all $1 \leq i \leq d$, there are $\mathbf{p}, \mathbf{q} \in P$ with $p_i \neq q_i$. Let $\mathbf{s}$ be a Steiner point in an optimal Steiner tree of P. Then, for all $1 \leq i \leq d$ it holds that*

$$\min_{\mathbf{p} \in P} p_i < s_i < \max_{\mathbf{p} \in P} p_i.$$

Proof. Assume not. Without loss of generality, we may assume that the statement does not hold for $i = 1$ and the bounds on the coordinate are $\min_{\mathbf{p} \in P} p_1 = 0$ and $\max_{\mathbf{p} \in P} p_1 = 1$. We prove the lower bound and the upper bound follows analogously.

Let T be an optimal Steiner tree for P. Suppose some Steiner point has first coordinate 0. Observe that some neighbor of the Steiner point must also have first coordinate 0 or else increasing the first coordinate of the Steiner point by an infinitesimal amount decreases the cost of the tree.

Now, since some terminal has nonzero first coordinate, there exists some Steiner point $\mathbf{s}$ with first coordinate 0 neighboring a point $\mathbf{x}$ with positive first coordinate. This uses the fact that T is contained in the convex hull of P by Theorem 3. By the above, $\mathbf{s}$ also has a neighbor $\mathbf{y}$ with first coordinate 0. Now recall Theorem 1 and Corollary 1: there are exactly three coplanar lines incident to $\mathbf{s}$. Any plane is defined by precisely two linearly independent lines. Using $\overleftrightarrow{\mathbf{sy}}$ as one of the two lines defining the plane, the other line must have non-fixed first coordinate. But we claim that the 120 degree angle property and coplanarity imply then that the 3$^{\text{rd}}$ neighbor of $\mathbf{s}$, $\mathbf{z}$, has negative first coordinate. To see this, note that $\overleftrightarrow{\mathbf{sy}}$ cuts the plane containing the lines incident to $\mathbf{s}$ into two parts. One side strictly contains $\mathbf{x}$ and the other strictly contains $\mathbf{z}$. Since the other line defining the plane has non-fixed first coordinate, this yields the claim.

However, we know from Theorem 3 that optimal Euclidean Steiner trees are contained in the convex hull of the terminal set, so this contradicts the optimality of T. $\square$

In fact, we can apply this lemma to prove that all Steiner points must be strictly contained in the convex hull of the terminal configuration.

Corollary 2. *For every finite $P \subseteq \mathbb{R}^d$, in any optimal Steiner tree T of P, all Steiner points in T are strictly contained in the convex hull of P.*

Proof. Suppose not. Suppose without loss of generality that the point configuration P cannot be embedded in fewer than d dimensions. Then, the convex hull of P is the intersection of $(d-1)$-dimensional hyperplanes (and the Steiner tree T is contained in the intersection of half-spaces). For each hyperplane composing part of the boundary of the convex hull, there is some terminal not contained in that hyperplane (or else the point configuration is embeddable in $\mathbb{R}^{d-1}$). Now, by rotating and translating the point configuration, we may assume that that hyperplane is a coordinate hyperplane corresponding to the first coordinate and that the interior of the convex hull is contained in the halfspace given by $\{\mathbf{x} \in \mathbb{R}^d : x_1 \geq 0\}$. Namely, 0 is a lower bound on the first coordinate of each Steiner point and the upper bound is strictly greater than 0 (since some terminal is not contained in the hyperplane). Then, by Lemma 1, no Steiner point can lie on this coordinate hyperplane and, hence, no Steiner point could lie on the hyperplane before translation and rotation either.

The same procedure applies to all hyperplanes making up the convex hull of P and hence the result follows. □

3.3 Degree constraints on terminals

We give a coordinate-based sufficient condition for a terminal being a leaf node in an optimal Steiner tree.

Lemma 2. *Let $P \subseteq \mathbb{R}^d$. Suppose there is some point $\mathbf{p} = (p_1, \ldots, p_d) \in P$ such that for each $i \in [d]$ we have $p_i = \max\{q_i : \mathbf{q} \in P\}$ or $p_i = \min\{q_i : \mathbf{q} \in P\}$. Then, $\mathbf{p}$ is a leaf node in every optimal Steiner tree T of P.*

Proof. Let T be a relatively minimal Steiner tree of P. Suppose that $\mathbf{p}$ has two lines incident to it with direction vectors $\vec{u}$ and $\vec{v}$ from $\mathbf{p}$ to the other endpoint of the edges, respectively. From Theorem 3, it follows that the other endpoints must be contained in the convex hull of P (whether the other endpoint be another terminal or a Steiner point). Therefore, in each coordinate $\vec{u}$ and $\vec{v}$ are either both non-negative or non-positive, depending on whether $\mathbf{p}$ is maximal or minimal in that coordinate.

Every pair of edges in T sharing a node intersect at an angle of at least 120°. But, $\vec{u} \cdot \vec{v} \geq 0$ and thus they form an angle of at most 90°, contradicting the optimality of T, as desired. □

4 The topology of Steiner trees of the regular simplex

In this section, we consider a conjecture of Smith about the topology of the optimal Steiner tree of the (vertices of the) regular simplex (Conjecture 2 of [34]). This conjecture extends the conjecture of [6] to regular simplices of all sizes. Smith verified the conjecture up to the regular 11-simplex (by running Smith's algorithm, we confirm that it holds for the regular 12-simplex as well). We provide new intuition for the conjecture and observe that trees with the conjectured topology have important extremal combinatorial properties with ties to chemical graph theory and the study of phylogenetic trees in computational biology.

4.1 The conjectured topology

From Lemma 2, we know that in any optimal Steiner tree of (the vertices of) a regular simplex, the leaf nodes are exactly the terminal nodes. Hence, there are exactly $n-2$ Steiner points (since each Steiner point is of degree precisely 3).

Let $\mathbf{e_i}$ and $\mathbf{e_j}$ be a pair of terminals with a topology-preserving coordinate permutation $\sigma : [d] \to [d]$ between them in some optimal Steiner tree of the regular simplex, T. Consider rooting T at $\mathbf{e_i}$. Then, we apply σ to each level of T rooted at $\mathbf{e_i}$ to get T rooted at $\mathbf{e_j}$. Such topology-preserving coordinate permutations are hence very restrictive and lead to extensive symmetries in the Steiner trees.

When does a topology-preserving coordinate permutation exist? Suppose that there exists an induced full binary subtree rooted at some Steiner point, with all its leaf nodes terminals. Then, the two subtrees induced by the children of the root can be interchanged by a permutation swapping the coordinates corresponding to the terminals in each subtree. Indeed, this observation may be repeated to yield a topology preserving coordinate permutation between any pair of terminals in the full subtree. We revisit this idea more rigorously in Section 5.

When $d = 2^k$, it is even possible to have topology-preserving coordinate permutation between every pair of terminals. One such topology permitting this is two full binary trees with 2^{k-1} terminal leaves each with their Steiner point root nodes connected by an edge (see Figure 2).

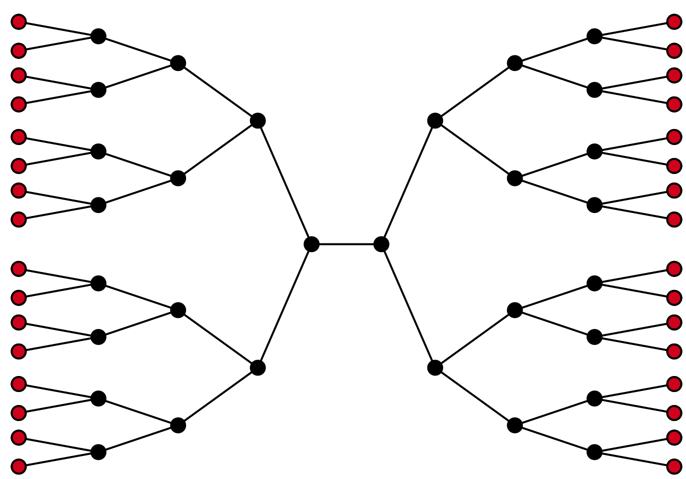

Figure 2: Two full binary trees on 16 terminals connected together.

Given the rigid structure induced by topology-preserving coordinate permutations, it feels plausible that trees exhibiting large full binary subtree structures are those of minimal cost. The topologies of the optimal Steiner trees (derived computationally via Smith's algorithm) are shown in Figure 3.

These topologies interpolate between the pair of full binary tree topologies for number of terminals a power of 2. We make this notion rigorous. We define a *good* binary tree of

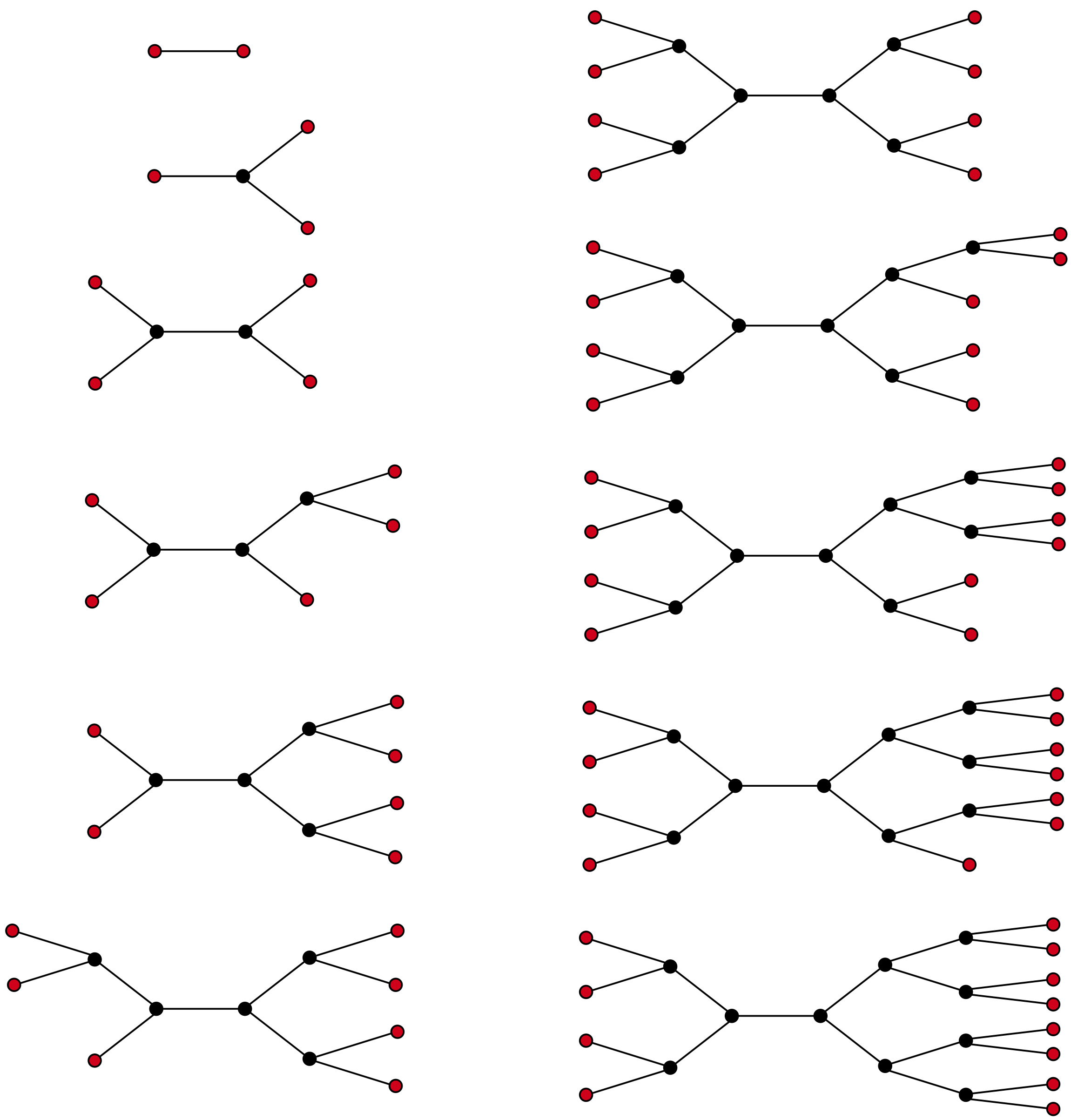

Figure 3: The optimal topology of the Euclidean Steiner tree of the regular simplex with up to 12 vertices, terminals marked red.

height k recursively. For height 0, it is a single node. For height $k > 0$, at most one subtree of the children of the root is a binary tree of height $k-1$ and the remaining subtrees are full binary trees of height $k-1$ or $k-2$. To avoid any confusion, note that this is not quite the structure of the trees shown in Figure 3. The connection between good binary trees and the trees in Figure 3 is made explicit in Conjecture 4.

Observe that in any good binary tree of height k the shortest distance from a root to a leaf node must be at least $k-1$ (this follows by a simple inductive argument). Hence, a good binary tree of height k contains strictly more than 2^{k-1} leaf nodes (and at most 2^k leaf nodes).

Lemma 3. *For $k \geq 1$ and $2^k < d \leq 2^{k+1}$ leaf nodes, there is a unique good binary tree of height $k+1$ (up to isomorphism) with that number of leaf nodes.*

Proof. We prove this by induction. This is clear for $d = 2$ leaves: the tree must be height 1 and hence must be a full binary tree of height 1.

Now, assume this holds for all $d < r$ and assume $2^k < r \leq 2^{k+1}$. Then, if $r \leq 2^k + 2^{k-1}$, by definition of a good binary tree of height $k+1$ and the fact that any good binary tree of height k contains strictly more than 2^{k-1} leaf nodes, one of the subtrees of the children of the root must be a full binary tree of height $k-1$. Then the other subtree must be a good subtree of height $k-1$ on $r - 2^{k-1}$ leaves, which, by induction, is unique up to isomorphism.

If $r > 2^k + 2^{k-1}$, since a good binary tree of height k contains at most 2^k leaf nodes, one of the subtrees of the children of the root must be a full binary tree of height k. Then, the other subtree must be a good subtree of height $k-1$ on $r-2^k$ leaves, yielding the desired via the inductive hypothesis. □

Finally, we can state the conjecture, a reformulated version of a conjecture of Smith [34].

Conjecture 4 (Optimal Topology of Steiner Trees of the Regular Simplex, Conjecture 2 of [34])**.** *Let $2 \leq 2^k < d \leq 2^{k+1}$. The topology of the optimal Steiner tree of a regular d-simplex is formed by taking the good binary tree of height $k+1$ on d leaf nodes, removing the root node, and reconnecting the tree via an edge between the former children of the root.*

In the next section we provide additional motivation for this topology, remarking that these trees are extremal with respect to a well-studied index of acyclic graphs from chemical graph theory.

4.2 Indices from chemical graph theory

Throughout this subsection, we will consider trees of the form of full Steiner trees: that is, trees with all non-leaf nodes of degree exactly three. Our connection to computational biology is simple: phylogenetic trees are precisely trees with this structure. We begin by defining several notions from chemical graph theory. The *Wiener index* [40] of a tree is the sum of pairwise hop-distances between nodes in the tree. I.e., for a tree T,

$$W(T) = \sum_{u,v \in V(T)} d_T(u,v).$$

Since its introduction in 1947, this has been one of the most widely used metrics in the study of quantitative structure-activity relationships in chemistry. See [10] for a thorough survey.

A related, more recently introduced index is the *terminal Wiener index* [17] of a tree, the Wiener index restricted only to pairs of leaf nodes. This index has garnered significant attention since its introduction [9, 4, 19, 42, 41, 32, 36]. Formally, let T be a tree and H an induced subgraph of T. Then, let $\ell(H)$ be the set of leaf nodes from T contained in H. For any edge $(u, v) \in E(T)$, let (C_u, C_v) be the cut induced by the edge. We have that

$$\Gamma(T) = \sum_{u,v \in \ell(T)} d_T(u, v) = \sum_{(u,v) \in E(T)} |\ell(C_u)||\ell(C_v)|.$$

This brings us to our main connection to these indices.

Theorem 6 ([19, 37])**.** *The trees of the form described in Conjecture 4 are the unique full Steiner trees minimizing the terminal Wiener index.*

Indeed, [19] reveals several other interesting properties of this extremal topology.

Definition 1 (Semi-regularity)**.** *Given a full Steiner tree T and some pair u, v of Steiner points, let T_u^1 and T_u^2 denote the subtrees rooted at the children of u upon removing the path $u \rightsquigarrow v$. Similarly define T_v^1 and T_v^2. For H an induced subtree of T, let $P(H)$ denote set of terminals in H. The pair (u, v) is semi-regular if*

$$\min(|P(T_v^1)|, |P(T_v^2)|) \geq \max(|P(T_u^1)|, |P(T_u^2)|)$$

or

$$\min(|P(T_u^1)|, |P(T_u^2)|) \geq \max(|P(T_v^1)|, |P(T_v^2)|).$$

The tree T is semi-regular if every pair of Steiner points is semi-regular.

If a pair were not semi-regular, then swapping a larger and a smaller subtree would result in a more balanced tree. Intuitively, this should not occur in optimal Steiner trees of the regular simplex due to its myriad symmetries. Indeed, we have the following.

Theorem 7 ([37])**.** *The unique semi-regular full Steiner trees are exactly the trees of the form described in Conjecture 4.*

5 Steiner trees of the regular simplex

In this section we explicitly compute Steiner trees of the regular simplex. Our constructions are a stronger version of the results of [6]. In the first subsection, we show several useful properties about Steiner trees of the regular simplex. In the second subsection, we describe our candidate construction for optimal Steiner trees. In the third subsection, we will apply this construction to give explicit coordinates for the candidate-optimal Steiner trees on $d = 2^k$ terminals and use these explicit coordinates to analyze the limiting Steiner ratio of the regular simplex.

5.1 Structural properties of Steiner trees of the regular simplex

The following definition will be useful.

Definition 2 (Extending Line)**.** *Let T be a tree in the Euclidean space. Let $\mathbf{x}, \mathbf{y} \in V(T)$ be two adjacent points in T. The* extending line *of the edge $(\mathbf{x}, \mathbf{y})$ is the line containing the segment corresponding to the edge $(\mathbf{x}, \mathbf{y})$.*

Applying Theorem 4 for Steiner trees of the regular simplex, we give the following lemma.

Lemma 4. *Let T be a relatively minimal Steiner tree of the regular n-simplex. Let T' be an induced full binary subtree of T, with all leaf nodes of T' terminals. Let $P(T')$ be the set of terminals in T' and $\mathbf{r_{T'}}$ the root Steiner point of T'. Let $e_{T'}$ be the edge incident to $\mathbf{r_{T'}}$ that does not lie in T'. Then the following hold:*

1. *For all Steiner points $\mathbf{s}$ in $(T \setminus T') \cup \{\mathbf{r_{T'}}\}$, for all coordinates i, j such that terminals $\mathbf{e_i}, \mathbf{e_j} \in P(T')$, it holds that $s_i = s_j$.*
2. *Let $\ell_{T'}$ be the line extending the edge $e_{T'}$. Then $\ell_{T'}$ passes through the centroid of the terminals in $P(T')$.*

The proof of this lemma uses permutations of the labels of the terminals, as informally sketched in Section 4.1. We formalize that notion here using labeled full binary trees.

Definition 3 (Labelling Full Binary Trees)**.** *Let T be a full binary tree (with a fixed choice of left and right children for every non-leaf node). Then, labelling the tree with respect to (a binary string) g is defined as follows.*

1. *The root of T is labeled as g.*
2. *Then, while there exists some labeled node v with unlabeled children, label the left child of v by appending 0 to the label of v and label the right child of v by appending 1 to the label of v. E.g., if v had binary string b as its label, its children will be labeled $b0$ and $b1$.*

We denote T_g as the result of labelling T with respect to g.

Let T be a Steiner tree of the regular simplex and let T'_g be a labeled induced full binary subtree with terminal leaf nodes (with an arbitrary choice of left and right children). Let $\mathbf{s}$ be a Steiner point in T'_g. Consider the subtree of T'_g rooted at $\mathbf{s}$. Each node in the left subtree has its label prepended by $b_{\mathbf{s}}0$ and each node in the right subtree has its label prepended by $b_{\mathbf{s}}1$. Swapping the left and right children of $\mathbf{s}$ amounts to making the labels of the nodes in the left subtree prepended by $b_{\mathbf{s}}1$ and the labels of the nodes in the right subtree instead prepended by $b_{\mathbf{s}}0$ (via Definition 3).

Observation 1. *Let T be a Steiner tree of the regular simplex and let T'_g be a labeled induced full binary subtree with terminal leaf nodes. Let $\mathbf{s}$ be a Steiner point in T'_g. Swapping the left and right children of $\mathbf{s}$ corresponds to a topology-preserving coordinate permutation in T.*

Proof. The coordinate permutation is precisely the composition of the involutions of each pair of terminals whose labels are $b_{\mathbf{s}}0c$ and $b_{\mathbf{s}}1c$. Namely, their labels differ exactly in the bit after the label of $\mathbf{s}$.

Since each pair of swapped terminals is between terminals in the corresponding position in the other subtree of $\mathbf{s}$ (and the subtrees have the same overall structure since T'_g is an induced full binary subtree with terminal leaf nodes), this permutation of the terminals preserves the topology of T. □

Finally, we can return to Lemma 4.

Proof. First, label T' with respect to the empty string ε to obtain T'_ε. We claim that for every pair of terminals $\mathbf{e_i}, \mathbf{e_j} \in T'$ there is a topology-preserving coordinate permutation of T that swaps $\mathbf{e_i}$ and $\mathbf{e_j}$. Namely, it is the composition of topology-preserving coordinate permutations induced by swapping the left and right children of Steiner points in T'_ε (via Observation 1). Index the bits of the labels of the nodes from last added to first (via Definition 3). Suppose that the labels of $\mathbf{e_i}$ and $\mathbf{e_j}$ differ on bits $a_1, a_2, \ldots, a_r$. Swapping the left and right children of each of the ${a_1}^{\text{th}}$, ${a_2}^{\text{th}}$, $\ldots$, ${a_r}^{\text{th}}$ ancestors of $\mathbf{e_i}$ and $\mathbf{e_j}$ (where the first ancestor is the parent of $\mathbf{e_i}$, the second ancestor is the grandparent, etc., and we only swap the children of a node at most once) swaps the labels of $\mathbf{e_i}$ and $\mathbf{e_j}$ (for example see Figure 4). The composition of the corresponding topology-preserving coordinate permutations is a topology-preserving coordinate permutation swapping $\mathbf{e_i}$ and $\mathbf{e_j}$. But, by Theorem 4, T must be fixed (up to isomorphism) under this map.

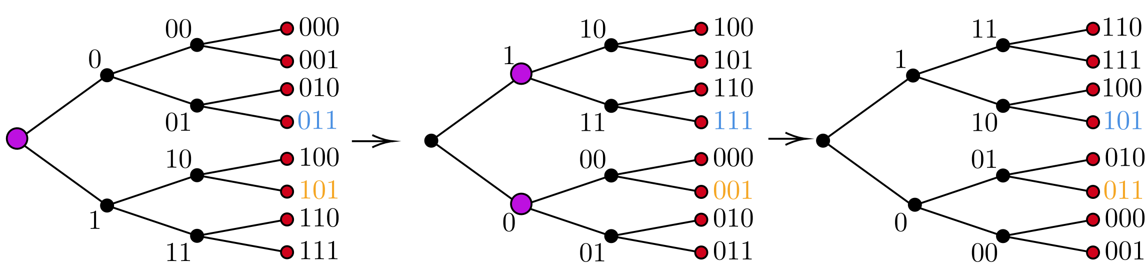

Figure 4: A sequence of topology-preserving coordinate permutations swapping the blue and the orange label. The purple vertices indicates the Steiner points whose children are to be swapped in the next step.

The topology of $(T \setminus T') \cup \{\mathbf{r_{T'}}\}$ is fixed under this topology-preserving coordinate permutation and each terminal is fixed. Hence, the Steiner points in this part of the tree must be fixed (or else we would violate Theorem 4). Hence, for each such Steiner point $\mathbf{s}$, we must have $s_i = s_j$. This holds for all $\mathbf{e_i}, \mathbf{e_j} \in T'$, yielding the first part of the result.

Observe that $e_{T'}$ is an edge between two Steiner points such that the first property holds. Hence, for every point on the extending line $\ell_{T'}$, $s_i = s_j$ for all pairs of terminals

$\mathbf{e_i}, \mathbf{e_j} \in T'$. Using this observation, we prove the second part of the result by induction on the number of levels in the induced full binary subtree T'. When there is only one level, T' is a Steiner point $\mathbf{r_{T'}}$ connected to two terminals, $\mathbf{e_i}$ and $\mathbf{e_j}$. By Corollary 1, the edge $e_{T'}$ and the edges from $\mathbf{r_{T'}}$ to $\mathbf{e_i}$ and $\mathbf{e_j}$ are all coplanar. Consider $\triangle \mathbf{r_{T'}e_ie_j}$. By coplanarity, $\ell_{T'}$ lies in the same plane as this triangle. By the observation about the extending line above, $\ell_{T'}$ must be coincident with the perpendicular bisector of the line segment joining $\mathbf{e_i}$ and $\mathbf{e_j}$. Hence, $\ell_{T'}$ passes through the midpoint of this segment, the centroid of $\mathbf{e_i}$ and $\mathbf{e_j}$.

The inductive step is similar: suppose the result holds for full binary subtrees with at least r levels. Then, consider the edges other than $e_{T'}$ incident to the root $\mathbf{r_{T'}}$ of T'. Namely, with T_L the left subtree of $\mathbf{r_{T'}}$ and T_R similarly defined, these edges are precisely e_{T_L} and e_{T_R}. By the inductive hypothesis, ℓ_{T_L} and ℓ_{T_R} pass through $\mathbf{c_{T_R}}$ and $\mathbf{c_{T_L}}$, the centroids of $P(T_R)$ and $P(T_L)$, respectively. Now, consider $\triangle \mathbf{r_{T'}c_{T_R}c_{T_L}}$. Again, coplanarity and the observation about the extending line imply that $\ell_{T'}$ is coincident to the perpendicular bisector of the line segment joining $\mathbf{c_{T_R}}$ and $\mathbf{c_{T_L}}$. Hence, it passes through the midpoint of $\mathbf{c_{T_R}}$ and $\mathbf{c_{T_L}}$, the centroid of $P(T')$, yielding the desired result. □

We need to say that the terminals of an optimal Steiner tree for the n-simplex have to be its leaf nodes. Luckily, this follows from a previous structural lemma.

Corollary 3. *In any relatively minimal Steiner tree of the regular n-simplex, all terminals are leaf nodes.*

Proof. Consider the regular n-simplex with terminals $\mathbf{p_i} = \mathbf{e_i}$. The result then follows from Lemma 2. □

Next, we will restrict the intersection of the extending lines of edges incident to Steiner points.

Lemma 5. *Let $F_i = \{\mathbf{x} \in \mathbb{R}^n : x_i = 0, ||\mathbf{x}||_1 = 1, x_j \geq 0\ \forall j \in [n]\}$ be a face of the regular n-simplex. Let T be an optimal Steiner tree of the regular n-simplex. Let $\mathbf{s} \in V(T)$ be a Steiner point, with $\mathbf{a}, \mathbf{b}, \mathbf{c} \in V(T)$ the neighbors of $\mathbf{s}$. Suppose that the ray $\overrightarrow{\mathbf{as}}$ does not intersect the convex hull of the n-simplex at F_i. Then at least one of the rays $\overrightarrow{\mathbf{sb}}, \overrightarrow{\mathbf{sc}}$ also does not intersect the convex hull of the n-simplex at F_i.*

Proof. For the sake of contradiction, suppose that both $\overrightarrow{\mathbf{sb}}, \overrightarrow{\mathbf{sc}}$ intersect F_i and $\overrightarrow{\mathbf{as}}$ does not, instead intersecting some F_j, for $j \neq i$. Define $\mathbf{a}_F \in F_j$ and $\mathbf{b}_F, \mathbf{c}_F \in F_i$ to be the intersections of these rays with faces. By Corollary 1, $\mathbf{a}, \mathbf{b}, \mathbf{c}$, and $\mathbf{s}$ are coplanar, and so $\mathbf{a}_F, \mathbf{b}_F, \mathbf{c}_F$, and $\mathbf{s}$ are also coplanar. Hence, the lines $\overleftrightarrow{\mathbf{b}_F\mathbf{c}_F}$ and $\overleftrightarrow{\mathbf{sa}_F}$ intersect at some point $\mathbf{x}$. Note that $\mathbf{sa}_F$ includes an angle of exactly $60°$ with each of $\mathbf{sb}_F$ and $\mathbf{sc}_F$ (by Theorem 1). So, in particular, coplanarity implies that $\mathbf{b}_F\mathbf{c}_F$ intersects the ray $\overrightarrow{\mathbf{sa}_F}$. Finally, all the points on $\mathbf{b}_F\mathbf{c}_F$ are contained in the simplex (by convexity), so $\mathbf{x}$ must be in the simplex as well. By Theorem 3, $\mathbf{s}$ is contained in the simplex, so all the points contained in the simplex and on the ray $\overrightarrow{\mathbf{sa}_F}$ are contained in the segment $\mathbf{sa}_F$. Namely, $\mathbf{x}$ must be contained in the segments $\mathbf{b}_F\mathbf{c}_F$ and $\mathbf{sa}_F$ (see Figure 5).

Finally, since $[b_F]_i = [c_F]_i = 0$, we have $x_i = 0$. But, then, since $[a_F]_i > 0$, we get $a_i < 0$, contradicting Theorem 3. □

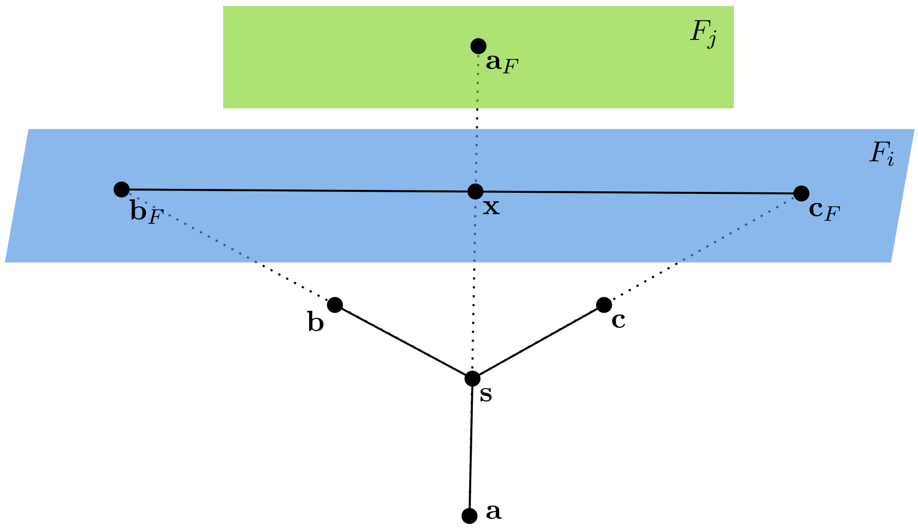

Figure 5: The intersection of the line segments $\mathbf{b}_F\mathbf{c}_F$ and $\mathbf{s}\mathbf{a}_F$ is the point $\mathbf{x}$.

Corollary 4. *Let T be an optimal Steiner tree of the regular simplex. Let $\mathbf{s}$ be a Steiner point adjacent to a terminal $\mathbf{e_i}$ in T. Then, the rays extending the other edges of $\mathbf{s}$, both with endpoints $\mathbf{s}$, intersect the regular simplex at the face $F_i = \{\mathbf{x} \in \mathbb{R}^n : x_i = 0, ||\mathbf{x}||_1 = 1, x_j \geq 0 \; \forall j \in [n]\}$.*

Proof. It holds that in every full, optimal Steiner tree, there are exactly $n-2$ Steiner points. It will suffice to use Lemma 5 until we run out of possible Steiner points. Let $\mathbf{a}_F$ be a point of intersection between a ray extending an edge of $\mathbf{s}$ (not to $\mathbf{e_i}$) with endpoint $\mathbf{s}$. For the sake of contradiction, assume that $\mathbf{a}_F \notin F_i$.

Let $\mathbf{s_0} = \mathbf{s}$ and let us proceed by induction on k. Let $\ell_k = (\mathbf{s_{k-1}}, \mathbf{s_k})$ be the edge such that the ray with endpoint $\mathbf{s_{k-1}}$ extending the edge ℓ_k does not intersect F_i (e.g., ℓ_1 is the edge whose extending ray has endpoint $\mathbf{a}_F$). If $\mathbf{s_k}$ is a terminal, since the i^{th} coordinate is greater than 0, $\mathbf{s_k} = \mathbf{e_i}$ and we found a cycle in our tree T, a contradiction. Otherwise, we iterate using Lemma 5 over up to all $n-2$ Steiner points in a path. Eventually then $\mathbf{s_k}$ must be a terminal since there are finitely many Steiner points, yielding a contradiction. □

Finally, we are prepared to prove the following theorem.

Theorem 8. *Let $n \in \mathbb{N}$ and let T be an optimal Steiner tree for the regular n-simplex. Consider a terminal $\mathbf{p} \in T$ and let $\mathbf{s}$ be the Steiner point adjacent to $\mathbf{p}$. Then, $||\mathbf{s}-\mathbf{p}|| > \frac{1}{\sqrt{3}}$.*

Proof. Without loss of generality, suppose $\mathbf{p} = \mathbf{e_1}$. By Corollary 3.2, we may assume that $\mathbf{s}$ is strictly contained in the n-simplex. Now consider the two other edges incident to $\mathbf{s}$. The rays with endpoint at $\mathbf{s}$ extending these edges must intersect the boundary of the n-simplex in some points $\mathbf{a}$, $\mathbf{b}$. Let $F_1 = \{\mathbf{x} \in \mathbb{R}^n : x_1 = 0, ||\mathbf{x}||_1 = 1, x_j \geq 0 \; \forall j \in [n]\}$.

By Corollary 4, we know that $\mathbf{a}$, $\mathbf{b}$ lie in F_1. We will show that $||\mathbf{s}-\mathbf{p}|| > \frac{1}{\sqrt{3}}$. Since $\mathbf{a}, \mathbf{b} \in F_1$, it holds that

$$\mathbf{a} = (0, a_2, \ldots, a_n)\,,$$
$$\mathbf{b} = (0, b_2, \ldots, b_n)\,,$$

where $\sum_{i=2}^{n} a_i = \sum_{i=2}^{n} b_i = 1$.

Now consider $\triangle\mathbf{pab}$. It has a unique Fermat point and that must be $\mathbf{s}$. We will use a calculation based on [6] to determine the lower bound for $||\mathbf{s}-\mathbf{p}||$. Let $L_{\mathbf{s}} = ||\mathbf{s}-\mathbf{p}|| + ||\mathbf{s}-\mathbf{a}|| + ||\mathbf{s}-\mathbf{b}||$. Without loss of generality, suppose that $||\mathbf{p}-\mathbf{a}|| \geq ||\mathbf{p}-\mathbf{b}||$. We will now show that $||\mathbf{a}-\mathbf{b}|| \leq ||\mathbf{p}-\mathbf{b}||$. It holds that

$$\begin{aligned} ||\mathbf{a}-\mathbf{b}||^2 &= \sum_{i=2}^{n}(a_i - b_i)^2 \\ &= \sum_{i=2}^{n}(a_i^2 - 2a_ib_i + b_i^2) \\ &= ||\mathbf{p}-\mathbf{b}||^2 - 1 + \sum_{i=2}^{n}(a_i^2 - 2a_ib_i) \\ &\leq ||\mathbf{p}-\mathbf{b}||^2, \end{aligned}$$

since $\sum_{i=2}^{n} a_i^2 = \left(\sum_{i=2}^{n} a_i\right)^2 - \sum_{i\neq j} 2a_ia_j = 1 - \sum_{i\neq j} 2a_ia_j \leq 1$. The third step uses that $\mathbf{p} = \mathbf{e_1}$ and $\mathbf{b} \in F_1$, so $\mathbf{p}$ and $\mathbf{b}$ are orthogonal.

From the proof of the Gilbert-Pollak Steiner ratio conjecture for 3 points (§10 of [16]), it is known that for $L = ||\mathbf{a}-\mathbf{b}|| + ||\mathbf{p}-\mathbf{b}||$ it holds that

$$L \geq L_{\mathbf{s}} \geq \frac{\sqrt{3}}{2}L,$$

by considering $\mathbf{p}$, $\mathbf{a}$, $\mathbf{b}$ as a set of terminals for the Steiner Tree problem. Next, it is important to note that $||\mathbf{p}-\mathbf{b}|| > 1$ and $\mathbf{b} \in F_1$. Finally, we can use formula (18) of [6] to compute a lower bound for $||\mathbf{s}-\mathbf{p}||$:

$$\begin{aligned} ||\mathbf{s}-\mathbf{p}|| &= \frac{L_{\mathbf{s}} + \frac{||\mathbf{p}-\mathbf{b}||^2 + ||\mathbf{p}-\mathbf{a}||^2 - 2||\mathbf{a}-\mathbf{b}||^2}{L_{\mathbf{s}}}}{3} \\ &\geq \frac{\frac{\sqrt{3}}{2}L^2 + ||\mathbf{p}-\mathbf{b}||^2 + ||\mathbf{p}-\mathbf{a}||^2 - 2||\mathbf{a}-\mathbf{b}||^2}{3L}. \end{aligned}$$

Then,

$$
\begin{aligned}
&||\mathbf{s}-\mathbf{p}|| \\
&\geq \frac{||\mathbf{a}-\mathbf{b}||^2\left(\frac{\sqrt{3}}{2}-2\right)+||\mathbf{p}-\mathbf{b}||^2\left(\frac{\sqrt{3}}{2}+1\right)+||\mathbf{p}-\mathbf{a}||^2+\sqrt{3}||\mathbf{a}-\mathbf{b}||||\mathbf{p}-\mathbf{b}||}{3\left(||\mathbf{a}-\mathbf{b}||+||\mathbf{p}-\mathbf{b}||\right)} \\
&= \frac{||\mathbf{p}-\mathbf{a}||^2-||\mathbf{a}-\mathbf{b}||^2+\left(||\mathbf{a}-\mathbf{b}||+||\mathbf{p}-\mathbf{b}||\right)\left(||\mathbf{a}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}-1\right)+||\mathbf{p}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}+1\right)\right)}{3\left(||\mathbf{a}-\mathbf{b}||+||\mathbf{p}-\mathbf{b}||\right)} \\
&= \underbrace{\frac{||\mathbf{p}-\mathbf{a}||^2-||\mathbf{a}-\mathbf{b}||^2}{3\left(||\mathbf{a}-\mathbf{b}||+||\mathbf{p}-\mathbf{b}||\right)}}_{\geq 0}+\frac{1}{3}\cdot\left(||\mathbf{a}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}-1\right)+||\mathbf{p}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}+1\right)\right).
\end{aligned}
$$

Finally, since $\frac{\sqrt{3}}{2}-1<0$ and $||\mathbf{a}-\mathbf{b}|| \leq ||\mathbf{p}-\mathbf{b}||$, it holds that

$$
\begin{aligned}
||\mathbf{a}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}-1\right)+||\mathbf{p}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}+1\right) &\geq ||\mathbf{p}-\mathbf{b}||\left(\frac{\sqrt{3}}{2}-1+\frac{\sqrt{3}}{2}+1\right) \\
&> \sqrt{3}.
\end{aligned}
$$

Therefore, $||\mathbf{s}-\mathbf{p}|| > \frac{1}{\sqrt{3}}$. □

Remark 1. *From Lemma 4 we already know that the lengths for a pair of terminals adjacent to the same Steiner point are the same and can hence compute the lengths using Theorem 1. In contrast, we did not previously know how to lower bound the length of an edge between a Steiner point and a terminal when the Steiner point is adjacent to only one terminal. Theorem 8 now provides such a bound.*

5.2 Constructing Steiner trees for the regular simplex

To describe our construction of Steiner trees of the regular simplex, we need one more definition.

Definition 4 (The Split of a Point)**.** *For $\mathbf{x} \in \mathbb{R}^d$, we define the split of $\mathbf{x}$ to be $\mathbf{x}' \in \mathbb{R}^{2d}$ such that $\mathbf{x}' = \left(\frac{x_1}{2}, \frac{x_1}{2}, \ldots, \frac{x_d}{2}, \frac{x_d}{2}\right)$.*

Lemma 6. *Let $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^d$ such that the angle included by $\mathbf{x}-\mathbf{y}$ and $\mathbf{z}-\mathbf{y}$ is α. Let $\mathbf{x}', \mathbf{y}'$, and $\mathbf{z}'$ denote the splits of $\mathbf{x}, \mathbf{y}$, and $\mathbf{z}$, respectively. Then, the angle included by $\mathbf{x}'-\mathbf{y}'$ and $\mathbf{z}'-\mathbf{y}'$ is α.*

Proof. Let $\mathbf{u} = (\mathbf{x}-\mathbf{y})$, $\mathbf{v} = (\mathbf{z}-\mathbf{y})$, $\mathbf{u}' = (\mathbf{x}'-\mathbf{y}')$ and $\mathbf{v}' = (\mathbf{z}'-\mathbf{y}')$. Now $\mathbf{u}\cdot\mathbf{v} = 2\mathbf{u}'\cdot\mathbf{v}'$, $||\mathbf{u}|| = \sqrt{2}||\mathbf{u}'||$ and the same with the norms of $\mathbf{v}$ and $\mathbf{v}'$. Now it is easy to see $\frac{\mathbf{u}\cdot\mathbf{v}}{||\mathbf{u}||||\mathbf{v}||} = \frac{\mathbf{u}'\cdot\mathbf{v}'}{||\mathbf{u}'||||\mathbf{v}'||}$. □

We will show how to leverage this idea of split to explicitly construct candidate-optimal Steiner trees of the regular simplex from optimal Steiner trees of smaller regular simplices (which can be computed directly). We formalize this in the following definition.

Definition 5 (Candidate-optimal Steiner tree)**.** *A Steiner tree T of a point configuration is called a candidate-optimal Steiner tree if each pair of edges incident to a common vertex in T include an angle of at least 120 degrees and each Steiner point is of degree exactly* 3*.*

Finally, we describe how to construct a candidate-optimal, full Steiner tree of the regular $2d$-simplex from a candidate-optimal full Steiner tree of the regular d-simplex. In the following, we will use the fact that all terminals are leaf nodes in an optimal Steiner tree if and only if it is full. This is clear by computing the degree sum of the tree in two ways: using that Steiner points are all degree 3 and that a full Steiner tree on n terminals is a tree on $2n-2$ total nodes. Recall also from Section 2 that Fermat points are the Steiner points of optimal Steiner trees of a triangle (when the optimal Steiner trees include a Steiner point).

Theorem 9 (Doubling the Tree)**.** *Let $d \geq 3$ and let T be an optimal Steiner tree of a regular d-simplex. Let S be the set of Steiner points in T. Then by the following procedure, we obtain a full, candidate-optimal Steiner tree T' of the regular $2d$-simplex:*

1. *For each $\mathbf{s} \in S$, denote the split of $\mathbf{s}$ by $\mathbf{s}'$. The set $\{\mathbf{s}' : \mathbf{s} \in S\}$ is a subset of the Steiner points S' in T'.*
2. *For all $\mathbf{r}, \mathbf{s} \in S$ such that $(\mathbf{r}, \mathbf{s}) \in E(T)$, let $(\mathbf{r}', \mathbf{s}') \in E(T')$.*
3. *For each terminal $\mathbf{e_i} \in V(T)$, let $\mathbf{s_i}$ be the adjacent Steiner point. Then we obtain new Steiner points $\mathbf{x_i}$ in T' by finding the Fermat points of the triangles formed by $\mathbf{e_{2i-1}}, \mathbf{e_{2i}}, \mathbf{s_i'}$.*
4. *Add edges $(\mathbf{e_{2i-1}}, \mathbf{x_i})$, $(\mathbf{e_{2i}}, \mathbf{x_i})$ and $(\mathbf{x_i}, \mathbf{s_i'})$ to T'.*

Proof. Note that, assuming that the Fermat points of the triangles of the form $\triangle \mathbf{e_{2i-1}}\mathbf{e_{2i}}\mathbf{s_i'}$ exist, T' is a full Steiner tree of the regular $2d$-simplex. The set of Steiner points $\{\mathbf{s}' : \mathbf{s} \in T\}$ are connected via the same tree topology as the Steiner points in T. Then, for each $i \in [d]$, each terminal $\mathbf{e_{2i}}$ or $\mathbf{e_{2i-1}}$ is connected to this tree via the Steiner tree of the triangle $\triangle \mathbf{e_{2i-1}}\mathbf{e_{2i}}\mathbf{s_i'}$ (via the additional Steiner point $\mathbf{x_i}$). Since one Steiner point is added to T' for each Steiner point and terminal in T and T is a full Steiner tree of the regular d-simplex, T' has $2d-2$ total Steiner points and is also full (this uses Corollary 3 and the discussion preceding this theorem).

We need to verify two claims. First, we need to show that the Fermat points always exist for the third step of the construction. Secondly, we need to prove that every included angle between two adjacent edges is 120° (so that T' is a candidate-optimal Steiner tree). First, consider the terminal $\mathbf{e_i}$ in T.

To prove the first claim, we distinguish between two cases. First, suppose that $\mathbf{e_i}$ shares its neighboring Steiner point with another terminal in T. In our coordinate system, the distance between every two terminals is exactly $\sqrt{2}$. By Theorem 4, it holds

$$||\mathbf{e_i} - \mathbf{s_i}|| = ||\mathbf{e_j} - \mathbf{s_i}|| = \sqrt{\frac{2}{3}},$$

applying Lemma 4 and Theorem 1.

Now, we denote the center of the segment $\mathbf{e_{2i-1}e_{2i}}$ by $\mathbf{c_i}$. It holds that $\mathbf{c_i}$ is the split of $\mathbf{e_i}$. Therefore (following from the proof of Lemma 6),

$$||\mathbf{c_i} - \mathbf{s_i'}|| = \frac{1}{\sqrt{2}}||\mathbf{e_i} - \mathbf{s_i}|| = \frac{1}{\sqrt{3}}.$$

To get the Fermat point of $\triangle \mathbf{e_{2i-1}e_{2i}s_i'}$, basic trigonometry tells us that we need to find a point at distance $\frac{1}{\sqrt{6}}$ from $\mathbf{c_i}$ in the direction of $\mathbf{s_i'}$ (see Figure 6). Since $||\mathbf{c_i} - \mathbf{s_i'}|| > \frac{1}{\sqrt{6}}$, the Fermat point $\mathbf{x_i}$ does exist.

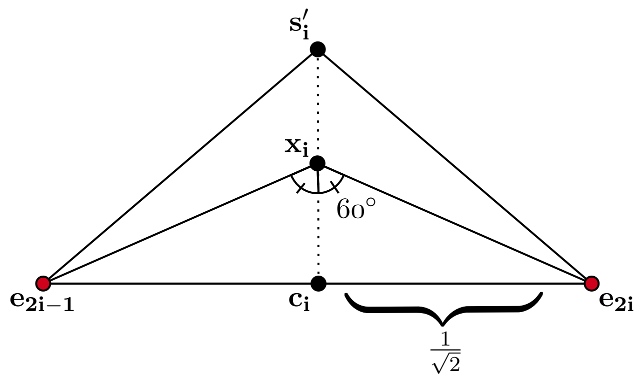

Figure 6: Diagram showing the existence of the Fermat point $\mathbf{x_i}$. Note that $||\mathbf{c_i} - \mathbf{s_i'}|| > \frac{1}{\sqrt{2}}\cot(60°) = \frac{1}{\sqrt{6}}$.

In the case that $\mathbf{e_i}$ does not share its neighboring Steiner point with another terminal in T, $\mathbf{c_i}$ is still well-defined as above. Using $||\mathbf{c_i} - \mathbf{s_i'}|| = \frac{1}{\sqrt{2}}||\mathbf{e_i} - \mathbf{s_i}||$ and that $||\mathbf{e_{2i-1}} - \mathbf{s_i'}|| = ||\mathbf{e_{2i}} - \mathbf{s_i'}||$ by definition of split, we need to find a point at distance $\frac{1}{\sqrt{6}}$ from $\mathbf{c_i}$ in the direction of $\mathbf{s_i'}$ to find a Fermat point of $\triangle \mathbf{e_{2i-1}e_{2i}s_i'}$. Hence, a Fermat point of this triangle exists if and only if $||\mathbf{e_i} - \mathbf{s_i}|| > 1/\sqrt{3}$ and a Fermat point then exists by Theorem 8.

To prove the second claim, observe that all such the angles were equal to 120° in T (by Theorem 1). Lemma 6 then implies that the angles stay the same size in the induced subtree on Steiner points in $\{\mathbf{s'} : \mathbf{s} \in T\}$. We already established that $\mathbf{c_i}$ is the split of $\mathbf{e_i}$, so, $\mathbf{e_i}$ and $\mathbf{e_j}$ share an adjacent Steiner point in T and $\mathbf{c_j}$ is the center of the segment $\mathbf{e_{2j-1}e_{2j}}$, then $|\angle \mathbf{c_i s_i' c_j}|$ in T' is equal to $|\angle \mathbf{e_i s_i p_j}|$ in T which is 120° by Theorem 1. Since the points $\mathbf{c_i}, \mathbf{x_i}, \mathbf{s_i'}$ and $\mathbf{c_j}, \mathbf{x_j}, \mathbf{s_i'}$ are colinear from the second part of Lemma 4 we have that

$$|\angle \mathbf{x_i s_i' x_j}| = 120°.$$

Finally, the remaining angles involve the Steiner points added which were computed as Fermat points of triangles. By definition of Fermat points, the edges sharing an endpoint at these Steiner points include angles of exactly 120°. □

Corollary 5. *Let $d \geq 3, k \geq 0$ and let T be an optimal Steiner tree of a regular d-simplex. Repeating the procedure in Theorem 9 k times, yields a full, candidate-optimal Steiner tree T' of a regular $2^k d$-simplex.*

Proof. Optimality of T handles $k = 0$ (using that the optimal Steiner tree of the regular simplex is full, using the discussion preceding Theorem 9 and Lemma 2). Theorem 9 handles the case of $k = 1$. Assume the result holds for up to some $r \geq 1$ and let T be the optimal tree with Steiner points S. We show the result for $k = r + 1$. The same proof as in Theorem 9 shows that T' computed from T by the procedure in Theorem 9 is a full Steiner tree of the regular simplex, assuming that the relevant Fermat points exist.

It remains to show that the Fermat points exist in each subsequent iteration and all the angles formed by edges at a common endpoint are 120°.

First, note that, since we assumed $r \geq 1$, by the procedure in Theorem 9, each terminal in T shares an adjacent Steiner point with another terminal. Namely, $\mathbf{e_{2i}}$ shares an adjacent Steiner point $\mathbf{s_{2i}}$ with $\mathbf{e_{2i-1}}$ for each $i \in [2^{r-1}d]$. The third neighbor $\mathbf{r}$ of $\mathbf{s_{2i}}$ in T is the split of the Steiner point neighboring $\mathbf{e_i}$ in the tree preceding T. In particular, then $||\mathbf{r} - \mathbf{e_{2i}}|| = ||\mathbf{r} - \mathbf{e_{2i-1}}||$, so $\triangle \mathbf{r e_{2i-1} e_{2i}}$ is isosceles. Hence, $\mathbf{s_{2i}}$, the Fermat point of this triangle must be equidistant to $\mathbf{e_{2i-1}}$ and $\mathbf{e_{2i}}$. Then,

$$||\mathbf{e_{2i-1}} - \mathbf{s_{2i}}|| = ||\mathbf{e_{2i}} - \mathbf{s_{2i}}|| = \sqrt{\frac{2}{3}}$$

using that the angles includes by the edges to $\mathbf{s_{2i}}$ must be 120° (since it is a Fermat point) and the distance between terminals is $\sqrt{2}$. Now, as in Theorem 9, for the Fermat point of $\triangle \mathbf{e_{4i} e_{4i-1} s'_{2i}}$ to exist in T', we need that the center of $\mathbf{e_{4i} e_{4i-1}}$, $\mathbf{c_{2i}}$, is at least $\frac{1}{\sqrt{6}}$ from $\mathbf{s'_{2i}}$. But, $\mathbf{c_{2i}}$ is the split of $\mathbf{e_{2i}}$ and $||\mathbf{e_{2i}} - \mathbf{s_{2i}}||$ is $\sqrt{\frac{2}{3}}$ from the above. Hence, by Lemma 6, we have $||\mathbf{c_{2i}} - \mathbf{s'_{2i}}|| = \frac{1}{\sqrt{3}} > \frac{1}{\sqrt{6}}$, as necessary. So, the Fermat points exist in constructing T'.

Finally, we need to show that all included angles between edges sharing an endpoint are at least 120° in T'. The argument here is identical to the argument in Theorem 9 (after applying the inductive hypothesis), completing the proof. □

Consider the Steiner trees of d-dimensional simplices for some small value of d where we can determine explicit coordinates for every Steiner point (e.g., $d = 3, 4$). The construction described in Theorem 9 yields the same Steiner points as the numerical algorithm in [34] for $d = 6, 8, 12$ (up to small errors presumably caused by the approximate nature of Smith's algorithm). For higher values of d it was not checked due to computational limitations.

5.3 Explicit construction for $d = 2^k$

Applying Corollary 5 starting from $d = 4$ yields an explicit construction for Steiner trees of regular simplices on $n = 2^k$ terminals. We analyze that construction in detail in this section. To start, find explicit coordinates for the Steiner points of a Steiner tree of the simplex on $d = 4$ terminals. Then, apply Theorem 9, $(k - 2)$ many times.

Our topology will be given by two full binary trees T^0, T^1, each on 2^{k-1} terminals, and an edge connecting both roots. Now recall Definition 3 and label T^0 with respect to 0 and T^1 with respect to 1. This is the representation of our tree that we will work with (see Figure 7). For simplicity, when we will talk about coordinates related to a terminal, we will use their unique binary label instead. The labels i will be in the range from 0 to $d-1$ (in binary). Therefore, the terminal with label i will be $\mathbf{e_{i+1}}$.

For $k \in \mathbb{N}$, let $\{T_m\}_{m=2}^{k}$ denote the sequence of trees from our construction. Each vertex has a superscript and a subscript—the superscript m refers to the vertex belonging to the vertex set of T_m and the subscript refers to the assigned binary string label. Steiner points obtained by splitting will retain the same binary string label. Those obtained as a new Fermat point will adopt the binary string label of the terminal whose binary label was appended to form the two terminal endpoints of the triangle. E.g., the Steiner point obtained as the split of $\mathbf{s_b^k}$ will be $\mathbf{s_b^{k+1}}$. The Steiner point obtained as the Fermat point of $\triangle \mathbf{s_b^{k+1}} \mathbf{p_{b00}^{k+1}} \mathbf{p_{b01}^{k+1}}$ will be $\mathbf{s_{b0}^{k+1}}$.

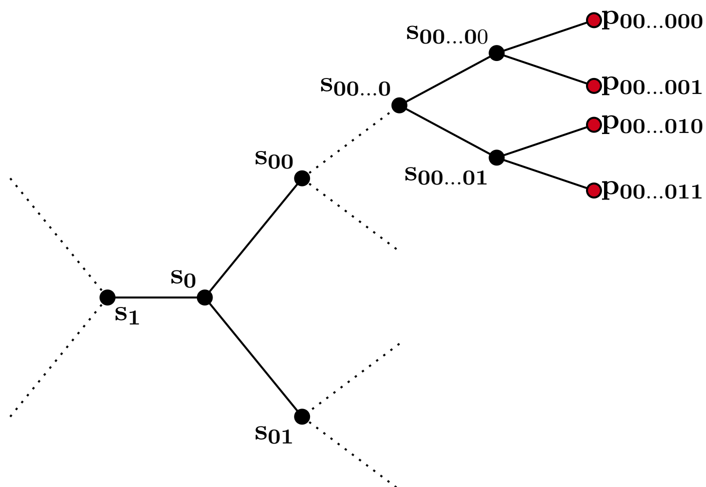

Figure 7: Binary representation of terminals and Steiner points for $n = 2^k$.

For $k = 1$, T_1 is just the line segment $\mathbf{p_0^1 p_1^1}$ connecting two terminals. For $k = 2$, we need to find the Steiner points $\mathbf{s_0^2}$ and $\mathbf{s_1^2}$. Lemma 4 gives us the following: the edge between $\mathbf{s_0^2}$ and $\mathbf{s_1^2}$ passes through $\mathbf{c} = \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)$, the centroid of the terminals. Then, it holds that $\mathbf{s_0^2}$ and $\mathbf{s_1^2}$ are the Fermat points of $\triangle \mathbf{p_{00}^2 p_{01}^2 c}$ and $\triangle \mathbf{p_{10}^2 p_{11}^2 c}$, respectively. Therefore, we get:

$$\mathbf{s_0^2} = \left(\frac{1}{2} - \frac{1}{2\sqrt{6}}, \frac{1}{2} - \frac{1}{2\sqrt{6}}, \frac{1}{2\sqrt{6}}, \frac{1}{2\sqrt{6}}\right),$$
$$\mathbf{s_1^2} = \left(\frac{1}{2\sqrt{6}}, \frac{1}{2\sqrt{6}}, \frac{1}{2} - \frac{1}{2\sqrt{6}}, \frac{1}{2} - \frac{1}{2\sqrt{6}}\right).$$

For $k \geq 3$, let $\{b_j\}_{j=1}^{k-1}$ be the sequence of binary strings of j zeros. For brevity, we will only show the coordinates of points $\mathbf{s_{b_j}^k}$. To obtain explicit formulas for other Steiner points, it suffices to apply suitable topology-preserving coordinate permutations.

Firstly, based on Theorem 9, we know that we obtain $\mathbf{s_0^k}$ by splitting $\mathbf{s_0^{k-1}}$. Repeat-

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edly applying this, we have

$$\mathbf{s_0^k} = \frac{1}{2^{k-2}} \left(\underbrace{\frac{1}{2} - \frac{1}{2\sqrt{6}}, \cdots,}_{2^{k-1}\,\text{times}} \frac{1}{2\sqrt{6}}, \cdots, \frac{1}{2\sqrt{6}} \right).$$

Now for each $2 \le j \le k-1$, let us find the first tree in our sequence that has a Steiner point with the binary representation of b_j. It is T_{j+1}. In this tree, the point $\mathbf{s_{b_j}^{j+1}}$ was constructed as the Fermat point of $\triangle \mathbf{p_{b_j0}^{j+1} p_{b_j1}^{j+1} s_{b_{j-1}}^{j+1}}$. If we denote the center of $\mathbf{p_{b_j0}^{j+1} p_{b_j1}^{j+1}}$ as $\mathbf{c}^{j+1}$, we already know from the proof of Corollary 5 that

$$||\mathbf{c}^{j+1}\mathbf{s_{b_j}^{j+1}}|| = \frac{1}{\sqrt{2}}||\mathbf{c}^{j+1}\mathbf{s_{b_{j-1}}^{j+1}}||.$$

From this it follows that

$$\begin{aligned} \mathbf{s_{b_j}^{j+1}} &= \mathbf{c}^{j+1} + \frac{1}{\sqrt{2}}\left(\mathbf{s_{b_{j-1}}^{j+1}} - \mathbf{c}^{j+1}\right) \\ &= \frac{1}{\sqrt{2}}\mathbf{s_{b_{j-1}}^{j+1}} + \left(1 - \frac{1}{\sqrt{2}}\right)\left(\frac{1}{2}, \frac{1}{2}, 0, \cdots, 0\right) \\ &= \frac{1}{\sqrt{2}}\mathbf{s_{b_{j-1}}^{j+1}} + \left(\frac{1}{2} - \frac{1}{2\sqrt{2}}, \frac{1}{2} - \frac{1}{2\sqrt{2}}, 0, \cdots, 0\right). \end{aligned}$$

After that, we need to split $\mathbf{s_{b_j}^{j+1}}$ a total of $(k-j-1)$ times to obtain $\mathbf{s_{b_j}^k}$. Splitting is linear and can be done separately on both summands

$$\mathbf{s_{b_j}^k} = \frac{1}{\sqrt{2}}\mathbf{s_{b_{j-1}}^k} + \frac{1}{2^{k-j-1}} \left(\underbrace{\frac{1}{2} - \frac{1}{2\sqrt{2}}, \cdots,}_{2^{k-j}\,\text{times}} 0, \cdots, 0 \right).$$

We can then repeat this step with $\mathbf{s_{b_{j-1}}^k}$ and so on until we get to $\mathbf{s_0^k}$

$$\mathbf{s^k_{b_j}} = \left(\frac{1}{\sqrt{2}}\right)^{j-1}\mathbf{s^k_0} + \frac{1}{2^{k-j-1}}\left(\underbrace{\frac{1}{2}-\frac{1}{2\sqrt{2}},\cdots,}_{2^{k-j}\text{ times}}0,\cdots,0\right)$$
$$+\frac{1}{\sqrt{2}\cdot 2^{k-j}}\left(\underbrace{\frac{1}{2}-\frac{1}{2\sqrt{2}},\cdots,}_{2^{k-j+1}\text{ times}}0,\cdots,0\right)$$
$$\vdots$$
$$+\frac{1}{(\sqrt{2})^{j-1}2^{k-2}}\left(\underbrace{\frac{1}{2}-\frac{1}{2\sqrt{2}},\cdots,}_{2^{k-1}\text{ times}}0,\cdots,0\right).$$

Note that this type of construction is not restricted to powers of two: the same can be done for any initial known Steiner tree. For example we can explicitly write down the coordinates for $d = 3\cdot 2^k$, $k \in \mathbb{N}$, where the only part of the expression that changes is the point $\mathbf{s^k_0}$. Or, by running some exact algorithm, e.g., Smith's algorithm, we can compute numerical approximations for the Steiner points of the optimal Steiner tree for $d = c$ for some some small constant c and then apply the same technique to write down the coordinates for $d = c\cdot 2^k$, $k \in \mathbb{N}$.

Conjecture 5. *This construction yields an optimal Steiner tree for every regular d-simplex, where $d = 2^k$, $k \geq 1$. Moreover, the natural generalization yields the optimal Steiner tree for every regular d-simplex, $d \geq 3$.*

The construction is closely related to the construction in [6]. The outcome in both cases is that, instead of considering every terminal, it is enough to represent each full binary tree by the centroid of its terminals. In essence, this is the second property of optimal Steiner trees of the regular simplex that we formalize in Lemma 4. It is not surprising to notice that the asymptotic length of our constructions are the same (although our constructions match the conjecture of Smith for all d, unlike [6]):

Proposition 1. *Let T_0 be a Steiner tree of the regular d-simplex. Let $\{T_k\}_{k=0}^{\infty}$ be the sequence of Steiner trees of the regular simplex created by repeatedly applying Theorem 9 to T_0 and let ℓ_k denote the Steiner ratio for T_k. If $\lim_{k\to\infty}\ell_k$ exists, then $\lim_{k\to\infty}\ell_k = \frac{\sqrt{3}}{\sqrt{2}(2\sqrt{2}-1)}$.*

Proof. Suppose that we know ℓ_0. Then we can recursively write

$$\ell_{k+1} = \frac{\ell_k\left(d2^k-1\right) - \frac{d2^k}{\sqrt{6}} + d2^{k+1}\sqrt{\frac{2}{3}}}{\left(d2^{k+1}-1\right)\sqrt{2}}. \qquad (*)$$

The distance between all pairs of terminals is $\sqrt{2}$, yielding the denominator. The tree resultant from taking the split of every node in T_k (and retaining the same topology) is nearly T_{k+1} and has cost $\sqrt{2} \cdot \frac{\ell_k(d2^k-1)}{\sqrt{2}}$ by Lemma 6. However, we do not include the entirety of each edge to the split of terminal $\mathbf{p}$ in T_k; we only continue along the edge to $\mathbf{p}$ to the Fermat point of the triangle with the two new terminals corresponding to $\mathbf{p}$. As argued in Corollary 5, this removes a length of $\frac{1}{\sqrt{6}}$ per terminal in T_k. Finally, for each terminal in T_{k+1} we connect it to the Fermat point of its respective triangle. Each such edge is of length $\sqrt{\frac{2}{3}}$ as argued in Corollary 5. Combining these quantities yields the numerator.

If we assume that there exists $\ell = \lim_{k\to\infty} \ell_k$, then by taking limits of both sides of $(*)$, we get

$$\ell = \frac{\ell}{2\sqrt{2}} - \frac{1}{4\sqrt{3}} + \frac{1}{\sqrt{3}}.$$

Therefore, by expressing ℓ, we obtain

$$\ell = \frac{\sqrt{3}}{\sqrt{2}\left(2\sqrt{2}-1\right)}.$$

□

To show that the limit exists, it is enough to show that $\ell_0 > \frac{\sqrt{3}}{\sqrt{2}(2\sqrt{2}-1)}$—it then follows from the recursive formula that $\ell_k > \frac{\sqrt{3}}{\sqrt{2}(2\sqrt{2}-1)}$ and that the sequence $\{\ell_k\}_{k=0}^{\infty}$ is strictly decreasing. This holds for T_0 being the numerically computed optimal Steiner tree of the regular d-simplex for all $3 \le d \le 12$, for example.

6 Progress towards Conjecture 3

In this section, we consider Conjecture 3. For ease of notation throughout, we use $f : G(V,E) \to \mathbb{R}^{|V|}$ to denote the embedding of each edge in G as its characteristic vector (e.g., (i,j) is mapped to $\mathbf{e_i} + \mathbf{e_j}$). As evidence of the efficiency of the Steiner trees of regular simplices, we observe the following lemma.

Lemma 7. *For any fixed $m \ge 1$, the graph of size m whose embedding (as above) features the minimum cost Steiner tree has diameter at most 2.*

That is, the only embeddings of graphs that might have more efficient Steiner trees than the embedding of the star graph (which embeds as a regular simplex) have diameter at most 2. We actually prove an even stronger result. In the lemma which follows, the *closed neighborhood* of a vertex v is the union of the neighborhood of v and $\{v\}$

Lemma 8. *Let $G = (V,E)$ be a graph with $|E| = m$ having two vertices with disjoint closed neighborhoods. Then, there exists some $G'(V',E')$ with $|E'| = m$ and all closed neighborhoods of vertices pairwise overlapping such that $f(G')$ has a Steiner tree of total length less than the total length of the optimal Steiner tree of $f(G)$.*

Proof. Without loss of generality, let $V = [n]$. Let i and j be two vertices with disjoint neighborhoods. This implies that the two sets of endpoints of edges incident to i and j are disjoint.

Now let T be an optimum Steiner tree for $f(G)$ (f is the embedding function described at the beginning of this section and in Section 1). We transform T into a lower total length Steiner tree on $f(G')$ for G' a graph with the neighborhoods of any pair of vertices overlapping.

For each point $\mathbf{x} = (x_1, x_2, \dots x_n)$ in T, set the i^{th} coordinate equal to $\max(x_i, x_j)$ and then set the j^{th} coordinate equal to 0. First, note that this operation maps each embedding of an edge incident to j, $f(k, j)$, to a distinct embedding of an edge incident to i (namely, the embedding of the edge (k, i)). The resultant collection of embedded edges is the result of embedding G after contracting the vertices i and j (call the contraction of i and j the graph G'): there are no lost or repeated edges exactly because i and j have disjoint closed neighborhoods. Second, this fixes all the other embedded edges in the configuration.

Now, consider two points $\mathbf{x} = (x_1, x_2, \dots x_n)$ and $\mathbf{y} = (y_1, y_2, \dots y_n)$ in T with an edge between them. We want to show that the distance between them has not increased as a result of this map. The difference in each coordinate other than the i^{th} and j^{th} coordinates is fixed. So, it suffices to show that

$$(x_i - y_i)^2 + (x_j - y_j)^2 \geq (\max(x_i, x_j) - \max(y_i, y_j))^2.$$

Expanding both sides, we have to show that

$$x_i^2 + x_j^2 + y_i^2 + y_j^2 - 2x_iy_i - 2x_jy_j \geq \max(x_i, x_j)^2 + \max(y_i, y_j)^2 - 2\max(x_i, x_j)\max(y_i, y_j).$$

We have two cases to consider. First, suppose $\max(x_i, x_j) = x_i$ and $\max(y_i, y_j) = y_i$. Then we have

$$\begin{aligned}(x_i - y_i)^2 + (x_j - y_j)^2 &= (\max(x_i, x_j) - \max(y_i, y_j))^2 + (x_j - y_j)^2 \\ &\geq (\max(x_i, x_j) - \max(y_i, y_j))^2.\end{aligned}$$

Notably, we have an equality in the second line only if $x_j = y_j$. The case of the maxima in the j^{th} coordinates follows symmetrically (with equality only if $x_i = y_i$).

Now suppose $\max(x_i, x_j) = x_i$ and $\max(y_i, y_j) = y_j$. First note that we have

$$(x_i - x_j)y_j \geq (x_i - x_j)y_i$$

since $x_i \geq x_j$ and $y_j \geq y_i \geq 0$ (since $\mathbf{x}$ and $\mathbf{y}$ are in the convex hull of $f(G)$ by Theorem 3). This implies

$$2x_iy_j + 2x_jy_i \geq 2x_iy_i + 2x_jy_j. \tag{1}$$

Now,

$$\begin{aligned}&x_i^2 + x_j^2 + y_i^2 + y_j^2 - 2x_iy_i - 2x_jy_j \\ &= \max(x_i, x_j)^2 + \max(y_i, y_j)^2 + x_j^2 + y_i^2 - 2x_iy_i - 2x_jy_j \\ &= \max(x_i, x_j)^2 + \max(y_i, y_j)^2 + (x_j - y_i)^2 + 2x_jy_i - 2x_iy_i - 2x_jy_j.\end{aligned}$$

Then, (1) implies that

$$(x_i - y_i)^2 + (x_j - y_j)^2 \geq (\max(x_i, x_j) - \max(y_i, y_j))^2,$$

with equality exactly when $x_i = y_i = x_j$ or $x_j = y_j = y_i$. The case of $\max(x_i, x_j) = x_j$ and $\max(y_i, y_j) = y_i$ follows by symmetry.

Finally, note that equality holds in either case only when the smaller of the i^{th} and j^{th} coordinates of the two points are of equal magnitude. But, consider a Steiner point $\mathbf{s}$ adjacent to terminal node $\mathbf{p}$. Such an incidence must occur by Lemma 2. Since i and j are non-adjacent in G, either p_i or p_j are 0. But then in particular $\min(p_i, p_j) = 0$, so, in order to have equality in the above, s_i or s_j must equal 0, contradicting optimality as a result of Lemma 1. □

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A Inapproximability of the Euclidean Steiner Tree problem

In this section we formalize the reduction strategy for showing APX-hardness of the Euclidean Steiner tree sketched in Section 1.

Informally, we conjecture that regular simplicial complexes admit more efficient Steiner trees when they are composed of fewer simplices. Formally, we conjecture the following.

Conjecture 6 (Euclidean Steiner Tree for Regular Simplicial Complexes)**.** *For all constants $r \in (0,1)$ and $\alpha \in (0, 1/r - 1)$, there exist constants $s, \beta > 0$ and $M \in \mathbb{Z}^+$ sufficiently large so that, for all $m \geq M$, given a regular, unit, simplicial complex on m vertices:*

1. ***Completeness:*** *If the vertices can be partitioned into the vertices of at most rm unit, regular simplices, then the point configuration of the m vertices admits a Euclidean Steiner tree of cost at most sm.*

2. ***Soundness:*** *If the vertices cannot be partitioned into the vertices of fewer than* $(1+\alpha)rm$ *unit, regular simplices, then the point configuration of the* m *vertices does not admit a Euclidean Steiner tree of cost less than* $(1+\beta)sm$*.*

In the above, for simplicity, we consider a single point to be a regular, unit simplex with one vertex. Conjecture 6 is entirely analytical; it does not directly involve any computation. Nonetheless, we show that if Conjecture 6 holds (or indeed a somewhat weaker conjecture holds), then the Euclidean Steiner tree problem is APX-hard.

Theorem 10. *Conjecture 6 implies that the Euclidean Steiner tree problem is* APX*-hard.*

Proof. We reduce from the Vertex Cover problem on (bounded degree) triangle-free graphs. From [24], there exists $r \in (0,1)$ and $\alpha \in (0, 1/r-1)$, and a family of m-edge, n-node graphs such that the following decision problem is NP-hard (where n is a fixed function of m). Given an input graph G, decide which of the following cases holds.

- **Completeness:** There exists a vertex cover of G of size rm.
- **Soundness:** All vertex covers of G are of size at least $(1+\alpha)rm$.

We will now describe a reduction from the Vertex Cover problem on triangle-free graphs to the Euclidean Steiner tree problem. Define $f_n : [n]^2 \to \mathbb{R}^n$ where $f_n(i,j) = \frac{1}{\sqrt{2}} \cdot (\mathbf{e_i} + \mathbf{e_j})$, the sum of the i^{th} and j^{th} standard basis vectors. Since the choice of domain will always be clear from context, we will abuse notation and denote f_n by f. For a graph G of order n, let

$$f(G) = f(E(G)) = \{f(i,j) : (i,j) \in E(G)\}.$$

Now, given an input graph G to the Vertex Cover problem on triangle-free graphs described above, our corresponding instance of the Euclidean Steiner Tree problem will be the instance on the terminal set $f(G)$. This mapping takes $O(\text{poly}(m))$ time. Observe that $f(G)$ is exactly the collection of vertices of a regular, unit simplicial complex on m vertices. Let s and β be as in Conjecture 6 for r and α as in Conjecture 6 and m sufficiently large.

Completeness. If the completeness case holds, i.e., G admits a vertex cover C of size rm, then the points in $f(G)$ can be partitioned into the vertices of at most rm regular, unit simplices. Namely, if vertex $i \in C$, then the collection of points $S_i = \{f(i,j) : (i,j) \in E\} \subseteq f(G)$ (the embeddings of each edge incident to vertex i) forms the vertices of a regular, unit simplex. Since C is a vertex cover of G, every edge in G is incident to some vertex in C. Namely, $f(G) \subset \cup_{i \in C} S_i$. Since any subset of the vertices of a regular, unit simplex also forms the vertices of a regular, unit simplex (using the convention that a single vertex is the vertex of a regular, unit simplex on one vertex), any arbitrary partition of $f(G)$ among the S_i's is a partitioning of $f(G)$ into the vertices of at most rm unit, regular simplices. Hence, by the completeness case of Conjecture 6, $f(G)$ admits an Euclidean Steiner tree of cost at most sm.

Soundness. Now suppose that the soundness case holds, i.e., all vertex covers of G are of size at least $(1+\alpha)m$. We need to show that the points in $f(G)$ cannot be partitioned into the vertices of fewer than $(1+\alpha)rm$ regular, unit simplices (and, hence, the soundness case of Conjecture 6 applies). To do this, we make a series of claims.

Claim 1. *For $\{i,j\},\{k,\ell\} \in E(G)$ such that $\{i,j\} \cap \{k,\ell\} = \emptyset$, $f(i,j)$ and $f(k,\ell)$ cannot belong to the same regular, unit simplex in any partition of $f(G)$ into the vertices of regular, unit simplices.*

Proof. Note that $||f(i,j) - f(k,\ell)||_2 = \sqrt{2} \neq 1$. □

Claim 2. *For $S \subset E(G)$ with $|S| \neq \emptyset$ such that $\cap_{e\in S} e = \emptyset$, the points in $f(S)$ cannot all belong to the same regular, unit simplex in any partition of $f(G)$ into the vertices of regular, unit simplices.*

Proof. The case of $|S| = 1$ is trivial and the case of $|S| = 2$ follows immediately from Claim 1.

Now assume that $|S| \geq 3$. Suppose that $e_1 = \{i,j\} \in S$. By Claim 1, for all $e \in S$, either $i \in e$ or $j \in e$. Since $\cap_{e\in S} e = \emptyset$, there exists $e_2 \in S$ such that $i \in e_2$ and $j \notin e_2$ and $e_3 \in S$ such that $i \notin e_3$ and $j \in e_3$. Now, by Claim 1 again, e_2 and e_3 must share a vertex, so $e_2 = \{i,k\}$ and $e_3 = \{j,k\}$. But, G is triangle-free and e_1, e_2, and e_3 form a triangle, yielding a contradiction. □

Now, Claim 2 implies that in any partition $E_1 \sqcup E_2 \cdots$ of $E(G)$ corresponding to a partition of $f(G)$ into the vertices of regular, unit simplices, for each part E_i, there exists $v_i \in V$ such that $v_i \in \cap_{e\in E_i} e$. Indeed, the v_i's form a vertex cover of G, implying that G has a vertex cover of size at most the size of the partition of $f(G)$ into the vertices of regular, unit simplices. Hence, by our assumption in the soundness case of our hard instance of the Vertex Cover problem, the vertices in $f(G)$ cannot be partitioned into the vertices of fewer than $(1+\alpha)rm$ unit, regular simplices. Then, by the soundness case of Conjecture 6, $f(G)$ does not admit an Euclidean Steiner Tree of cost less than $(1+\beta)sm$ in this case.

Combining the analysis of the completeness and soundness cases, the Euclidean Steiner Tree problem is NP-hard to approximate within a factor of less than $(1+\beta)$, yielding the desired result. □

Note that we only used a weaker version of Conjecture 6 to prove Theorem 10. Indeed, we really only need that s and β exist for r and α induced by the inapproximability of Vertex Cover on triangle-free graphs.