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STEINER TREES FOR THE REGULAR SIMPLEX

BY

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Abstract. Ordinary minimal trees and Steiner minimal trees are two kinds of graphs which interconnect n given vertices A_i and have minimal length. Lines of ordinary minimal trees must be of the form A_iA_j. Steiner minimal trees may also have extra vertices S_i (Steiner points) in order to reduce the length further.

For points in the euclidean plane the Steiner minimal tree length L_S and the ordinary minimal tree length L_M were conjectured to satisfy $L_S/L_M \geq \frac{1}{2} \times 3^{1/2} = .86603$. Equality holds when $n=3$ and A_1, A_2, A_3 are vertices of an equilateral triangle. Likewise, in D-dimensional euclidean space it was conjectured that $L_S/L_M \geq \rho(D)$, where $\rho(D)$ is the ratio achieved for $n = D+1$ vertices at the corners of a regular simplex. However, $\rho(D)$ was not known for $D \geq 3$.

Here we find $\rho(3)$, $\rho(4)$, $\rho(5)$ and derive an upper bound on $\rho(D)$ for all larger D. Our bound approaches .669842 for large D. The bound is obtained by constructing trees which, for $D \leq 13$, satisfy the usual necessary conditions on trees which minimize length (Steiner trees).

Introduction. Minimal trees and Steiner minimal trees are two kinds of graphs interconnecting given points $A_1, \cdots, A_n$. The length of a graph is defined to be the sum of the lengths of its lines. The (ordinary) minimal tree has the least length of all n^{n-2} trees with $A_1, \cdots, A_n$ as vertices. The Steiner minimal tree has vertices $A_1, \cdots, A_n$ and may have other vertices $S_1, \cdots, S_s$, called Steiner points, to help minimize the length. Properties of these trees are reviewed by Gilbert and Pollak [1], who emphasize trees in the euclidean plane.

The minimal tree is easy to construct. By contrast, the Steiner minimal tree is found by constructing a finite, but often large, number of topologically different trees. These trees, called Steiner trees, satisfy certain requirements necessary for minimal length. The main requirement is that each Steiner point must be the end-point of three lines meeting at 120°.

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The length L_S of the Steiner minimal tree is typically smaller than the length L_M of the minimal tree by only a few percent. In the plane, the smallest known ratio of L_S/L_M is obtained by prescribing three points A_1, A_2, A_3 at the corners of an equilateral triangle. That configuration has $L_S/L_M = 3^{1/2}/2 = .86603$, which in [1] was proved to be the smallest ratio possible when $n = 3$ and was conjectured to be the smallest ratio, Min L_S/L_M, for any n points. Pollak [2] recently verified that conjecture for $n = 4$. Kallman [3] proved, for any n, that trees with only one Steiner point have length $\geq \frac{1}{2}3^{1/2}L_M$.

Some lower bounds on L_S/L_M are known. The simplest is $L_S/L_M \geq \frac{1}{2}$, which in [1] was proved to be best possible for trees in arbitrary metric spaces. Graham and Hwang [4] obtained a better bound $L_S/L_M \geq 3^{-1/2} = .57735$, for trees in euclidean spaces of any dimension. For euclidean space of given dimension D, it was also suggested in [1] that the ratio $\rho(D) = L_S/L_M$ for the $n = D + 1$ vertices of a regular simplex might be the Min L_S/L_M for all configurations of points. That conjecture, of course, is not proved, even for $D = 2$. Moreover, the ratio $\rho(D)$ and the Steiner minimal tree of a D-dimensional regular simplex are not known. In [1], short trees were given for simplexes of several dimensions D. Except when $D = 3$, 4, and 5, these trees were not even Steiner trees; however, they provided a bound on $\rho(D)$, and hence on Min L_S/L_M, close to $(1 + 3^{1/2})/4 = .68301$ in the limit of large D.

Here trees will be constructed for regular simplexes to get a bound on Min L_S/L_M which comes arbitrarily close to $C = (3/2)^{1/2} \cdot (2^{3/2} - 1)^{-1} = .66984$ for all sufficiently large D. In dimensions $D \leq 5$ these trees are proved to be Steiner minimal trees. In higher dimensions such that $D + 1$ is a sum of three powers of 2, the tree is a Steiner tree having a high degree of symmetry, but it is not proved to be Steiner minimal in general. In other dimensions the tree may not even be a Steiner tree. These trees supply upper bounds on $\rho(D)$ which appear in Table I. Although Min L_S/L_M must be a monotone decreasing function of D, the same is not obviously true of $\rho(D)$.

TABLE I. Upper Bound on $\rho(D) = L_S/L_M$ for a Simplex in Dimension D.

D	Bound
1	1.
2	.866026
3	.813053
4	.783748
5	.764564
6	.751427
7	.741264
8	.733982
9	.727434
10	.722504
11	.718118
12	.714967
13	.711555
14	.711033
15	.706485
16	.704923
17	.702721
18	.701083
19	.699453
20	.698390
40	.684995
80	.677754
160	.673921
large	$C = .669842$

2. **The regular simplex.** The simplex is a generalization, to D-dimensional euclidean space, of the 2-dimensional triangle and 3-dimensional tetrahedron. It has $n = D + 1$ vertices $A_1, \cdots, A_n$. If all $\frac{1}{2}nD$ distances $|A_i - A_j|$ between distinct vertices are equal, the simplex is called *regular*. We use a convenient D-dimensional space consisting of n-tuples $(X_1, \cdots, X_n)$ of real coordinates X_i which satisfy $X_1 + \cdots + X_n = 1$. Take $A_1 = (1, 0, \cdots, 0), \cdots, A_n = (0, 0, \cdots, 1)$, each A_i having $X_i = 1$ and all other coordinates 0. Then $|A_i - A_j|$

$= 2^{1/2}$. All trees with vertices $A_1, \cdots, A_n$ are minimal and have length

(1) $$L_M = 2^{1/2}D.$$

A Steiner tree with $n-2$ Steiner points is called *full* in [1]. All other Steiner trees have fewer Steiner points. A Steiner tree which is not full contains a vertex A_i at which 2 or more lines are incident. Then the Steiner tree is a union of smaller Steiner trees which are disjoint except for the common point A_i. One can easily show that any non-full Steiner tree for the regular simplex has length $\rho(D-1)L_M$ or more. We therefore particularly want to construct full Steiner trees.

Figure 1 illustrates the general form of our full Steiner tree for the regular simplex. The construction requires n to be written as a sum of powers of 2.

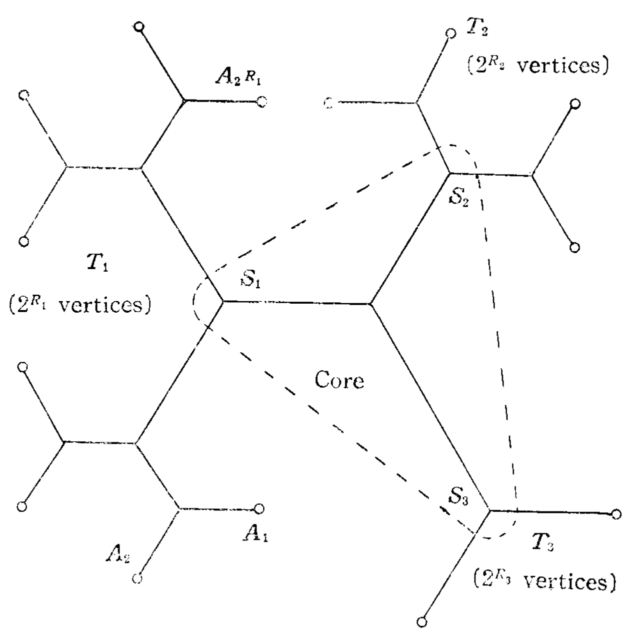

FIGURE 1. Binary trees T_k and core.

(2) $$n = 2^{R_1} + 2^{R_2} + \cdots$$

Partition the set of vertices $\{A_1, \cdots, A_n\}$ into disjoint subsets containing $2^{R_1}, 2^{R_2}, \cdots$ vertices. Each set of 2^{R_k} vertices will be connected through a ***binary tree*** T_k, to be derived presently, to a

Steiner point S_k. The Steiner tree will consist of the binary trees $T_1, T_2, \cdots$ and a central *core*, which is a Steiner tree connecting $S_1, S_2, \cdots$.

Although (2) can be the binary representation of the integer n, the $R_1, R_2, \cdots$ need not be distinct. Indeed, if $n = 2^R$, a power of 2, it will be necessary to write $n = 2^{R-1} + 2^{R-1}$, so that the core will not be empty. Since the core is itself a Steiner tree, Figure 1 will be useful only if (2) contains a small number of terms. With 2 terms, the core is just the line $S_1 S_2$. With 3 terms, as in Figure 1, the core contains one additional Steiner point, determined by the methods used in the plane (see §4). Only numbers n having binary representations containing 4 or more ones require more complicated cores.

3. **Binary trees.** The topology of each binary tree T_k in Figure 1 or 2 may be described in terms of a system of levels. The Steiner point S_k is the root of the tree, at level 0. Each Steiner point S at level j is connected to two points at level $j+1$. Then there are 2^j Steiner points at level j for $j = 0, 1, \cdots, R_k - 1$. The tree ends at level R_k with the 2^{R_k} vertices A_i.

Any Steiner point S in a binary tree for 2^R vertices determines a subtree containing all points which can be reached from S along paths on which the level increases. If S is at level j one can reach 2^{R-j} vertices A_i from S. This set of vertices will be called $V(S)$. An important point associated with S is the centroid of $V(S)$,

$$C(S) = 2^{j-R} \sum_{A \in V(S)} A, \tag{3}$$

the vector average of all 2^{R-j} vertices in $V(S)$. Note that (3) determines $C(S)$ even before coordinates of S are known.

The line which leads down from S to the next lower level will be called the *exit line* from S. If S is at level 0, the exit line is defined to be the line of the core at S.

One may expect the 2^{R-j} vertices of $V(S)$ to be arranged symmetrically with respect to the exit line at S. We therefore try to construct a tree in such a way that

(4) *the extended exit line at S passes through $C(S)$*

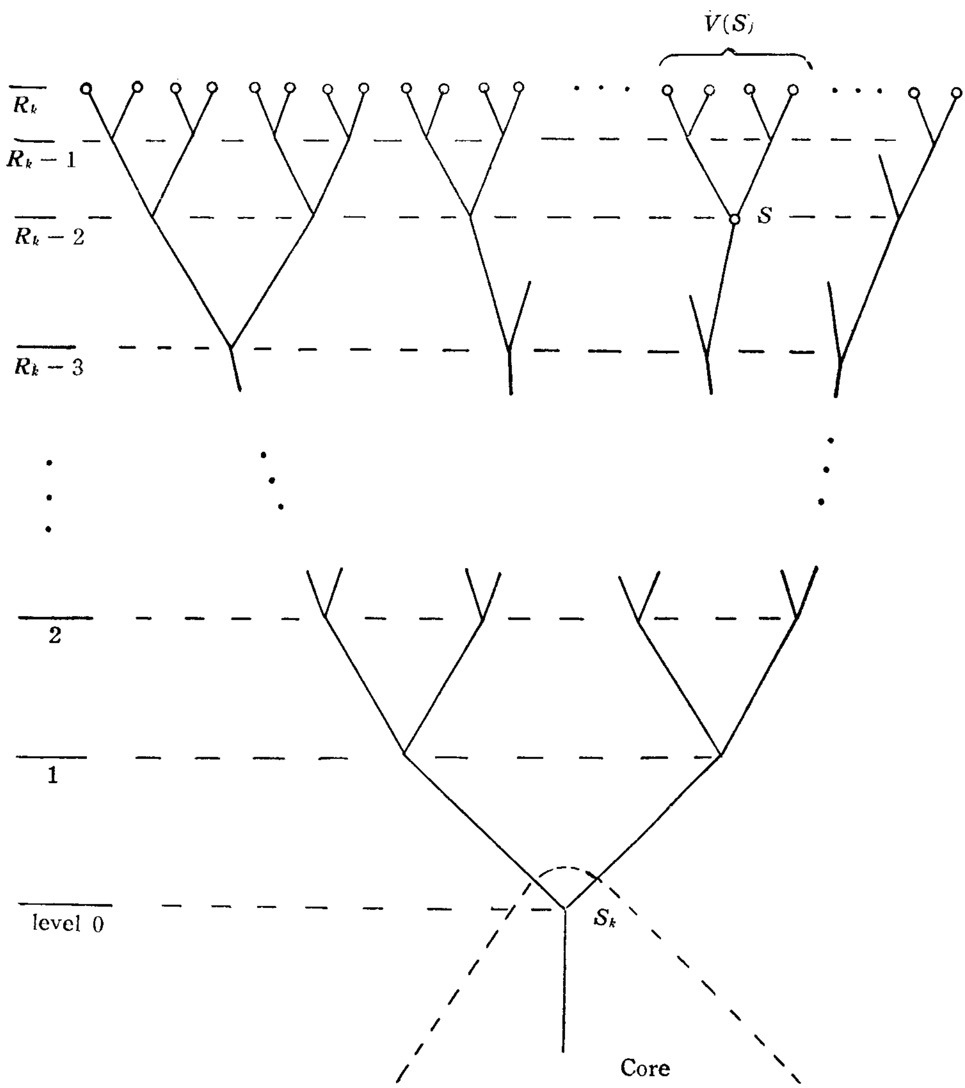

FIGURE 2. Level structure of binary tree T_k.

for every Steiner point S of every binary tree $T_1, T_2, \cdots$ in Figure 1. At this stage it is not necessary to prove (4). It will suffice that we finally do obtain a Steiner tree. A uniqueness theorem in [1] guarantees that this is the only Steiner tree with the given tree topology.

When (4) holds, S lies in a space spanned by $C(S)$ and the vertices A_i which do not belong to $V(S)$. Thus (4) implies

$$S = \alpha C(S) + V, \tag{5}$$

where α is a constant and V is a vector orthogonal to every A_j in $V(S)$. Now let S', S'' be the two points to which S is connected on the next higher level. Then $V(S) = V(S') \cup V(S'')$ and $C(S) = \frac{1}{2}\{C(S') + C(S'')\}$ while (5) shows that $C(S')$, S, $C(S'')$ determine an isosceles triangle. As shown in Figure 3, the median from S intersects the opposite side $C(S')C(S'')$ at $C(S)$ and is the perpendicular bisector of that side.

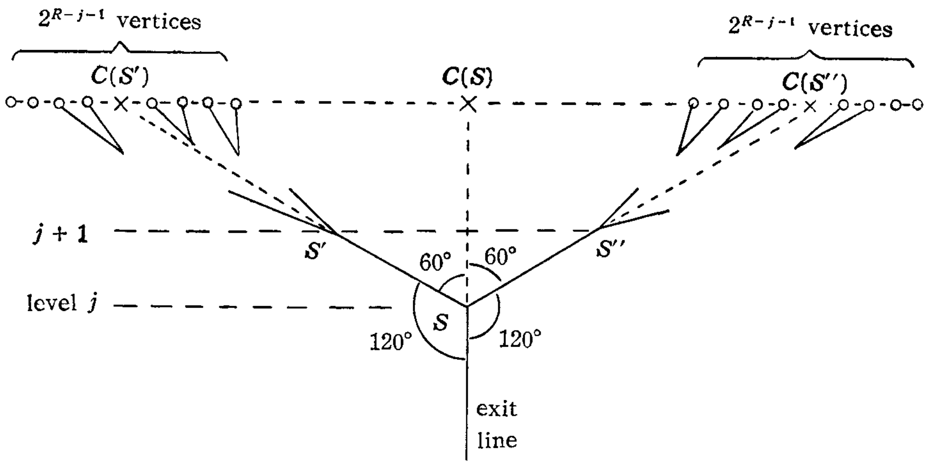

FIGURE 3. The isosceles triangle $C(S')\ S\ C(S'')$.

If S is at level $j < R$ in a binary tree for 2^R vertices, the vector $C(S') - C(S)$ has 2^{R-j} nonzero coordinates, all $\pm\, 2^{j+1-R}$. Then

$$|C(S') - C(S'')| = 2^{(j+2-R)/2}. \tag{6}$$

In order to obtain 120° angles at S, shown in Figure 3,

$$\begin{aligned} |S - C(S')| &= |C(S) - C(S')|(2/3^{1/2}) \\ &= |C(S'') - C(S')|/3^{1/2} \\ |S - C(S')| &= (2^{j+2-R}/3)^{1/2}. \end{aligned} \tag{7}$$

Also

$$|S - C(S)| = \tfrac{1}{2}|S - C(S')| = (2^{j-R}/3)^{1/2}. \tag{8}$$

These formulas determine the lengths of the lines between levels j and $j + 1$. Since S, S', $C(S')$ lie on a line,

$$|S - S'| = |S - C(S')| - |S' - C(S')|.$$

The first term is given by (7). The second is obtained from (8) by replacing j by $j+1$ (the level of S'). Then

(9) $$|S - S'| = \{(2^{1/2} - 1)/3^{1/2}\}2^{(1/2)(j+1-R)}.$$

Condition (4) determines the Steiner tree inductively, proceeding from the core out. The core is a Steiner tree for the (unknown) Steiner points $S_1, S_2 \cdots$ in Figure 1. However, (4) requires that the core, with lines extended beyond $S_1, S_2, \cdots$, be a Steiner tree for the known points $C(S_1), C(S_2), \cdots$. Thus all lines of the core may be constructed before locating $S_1, S_2, \cdots$.

Now consider any binary tree, such as T_1, in Figure 1. At level 0, the point S_1 lies on a line of the core which has been constructed to pass through $C(S_1)$. The location of S_1 on this line is determined by the distance $|S_1 - C(S_1)|$, given by (8) with $j = 0$. Knowing S_1 determines the two lines upward from S_1 to $C(S')$, $C(S'')$. The location of the points S', S'' (of level 1) on these lines is again determined by (8). Continuing in this way, (8) determines all the Steiner points in the binary tree.

4. **Steiner tree length.** The length L_T of the entire Steiner tree will be a sum of lengths of all binary trees plus the length of the core. It will be simpler to find the length L_C of the extended core connecting $C(S_1), C(S_2), \cdots$. Then each binary tree for 2^R vertices contributes additional length $f(R)$, the length of the binary tree minus the extra length $|S_i - C(S_i)|$ which was included in L_C.

Begin with a binary tree for 2^R vertices A_i. The cases $R = 0$ and 1 are atypical; consider first $2 \leq R$. For each $j = 0, 1, \cdots, R-2$, 2^{j+1} lines from Steiner points S at level j to Steiner points S' at level $j+1$. These lines have length given by (9). The total length is

(10) $$\{(2^{1/2} - 1)/3^{1/2}\}2^{(1/2)(3j+3-R)}.$$

Lines between levels $R-1$ and R are different because level R contains vertices A_i instead of Steiner points. The lengths are derived as in (7), where now $C(S')$ is a vertex A_i. The total contribution from the 2^R lines is

(11) $$(2/3)^{1/2}\, 2R.$$

Adding up the lengths (10) for $j = 0, \cdots, R-2$ and including

(11), we find the total length of the binary tree to be

$$L_B = 2^{1/2}C\{2^R - [4 - 2^{3/2})/3]\, 2^{-R/2}\}\,, \tag{12}$$

where

$$C = (3/2)^{1/2}/(2^{3/2} - 1)\,. \tag{13}$$

To get the contribution $f(R)$, defined above, we must subtract

$$|S_i - C(S_i)| = (2^{-R}/3)^{1/2},$$

as given by (8). The final result is

$$f(R) = 2^{1/2}C\{2^R - 2^{-R/2}\}\,. \tag{14}$$

Although the derivation assumed $2 \leq R$, note now that (14) also gives the correct results $f(0) = 0$, $f(1) = (3/2)^{1/2}$.

When $n = 2^{R_1} + {}^{R_2}$, the core is a single line from S_1 to S_2 and the extended core is the line from $C(S_1)$ to $C(S_2)$. An easy calculation gives the length L_C of the extended core

$$L_C = |C(S_1) - C(S_2)| = (2^{-R_1} + 2^{-R_2})^{1/2}\,. \tag{15}$$

Now (14) and (15) provide the length of the Steiner tree, $L_T = L_C + f(R_1) + f(R_2)$. This length may be compared with L_M, given by (1), to get a bound $\rho(D) \leq L_T/L_M$, or

$$\rho(D) \leq D^{-1}\{C(n - 2^{-R_1/2} - 2^{-R_2/2}) + ([2^{-R_1} + 2^{-R_2}]/2)^{1/2}\} \qquad (n = D + 1 = 2^{R_1} + 2^{R_2}). \tag{16}$$

This bound applies to dimensions $D = 1, 2, 3, 4, 5, 7, 8, 9, 11, 15, 16, 17, 19$, in Table I.

In order to verify that the tree just constructed is a legitimate Steiner tree we must check that the Steiner points lie on the line $C(S_1)\,C(S_2)$ in the order $C(S_1)$, S_1, S_2, $C(S_2)$. That requirement may be stated

$$|C(S_1) - S_1| + |C(S_2) - S_2| \leq |C(S_1) - C(S_2)|\,,$$

and verified with the help of (8) and (15) for any R_1, R_2.

When $n = 2^{R_1} + 2^{R_2} + 2^{R_3}$, the extended core is a Steiner tree for three points $C(S_1)$, $C(S_2)$, $C(S_3)$. As shown in Figure 4, it consists of lines from these points to a single Steiner point S_0. The distances between $C(S_1)$, $C(S_2)$, $C(S_3)$ are numbers b_1, b_2, b_3 having formulas like (15), e.g.

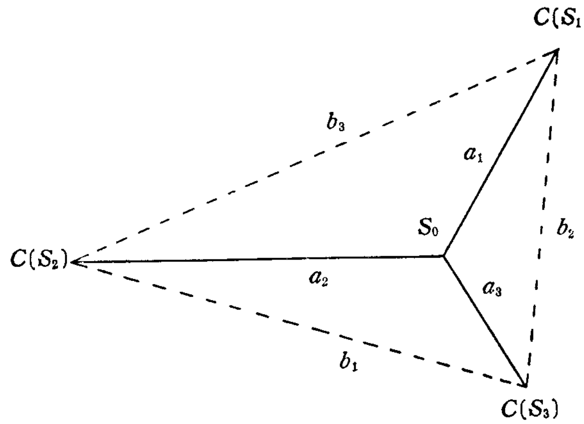

FIGURE 4. Extended core for three binary trees.

$$b_1 = |C(S_2) - C(S_3)| = (2^{-R_2} + 2^{-R_3})^{1/2}.$$

The line lengths

$$a_i = |C(S_i) - S_0|, \qquad i = 1, 2, 3,$$

can be determined by the usual methods for plane Steiner trees. The length $L_C = a_1 + a_2 + a_3$ of the extended core may be found from

$$(17) \quad L_C^2 = \tfrac{1}{2}\{b_1^2 + b_2^2 + b_3^2 + [6(b_1^2b_2^2 + b_2^2b_3^2 + b_3^2b_1^2) - 3(b_1^4 + b_2^4 + b_3^4)]^{1/2}\}.$$

Individual line lengths have formulas like

$$(18) \qquad a_1 = \{L_C + (b_2^2 + b_3^2 - 2b_1^2)/L_C\}/3.$$

Now the Steiner tree has length $L_T = L_C + f(R_1) + f(R_2) + f(R_3)$. An upper bound L_T/L_M on $\rho(D)$ may now be computed from (1), (14), and (17). This bound provided numbers for the other dimensions $D \neq 14$ in Table I. In these computations, (8) and (18) were used to check that

$$|C(S_i) - S_i| < a_i, \qquad i = 1, 2, 3.$$

Dimensions of the form

$$D = 3 \times 2^R - 1$$

afford a comparison between two constructions because

$$D + 1 = 2^R + 2^R + 2^R = 2^{R+1} + 2^R.$$

Actually the same Steiner tree is obtained whether the number of binary trees is taken to be 2 or 3. Using either (16) or (17) one obtains the bound

$$\rho(D) \leq D^{-1}\{Cn - [(9 \times 2^{1/2} - 6)/14]n^{-1/2}\} \tag{19}$$

for $n = D + 1 = 3 \times 2^R$.

5. **Other dimensions.** The bound (19) approaches C as $D \to \infty$ but applies only to dimensions D of special form. This section obtains a bound $\rho(D) \leq C + O(D^{-1})$, applicable for all D.

The bound will be obtained by modifying the construction in §2. Now (2) will be the binary representation of $D + 1$. Instead of using a Steiner tree for the core, we merely connect $S_1, S_2, \cdots$ directly to the same point $O = (1, 1, \cdots, 1)/n$, the centroid of the entire simplex. For the binary tree with 2^R vertices A_i, the extended core contains a line from O to $C(S_k)$ with length $(2^{-R_k} - n^{-1})^{1/2}$. Then the extended core has length

$$L_C = \sum (2^{-R_k} - n^{-1})^{1/2} < \sum 2^{-R_k/2}. \tag{20}$$

The length of the entire tree is

$$\begin{aligned} L_T &= L_C + \sum f(R_k), \\ L_T &< 2^{1/2}cn + (1 - 2^{1/2}c) \sum 2^{-R_k/2}, \end{aligned} \tag{21}$$

the inequality following from (2), (14), and (20). Since the R_k are now distinct integers,

$$\begin{aligned} \sum 2^{-R_k/2} &< 2^{-0} + 2^{-1/2} + (2^{-1/2})^2 + \cdots \\ &= 1/(1 - 2^{-1/2}). \end{aligned}$$

Then (21) simplifies to $L_T < 2^{1/2}c\{n + .22\}$ and

$$\rho(D) \leq L_T/L_M < c + 1.22/D. \tag{22}$$

When $D = 14$, $n = 15 = 2^0 + 2^1 + 2^2 + 2^3$, $L_C = 2.29407$, $L_T = 14.0777$ and one obtains the bound $\rho(14) \leq .711033$ in Table I.

6. **Steiner minimal trees.** The trees which were constructed for $D \leq 5$ in Table I are the Steiner minimal trees for these simplexes; the tabulated bound is actually the exact value of $\rho(D)$. That is easily proved when $D = 1$, 2, 3, or 4 by the following induc-

tion. When $D=1$ the minimal tree is the only possible tree; then $\rho(1)=1$. In higher dimensions D, any tree that is not full can be decomposed into a union of smaller trees to show that its length is at least $\rho(D-1)L_M$. But $\rho(D-1)$, is the value in Table I by the induction hypothesis, and so trees which are not full are all longer than the tree which gave the bound on $\rho(D)$. In [1], Figure 3 shows all possible topologies of full Steiner trees with $n \leq 9$ vertices. Aside from permutation of the n vertices, which does not affect the length of trees for a regular simplex, there is only one full topology for simplexes of dimension 1, 2, 3, and 4. Then if $D \leq 4$ the full Steiner tree that was constructed must be a Steiner minimal tree.

At $D=5$ the argument becomes complicated because there are two full topologies to consider. Table I used the tree based on the representation (2) $6=4+2$ or $6=2+2+2$. The other topology is shown in Figure 5. Again the construction of §3 applies but with a representation $6=(2+1)+(2+1)$. The core now must connect 4 points in a 3-dimensional arrangement.

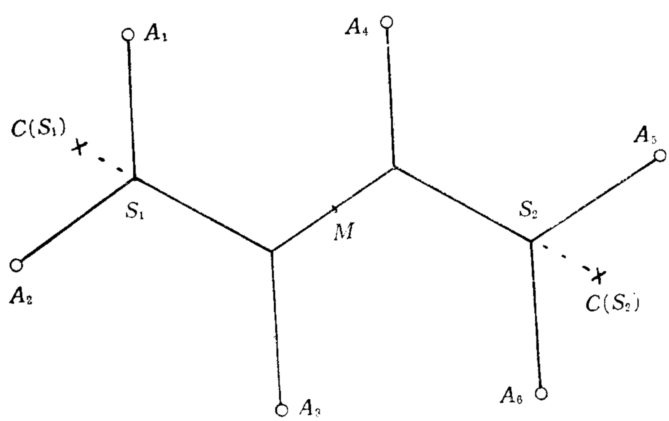

FIGURE 5. Another tree for $D=5$.

To simplify the problem we anticipate the core will have a center of symmetry M of the form

$$M=p(A_1+A_2+A_5+A_6)/4+q(A_3+A_4)/2,$$

where p, q are constants with $p+q=1$. Then the Steiner points can be found by first solving the triangles M, $C(S_1)$, A_3 and M, $C(S_2)$, A_4. Afterward p and q may be adjusted to minimize the length. This minimization also makes the two lines at M join smoothly. A tedious calculation finally produces a Steiner tree with $L_S/L_M = .7650$, larger than the earlier ratio .764564 which is now proved to be $\rho(5)$.

There are also only two full topologies when $D = 6$. The extra topology corresponds to $7 = (2 + 1) + 1 + (1 + 2)$. That requires a core connecting 5 points which has not been constructed. When $7 \leq D$ there are too many topologies to make this approach attractive.

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