On the Steiner ratio in 3-space

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Abstract — **The "Steiner minimal tree" (SMT) of a point set P is the shortest network of "wires" which will suffice to "electrically" interconnect P. The "minimum spanning tree" (MST) is the shortest such network when only *intersite line segments* are permitted. The "Steiner ratio" $\rho(P)$ of a point set P is the length of its SMT divided by the length of its MST. It is of interest to understand which point set (or point sets) in $\mathbf{R}^d$ have minimal Steiner ratio. In this paper, we introduce a point set in $\mathbf{R}^d$ which we call the "d-dimensional sausage." The 1 and 2-dimensional sausages have minimal Steiner ratios 1 and $\sqrt{3}/2$ respectively. (The 2-sausage is the vertex set of an infinite strip of abutting equilateral triangles. The 3-sausage is an infinite number of points evenly spaced along a certain helix.) We present extensive heuristic evidence to support the conjecture that the 3-sausage also has minimal Steiner ratio ($\approx 0.784190373377122$).**

Also: We prove that the regular tetrahedron minimizes ρ among 4-point sets to at least 12 decimal places of accuracy.

This is a companion paper to D-Z. Du and W.D.Smith: Three disproofs of the Gilbert-Pollak Steiner ratio conjecture in three or more dimensions, submitted Journal of Combinatorial Theory. We have tried to devote this paper more to 3D and the other paper more to general dimension, but the split is not clean.

Keywords — Gilbert-Pollak conjecture, Steiner Trees, steiner ratio, Minimum spanning trees, inequalities, sausage.

1 Introduction

Given a point set $P \subset \mathbf{R}^d$, its *Steiner Minimal Tree* (SMT) is the shortest network which will suffice to connect the points. Its *Minimum spanning tree* (MST) is the shortest such network if one is only allowed to use inter-site line segments. An open question is: what is the worst-case "*Steiner ratio*"

$$\rho_d = \inf_{P \subset \mathbf{R}^d} \rho(P) \quad \text{where} \quad \rho(P) = \frac{\ell \mathrm{SMT}(P)}{\ell \mathrm{MST}(P)}, \qquad (1)$$

of their lengths in $\mathbf{R}^d$? Point sets achieving this infimum may be thought of, colloquially, as "the point sets with the most short cuts."

It was shown by Du and Hwang [19], confirming an old conjecture of Gilbert and Pollak [27], that $\rho_2 = \sqrt{3}/2 \approx .866$. This is achieved when P is the vertices of an equilateral triangle.

Of course, when $d = 1$, the MST and SMT are identical and $\rho_1 = 1$.

For each $d \geq 3$, at present ρ_d is not known. (The conjecture of Gilbert and Pollak that ρ_d was achieved when P was the $d+1$ vertices of a regular d-simplex, has been shown [22] to be false for each $d \geq 3$.)

The purpose of this paper is to present a point set we call the d-dimensional sausage. The d-sausage achieves ρ_d when $d = 1$ and $d = 2$. We present extensive heuristic evidence – but no proof – in this paper to make this conjecture plausible:

Conjecture 1 (Main Conjecture) *The 3-sausage achieves ρ_3, and*

$$\rho_3 = \sqrt{\frac{283}{700} - \frac{3\sqrt{21}}{700} + \frac{9\sqrt{11-\sqrt{21}}\sqrt{2}}{140}}$$
$$\approx 0.78419037337712224710839547781568775265 4. \qquad (2)$$

It may also be that the d-sausage achieves ρ_d for some other value of d, such as $d = 4$ or $d = 5$. The d-sausage is in fact the current record holder (minimal known ρ-value) in every dimension d. (Some bounds on ρ_d that arise from the d-sausage were tabulated in [22].) In particular (2) is the best known upper bound on ρ_3. However, we advise caution for these two reasons:

1. We have not subjected any dimension $d \geq 4$ to the sort of scrutiny (which we will report on in this paper) that we have when $d = 3$.

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2. There is an argument [22] which makes it plausible that the d-sausage may not have minimal ρ in all sufficiently large dimensions d. In particular, if the d-sausage is non-minimal in any dimension d, it probably is non-minimal for every $d \geq 15$.

The best rigorous lower bound on ρ_3 is ≈ 0.6158277481, by D-Z. Du [20] [22].

2 Plan

The plan of the present paper is as follows. In §3, we'll survey previous work motivating this paper. We've already defined "Steiner ratio" our (and other people's) results on it; in particular our Main Conjecture that the 3-sausage is the point set with minimal Steiner ratio. The rest of the paper will be concerned with providing evidence to support and elaborate on this conjecture.

In §4 we will define some of the terminology we will use In § 5 we define the "d-sausage" point set. In §6 we give some elaborations on our main conjecture: we conjecture that certain finite subsets of the 3-sausage are the point sets of fixed cardinality having minimal Steiner ratio; we conjecture the Steiner trees of all of these sets, and we conjecture certain monotonicity properties.

In §7 we summarize the evidence for the Main Conjecture which we will present in the remainder (§8-10) of the paper. This evidence consists of theorems (partial results) and computer searches.

3 Why people care about Steiner ratio

Steiner minimal trees are of fundamental importance in path-metric spaces and in geometry, since they are the shortest interconnecting networks for a point set. They are important in network design for the same reason. For surveys of this area see [28] [19] [3] [43] [45] [40].

Unfortunately it is NP-hard to find the shortest Steiner tree (SMT) of a point set, even in the Euclidean plane [23]. The best known algorithms are discussed in [43] and [14]. One therefore is forced to either use an exponentially large amount of computer time, prove $P = NP$,[1] or else settle for an interconnecting network whose length may not be absolutely minimal – but which may be found in polynomial time.

One may then ask for a network whose length is *approximately* minimal. It is not known whether there is a "polynomial time approximation scheme" (that is, a sequence of polynomial time algorithms, such that the kth algorithm is guaranteed to find a tree at most $1 + \epsilon_k$ times the length of the SMT, where $\lim_{k \to \infty} \epsilon_k = 0$) for Steiner trees in any Euclidean d-space, $d \geq 2$. It has been shown [2] [5], however, that if P≠NP, there cannot be a polynomial time approximation scheme for SMTs in general *metric* spaces. On the other hand, it *is* possible to approximate within a factor of 2, since it is easy to see that, in any metric space, the MST is never longer than 2× the length of the SMT [27].

The minimum spanning tree (MST) has many advantages as an approximation to the SMT. It is easy to find the MST of an N-point set. Using Prim's algorithm [35], this may be accomplished in $O(N^2)$ steps, where each "step" may involve the computation of the "distance" between two points. Prim's algorithm will work in any space equipped with a distance function. If the points lie in the Euclidean plane and the distances are Euclidean distances, it may be accomplished [33] in only $O(N \log N)$ steps where a "step" may involve a real arithmetic operation. If the points lie in 3-space, it may be accomplished [1] in $O((N \log N)^{4/3})$ steps, in expectation, by a randomized algorithm. In [42], section III.C.8.2.1-3, is given a deterministic algorithm which will compute the MST of N points in 3-space in $O(N^{3/2}(\log N)^3)$ steps. It was shown in [42], section III.C.8.2.1-3, that one may find the minimum spanning tree of N points in $\mathbf{R}^d$, in $O(N^2 d / \log(Nd)^P)$ steps, where the constant implied by the "O" is independent of both N and d, and P is some positive constant.

We now see that constant-factor length-approximation in polynomial time is possible, but it may not be possible to do better. It is now an important open question to find good approximation algorithms and to find out what is the least ϵ that can be assured by a polynomial time algorithm. (In the plane: see [21] [4].) This question is presently too hard, however, which is why people first want merely to understand Steiner ratio.

4 Notation and definitions

For our graph-theoretic terms and notation, see [6]. For terminology relating to d-polytopes, see [26]. When we say "d-something," we mean that the something can be embedded in a $\mathbf{R}^d$ but not in a $\mathbf{R}^{d-1}$. For example, a "k-facet of a d-polytope" would refer to a facet of the polytope (embedded in a $\mathbf{R}^d$) which lies entirely inside a (translated and rotated) version of $\mathbf{R}^k$ inside this $\mathbf{R}^d$, $0 \leq k \leq d$. For Steiner tree terminology, see [28]. In particular a "full" Steiner tree is one in which the number of Steiner points is the same as the number of original sites, minus 2 (that is, the most it could possibly be).

When we use $\approx$ with a numerical quantity, we mean to imply unit last place accuracy unless otherwise stated.

An "algebraic" number [32] is one that is a root of a polynomial with integer coefficients. Its "degree" is the minimal degree of any such polynomial. (Thus the rational numbers are the algebraics of degree 1.) Numbers which are not algebraic are "transcendental."

We will sometimes (sloppily) refer to a polyhedron when we mean the point set consisting of its vertices. (For example, instead of saying "the point set consisting of the 8 vertices of a cube" we might just say "the cube.")

It is actually quite difficult to define "Steiner ratio" for point sets of possibly infinite cardinality in general

[1] Actually, since the Steiner Problem is not known to be in NP, even this might not help.

metric spaces. Of course, the definition for finite point sets in path metric spaces – namely the length of the Steiner minimal tree divided by the length of the minimum spanning tree – is trivial. With no qualms, we define the Steiner ratio of an infinite point set S in a Euclidean space, which has no accumulation points and which is *periodic*, to be the limit of the Steiner ratio of $S \cap B(\vec{x}, r)$ as $r \to \infty$, where $B(\vec{x}, r)$ is a ball centered at $\vec{x}$ and having radius r. It is easily seen that this limit exists and does not depend upon $\vec{x}$.

In this paper, we are not going to consider any other kinds of infinite point sets. This is fortunate, because the authors actually do not know how to define a "Steiner ratio" of the following rather well-behaved infinite point set P in the Euclidean plane (!). Let r be the distance to the origin. P is the union of the points of the square lattice $\mathbf{Z}^2$ satisfying $10^{2^n} + 1 \le r < 10^{2^{n+1}}$ for some *even* integer $n \ge 0$ with the points of the equilateral triangle lattice A_2 satisfying the same condition where n is odd.

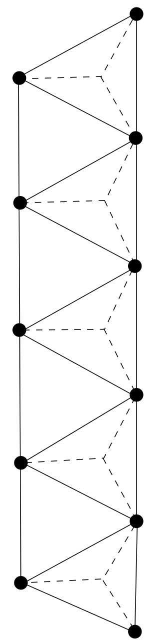

Figure 1: 11-point 2-Sausage, shown with SMT

5 Definition of the d-sausage

The d-dimensional point set which we call the "d-sausage" may be described as follows.

1. Start with a unit (diameter) ball in d-space.

2. Successively add unit balls so that the Nth ball you add, is always touching the $\min(d, N-1)$ most-recently-added balls.

This procedure uniquely (up to congruence) defines an infinite sequence of interior-disjoint numbered d-balls. The centers of these balls form a countably infinite discrete point set,which we call the d-sausage.

Indeed it is most convenient to consider the doubly infinite sausage in which there is a ball corresponding to every integer, both positive and negative (although this makes no difference to the Steiner ratio). A point set consisting of any N consecutive points of the d-sausage will be called the "N-point d-sausage."

The 1-sausage is simply the integers on the real line. Pictures of the 2-sausage and the 3-sausage are given in Figures 1 and 2.

All of the points of the 3-sausage are uniformly spaced along a helix[2] (shown in figure 2). Each successive sausage point is gotten from the previous sausage point by translating along the helix's axis by an amount T, and then rotating about it by an angle θ, where if R is the radius of the cylinder containing the helix, $T/R = \sqrt{10/27} \approx 0.6085806$, and $\theta = \arg(i\sqrt{5}-2) \approx 131.8103°$.

Another useful way to think of the sausage is as the vertices of an infinite simplicial complex made of regular tetrahedra glued together at common faces. Any 4 consecutively numbered sausage points form a regular tetrahedron (figure 3).

Convenient coordinates for a 3-sausage (which is a scale factor of $\sqrt{8}$ larger than the one we'd defined above) are as follows. The first four points are $\vec{p}_1 = (-1,-1,-1)$, $\vec{p}_2 = (-1,1,1)$, $\vec{p}_3 = (1,-1,1)$, $\vec{p}_4 = (1,1,-1)$. Succeeding points are given by $\vec{p}_n = \frac{2}{3}(\vec{p}_{n-1} + \vec{p}_{n-2} + \vec{p}_{n-3}) - \vec{p}_{n-4}$.

6 Some stronger conjectures

Conjecture 2 (The worst finite sets in $\mathbf{R}^3$) *The N-point 3-sausage has minimal Steiner ratio* among N-point subsets of $\mathbf{R}^3$, *whenever $N > 1$ is an integer and $N \ne 5$. The 5-point set with minimal Steiner ratio is the regular tetrahedron (= the 4-point 3-sausage) where the 5th point is infinitesimally near to the 4th.*

This strengthened conjecture is true when $N = 2$ and $N = 3$. (The latter as a result of the Du-Hwang theorem that $\rho_2 = \sqrt{3}/2$.) We will later show (theorem 13) that it is also true when $N = 4$ (at least to 12 decimal places of accuracy), and will provide heuristic evidence for its truth for other values of N.

Conjecture 3 (Monotonic decrease) *The N-point d-sausage has a smaller Steiner ratio than the $(N-1)$-point d-sausage if $N \ge 2d \ge 6$.*

A related conjecture, which we have also, frustratingly, been unable to prove (surely there must be an inductive proof?!), is that

Conjecture 4 (Topology of sausage's SMT) *The N-point 3-sausage, $N \ge 3$, has a unique SMT whose "topology" is as follows. There are $(N-2)$ Steiner points,*

[2] Any set of points spaced uniformly along a helix may be thought of as being spaced uniformly along h disjoint and intertwined helices, for any positive integer h. (The points on helix #k are the ones whose position on the original helix are k modulo h.) Since the choice $h = 3$ minimizes the separation between consecutive points, the human visual system prefers to see the sausage points as lying on a *triple* helix. See figure ??.

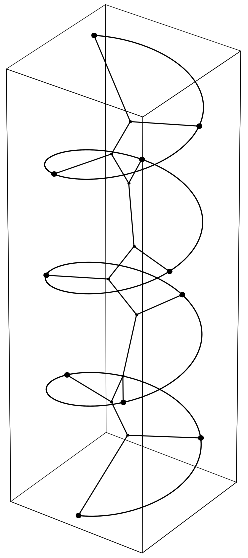

Figure 2: 11-point 3-sausage, shown with helix and SMT

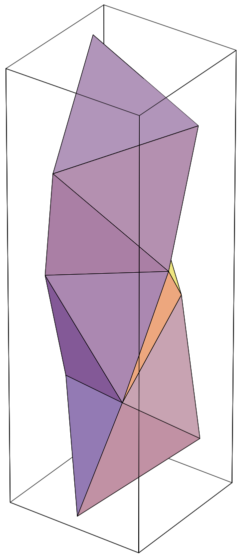

Figure 3: The same 11-point 3-sausage, now shown as a complex of 8 regular tetrahedra (only the outer skin is shown)

Steiner point i being connected to Steiner point $i+1$ for $i = 1 \ldots N-3$. Also sausage point i is attached to Steiner point $i-1$ for $i = 2 \ldots N-1$, and also sausage point 1 is attached to Steiner point 1 and sausage point N is attached to Steiner point $N-2$.

This topology was called the "path topology" in [22], since the Steiner points fall on a single path. We have shown that when $d = 3$ and $N = 3 \ldots 13$, conjectures 3 and 4 are true. (Proof: brute force computer computation of the SMTs of the (≤ 13)-point 3-sausages using the computer program given in [43]. See table 1.)

A related monotonicity statement which we have been able to prove, is

Fact 5 *The N-point d-sausage has a smaller ρ-value than the N-point $(d-1)$-sausage if $N > d \geq 3$.*

Proof Sketch. This is a consequence of the fact that the N-point $(d-1)$-sausage can be mapped onto the N-point d-sausage by "folding" $(d-1)$-space inside of d-space, much as you would fold a sheet of paper to make a 3-dimensional shape. The full proof was given in [22]. □

An immediate, and surprising, consequence of conjectures 2 and 3 would be

Conjecture 6 (The worst sets are infinite) *No finite point set in $\mathbf{R}^3$ has minimal ρ.*

This contrasts with the situation in the plane, where the infimal ρ for an N-point set is $\sqrt{3}/2$ regardless of the value of $N \geq 3$. (Although, for sets of $N \geq 3$ disjoint points in the plane, ρ_2 can only be exactly achieved when N is odd. [This is a consequence of the Du-Hwang proof [19], an impression confirmed by a private communication from F.K. Hwang.])

The assumption of conjecture 4 forces one, as was described in [22], to the conclusion that the 3-sausage's SMT must have the same symmetry group as the 3-sausage itself and must be "periodic" with the "unit cell" being the regular tetrahedron formed of any 4 consecutively numbered sausage points. A computation within this unit cell [22] (see also §10.2 of the present paper) then leads to the conclusion (subject to conjecture 4) that the 3-sausage has Steiner ratio ≈ 0.784190. Regardless of the truth of conjecture 4, this is still a valid upper bound on the 3-sausage's ρ-value, and hence on ρ_3. (Upper bounds on ρ_d derived from the d-sausages for some other values of d, may be found in [22].)

This is an algebraic number, and indeed any assumption of periodicity must always lead to an algebraic number[3]. We will describe how we found the closed form (2) in §10.2.

7 Summary of the evidence

I. We have found the Steiner ratios (or putative Steiner ratios) of thousands of interesting N-point subsets of $\mathbf{R}^3$,

[3] It is also possible to write a closed form expression for ρ(4−sausage), using only rational operations and radicals, again assuming that the path-topology is correct. (Apply the quartic formula and see a footnote in [22].) In dimensions higher than 4, though, we doubt any such closed forms are possible. We also suspect that the algebraic degree of ρ_d grows unboundedly. It is possible to conceive that ρ_d for some d might arise from an aperiodic infinite point set, in which case it would be possible for ρ_d to be transcendental. Unfortunately, we do not know whether that ever happens.

for various N. (The sets we tried will be described in §10.) None of them beat the N-point 3-sausage.

II. Numerical evidence indicates (although we do not claim to have proven it) that the N-point 3-sausages, $N = 6 \ldots 15$, are optimal to small perturbations. (See §10.9.)

III. The d-sausage was "designed" ([22] and see §10.3 of the present paper) to try to lower ρ as much below the d-simplex as possible.

IV. We believe that whatever the minimal-ρ point set P in $\mathbf{R}^d$ is, it will probably have these properties WLOG:

1. It has a large symmetry group.
2. It has a lot of regular simplices.
3. Every point of P lies on the convex hull of P.

For some motivation for some of these beliefs, see the end of §9. It will *certainly* have these properties WLOG:

4. There is no cone of diametric angle $\leq \operatorname{arcsec}(-3) - 60° \approx 49.47122063°$ and apex at a point of P, which contains P. (See theorem 11.)
5. It has a "full" Steiner tree, that is every point of P has valence 1 in the SMT. (See lemma 7.)

In fact:

1. the d-sausage has an infinite symmetry group, there being two symmetries for each integer. (Symmetry $k^{\pm}$, where k is any integer, will map sausage point m to sausage point $k \pm m$.)
2. It may be viewed as the vertices of a simplicial complex made by gluing together congruent regular d-simplices of unit side at common faces. (Sausage points $\{m, m+1, m+2, \ldots, m+d\}$ form such a d-simplex for each integer m. See figure 3.)
3. Every sausage point is an extreme point of the convex hull. (And see figure 2.)
4. The d-sausage may not be enclosed in any cone whose apex is a sausage point. (This cone-free property, of course, is not shared by any finite point set.)
5. The conjecture that the d-sausage, $d \geq 3$, has a unique full SMT, is implied by either conjecture 4 or conjecture 3.

8 Properties that a minimal-ρ point set must (WLOG) have

A well known fact is:

Lemma 7 (The worst sets have full SMTs) *Without loss of generality, a point set in a path-metric space with minimal Steiner ratio must have a "full" SMT topology. That is, every point of P has valence 1 in its Steiner minimal tree.*

Proof. Otherwise, find all the points in P of valence ≥ 2 and mentally "split" them, thus dividing the SMT of P into a forest of edge-disjoint full SMTs on subsets of P. The Steiner ratio of at least one of these subsets must be at least as small as the Steiner ratio of the full set P. □

Speaking of full topologies, it is an empirically observed fact that "typical" point sets in the plane usually do not have full SMTs (their SMTs tend to be unions of disjoint small full SMTs), but typical point sets in 3-space usually do have full SMTs, or at any rate are unions of very large full SMTs. A partial explanation for this phenomenon is provided by the following theorem. (This theorem is, strictly speaking, irrelevant to the main thrust of this paper. But it does provide some useful intuition.)

Theorem 8 (Converse of Rubinstein-Thomas theorem) *Consider a convex polyhedron P, which has triangular faces (by drawing in diagonals on faces if necessary, we may assume WLOG that any polyhedron has only triangular faces), and such that all of these triangles (with at most one exception) have all angles $< 120°$, and such that the MST of the vertices is a subgraph of P's edges. (This last will happen for any polyhedron P which is sufficiently "round;" for example if all the vertices of P lie on a sphere, the center of the sphere is inside P, and at most two edges of P are longer than the sphere's radius.) Then: The SMT of the vertices of P is never the same as the MST.*

Remark 9 *This is interesting because the Rubinstein-Thomas theorem [37] states that the SMT of n-gons in the plane whose vertices all lie on a circle and at most one of whose edges is longer than the circle's radius, is* always *the same as the MST.*

Remark 10 *Some assumption like the $< 120°$ assumption is required: to see this consider a very thin regular n-gonal antiprism.*

Proof. Suppose that the MST and SMT were the same. Then the planar dual $G*$ of the polyhedral graph G with the duals of the MST edges removed (that is, $G * - MST*$), is also a tree. Trees have at least 2 leafs. Hence, there are at least 2 MST vertices each with 2 MST edges incident, both edges sharing the same triangular face of P, hence at least one of them involves an angle $< 120°$. Since no angle in an SMT can be $< 120°$ [27], this is a contradiction. □

We now prove a theorem about enclosing cones.

Theorem 11 (No sharp cones) *If a d-dimensional point set P, $d \geq 3$, achieves minimal Steiner ratio, then WLOG it cannot be contained in any cone C, whose apex coincides with a point of P, and whose (diametric) apex angle is $\leq \operatorname{arcsec}(-3) - 60° \approx 49.471221°$.*

Proof. (By contradiction.) Four interior-disjoint cones with (diametric) apex angle $\operatorname{arcsec}(-3) \approx 109.47°$ and common apex exist in d-space if $d \geq 3$. (They arise from the regular tetrahedron. See [36], for example.) Put four copies of P inside cones of diametric angle $\approx 49.47°$ and common apex coaxially centered in these 4 cones. The resulting set P_4 (which has cardinality $4|P| - 3$) has a Steiner ratio $\rho(P_4) \leq \rho(P)$. In fact, if $|P| < \infty$, then $\rho(P_4) < \rho(P)$, because any tree with a 4-valent vertex is not minimal length hence improvable. Even if P is infinite, however, there can still be only a constant number (that is, depending only on d) of points $A \in P$ such that cones of diametric angle $\leq 50°$ and apex A contain P. This finiteness arises from Gauss's curvature integral theorem applied to the surface of the convex hull of P. Hence, after a finite number of these cone-quadrupling operations, we will obtain a point set with no larger Steiner ratio than P's, but obeying the hypothesis of the theorem. The 60-degree buffer zone assures the MST of P_4 is not shorter than $4\times$ the length of the MST of P. (Suppose it were. Then there must be an edge BC of MST(P_4) where B and C are in different copies of P, so that $\angle BAC > 60°$ where A is the common apex. Then remove BC and replace it with edge AB where $\ell(AB)$ is WLOG minimal, or else replace it with CB' where B' is the point corresponding to B but lying in C's copy of P. One obtains a contradiction.) □

Theorem 11 is in fact a special case of "Du's packing principle" given in [22].

9 The Du-Hwang minimax lemma meets 3D; The regular tetrahedron is the 4-point set with minimal ρ

The useful "Du-Hwang minimax lemma" is as follows. (It is theorem 3.1 of [19]. We have extended and reworded it slightly.)

Lemma 12 (Du-Hwang minimax lemma.) *Suppose $f(x) = \max_{i \in I} g_i(x)$ where I is a finite set and every $g_i(x)$ is a continuous concave-down function in a compact convex d-polytope X. Then the minimum value of $f(x)$ for $x \in X$ is achieved for some x in the strict interior of a k-facet of X (for some $k = 0 \ldots d$) and such that this x is a critical point of order $k+1$ within that k-facet.*

Here a "critical point of order z" is a point at which a maximal ("maximal" here meaning with respect to set-inclusion) set of $g_i(x)$ are equal to $f(x)$, and such that this set has cardinality $\geq z$.

Du and Hwang applied this lemma to the problem of characterizing planar point sets with minimal Steiner ratio.

The question is: can the Du-Hwang lemma be used to deduce properties of 3-dimensional point sets with minimal Steiner ratio? In this section we will see that the answer, unfortunately, appears to be "no." However, it turns out that the Du-Hwang lemma is powerful enough for us to establish the following.

Theorem 13 (Tetrahedon optimality) *The 4-point set with the smallest Steiner ratio is either a regular tetrahedron (with ratio $G = \frac{2\sqrt{3}+\sqrt{2}}{6} \approx 0.813$), or else is a tetrahedron that is regular to at least 12 decimal places.*

In order to use lemma 12 to investigate Steiner ratio for planar point sets, Du and Hwang introduced a convenient parameterization of the coordinates of the N points by use of the lengths of the $2N-3$ Steiner tree edges in some Steiner topology. These lengths suffice to determine the point set up to congruence, since the angles between Steiner tree edges are fixed (120°). They actually only used $2N-4$ parameters since by choice of scale they assumed the length of the Steiner tree was 1. They then observed that the length of the MST of the points was the minimum of several concave-up (in this coordinate system) functions, enabling them to use the lemma with f being the negated reciprocal Steiner ratio.

But, when you try to apply the Du-Hwang techniques to ≥ 3 dimensions, the convenient parameterization no longer suffices. In order to determine the point set uniquely, one also needs to specify (in 3D) the $N-2$ *twist angles* at the Steiner vertices. And then, the length of a spanning tree topology is *not* anymore a concave-up function of the $3N-6$ parameters. We know of no way to fix this fundamental flaw.

Proof of theorem 13. The 4-point set with minimal Steiner ratio of course forms a tetrahedron. (It is impossible for the set to be coplanar since then we would have $\rho > .866$.)

By lemma 7, there are only 3 possible topologies for the SMT of a 4-point set with minimal Steiner ratio. All these 3 topologies are actually the same topology but connected to different permutations of the sites; see the picture below.

```
1          4   1          2   1          2
 \        /     \        /     \        /
  \      /       \      /       \      /
   -------        -------        -------
  /      \       /      \       /      \
 /        \     /        \     /        \
2          3   3          4   4          3
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The idea is going to be that the Du-Hwang idea described 4 paragraphs ago works fine in 3D if the single twist angle θ is held *fixed.* We also assume the Steiner topology τ is being held fixed. The 4-point set is then being parameterized by 5 lengths (of the 5 Steiner tree edges in topology τ) and in fact we assume WLOG that the SMT has unit total length, so these 5 parameters really are restricted to a 4-dimensional set. (We are pretending we have already found the best twist angle θ and the best topology τ and are holding them fixed. We will later minimize over them.)

The "4-polytope X" involved in lemma 12 is then the regular 4-simplex in $\mathbf{R}^5$ with vertex coordinates being the rows of the 5×5 identity matrix. "x" is the 5-vector of parameter values. The "g_i" in lemma 12 are $\ell\text{SMT} - G\ell\text{MST}_i$ where $G = \frac{2\sqrt{3}+\sqrt{2}}{6} \approx 0.81305$ is the Steiner ratio of a regular tetrahedron. Here the i denotes a choice among the 16 possible spanning tree topologies and the "max" accomplishes the selection of the MST. Since we know by lemma 7 that the topology is full, no SMT edge length is zero so that x will be strictly interior to X and "k" in lemma 12 will be 4.

We then see that, to prove that the theorem is true, it will suffice to show that at any tetrahedron whose parameters x form a *critical point of order 5*, $f(x) \geq 0$ for every τ and θ, in particular the ones (which minimize f) arising from the SMT for that tetrahedron.

We then see that a 4-point set that is a critical point of order 5 must have at least 5 minimum spanning trees of equal length. In order for a tetrahedron to have at least 5 equally long MSTs, (one easily sees), one of the following two cases must apply.

I. It has 3 sides of length a forming an equilateral triangle, and of the remaining 3 sides, 2 have length b and the final side is c, where $a \leq b \leq c$.

II. It has one side a, and the other 5 sides have length b, and $a \leq b$.

In either case, the tetrahedron always has at least one equilateral triangular face T and the 4th vertex not on this face always lies in a *plane* P perpendicular to the plane of T and intersecting the plane of T along an altitude of T.

Thus lemma 12 has allowed us to reduce a high-dimensional optimization problem down to a 2-dimensional one, since we may now WLOG agree that the 3 points of T are $(0,1,0)$, $(0,-1/2,\sqrt{3}/2)$, and $(0,-1/2,-\sqrt{3}/2)$, and the 4th point is $(x,y,0)$, where x and y are as yet undetermined and $x > 0$.

Now, observe that the length of the MST, viewed as a continuous function of x and y, has slope nowhere exceeding 1. Similarly the length of the SMT has slope nowhere exceeding 1. The length of the MST and SMT are both at least 3 and the length of the MST is less than the length of the SMT. Hence, by consideration of the derivative formula $(p(t)/q(t))' = p'/q - pq'/q^2$, the slope of the Steiner ratio $\rho(x,y)$ is at most $2/3$. Also, $c < 58a$ since otherwise we would have $\rho > 0.87$. We conclude from these facts that if we examine a square grid of points lying within the semicircle $x^2 + y^2 < 3 \times 60^2$, $x > 0$, with grid spacing ϵ, then the minimal ρ that arises from choosing the fourth point on this grid, will be no greater than the minimal possible ρ for a 4-point set, plus 0.48ϵ. Of course, we may ignore all squares of the ϵ-grid whose corners's ρ values are $\geq G + 0.48\epsilon$. The remaining grid squares, which are rare, may be subdivided with ϵ reduced by a factor of 2 and the process continued.

A computer program then quickly shows that the minimum possible ρ value for a 4-point set is in the interval $[G - 10^{-13}, G]$ and the 4th point forms a regular tetrahedron with the first 3 except for a possible error of $\leq 10^{-12}$. □

Getting rid of the "10^{-12}" proviso would be painful. (It is no problem, of course, to get more decimal places. The problem is proving the regular tetrahedron has a smaller Steiner ratio than every other 4-point set, with no accuracy proviso.) It should presumably be possible to do this with the aid of a local analysis of $\rho(x,y)$ near the regular tetrahedron. We have not carried out such an analysis, however. The same sort of technique should make it possible to prove that a few more point sets are optimal to high accuracy (for example, the regular 4-simplex in $\mathbf{R}^4$), but we have not done this either.

Finally, some speculation. Although (as we've seen) the Du-Hwang minimax lemma is not directly applicable to the Steiner ratio problem in 3D, it still makes it plausible that the ratio-minimizing set has a lot of equally long MSTs. Point sets with a lot of symmetries and/or a lot of regular simplices are therefore plausible candidates.

10 A Plethora of point sets & their Steiner ratios

10.1 The ρ values for the N-point 3-sausages

By brute force computation using the computer program given in [43], we found the following ρ values for the N-point 3-sausages. All values should be accurate to unit last place.

N	rho	name
4	0.813052529585	(regular tetrahedron)
5	0.815469669674	(triangular bipyramid)
6	0.808064936179	("propane")
7	0.802859896946	(1 of 2 "chain butanes")
8	0.800899342742	pentane
9	0.798704227344	hexane
10	0.797013231353	heptane
11	0.795785747249	octane
12	0.794720989050	nonane
13	0.793838038891	decane
14	<= 0.7934	
15	<= 0.7926	
infinity	<= 0.784190373377122	3-sausage

TABLE 1. STEINER RATIOS FOR N-POINT 3-SAUSAGES.

When $N \geq 14$ we did not wait for the computer to complete an exhaustive search, hence the ρ values given are merely upper bounds and are not necessarily the correct answers (though in fact, we believe they are correct). In all cases mentioned, the ρ value given arose from the "path topology" described in conjecture 4.

10.2 The (putative) ρ value for the infinite 3-sausage

Let ρ denote the Steiner ratio of the 3-sausage, subject to the path-topology assumption of conjecture 4. In [22], it was described how to find ρ for the d-sausage (subject to essentially the same topology-assumption) by solving a certain $(d-1)$-dimensional concave-up minimization problem. In the present case $d = 3$, this 2-dimensional minimization problem is

$$\rho = \min_{u,v,w:u+v+w=1} \min\left(\sqrt{\frac{a^2+b^2+c^2}{4} + \sqrt{3Q^2}},\ \ell\right) \tag{3}$$

where

$$\begin{aligned} a^2 &= u^2 + v^2 + (w-1)^2 \\ b^2 &= u^2 + (v-1)^2 + w^2 \\ c^2 &= u^2 + (v-u)^2 + (w-v)^2 + w^2 \end{aligned} \tag{4}$$

and Q is the area of a triangle with sides a, b, c, that is

$$Q^2 = s(s-a)(s-b)(s-c) \quad \text{where} \quad s = \frac{a+b+c}{2}, \quad (5)$$

and ℓ is the length of the MST of that triangle, that is

$$\ell = 2s - \max(a, b, c). \quad (6)$$

Here u, v, w are the barycentric coordinates of the location on either face of the "unit cell" tetrahedron where the SMT leaves the cell. The minimization problem as we have formulated it arises from using coordinates for the unit cell tetrahedron's vertices being the rows of the 4×4 identity matrix (these convenient coordinates all lie in the hyperplane inside $\mathbf{R}^4$ having unit sum of coordinates). The piece of the SMT inside this unit cell is simply the SMT of a triangle, whose three vertices are $(u, v, w, 0)$, $(0, u, v, w)$, and $(0, 0, 1, 0)$ and whose sides are a, b, c.

The formula (3) arises from formula (2) of [43].

Since $v = 1-u-w$, the minimization problem is really only 2-dimensional. At and near the minimum (one sees by numerical investigation) ℓ is irrelevant, Q is bounded above 0, and hence ρ^2 is an analytic function of u, w in a neighborhood of this minimum. With great labor, one may confirm that the gradient of ρ^2 with respect to (u, w) is zero when $u = w = (21 - \sqrt{21})/70 \approx 0.2345346$. Due to the concave-up nature of the minimization problem, this is the unique minimum. The expression (2) then follows.

It is quite remarkable that this relatively simple closed form exists in 3D. The corresponding closed form in 4D is exceedingly complicated, and in 5 or more dimensions we are dubious that there is any closed form.

Regardless of the truth of conjecture 4, *the expression on the right hand side of (2) is a valid upper bound on the Steiner ratio of the 3-sausage, and on* ρ_3.

10.3 The sausage seems to be correctly designed locally

The reader will recall from [22] that the sausage was "designed" to bring ρ as far as possible below the value achieved by the regular simplex. This is because the d-sausage may be viewed as the union of an infinite number of d-simplices where two consecutive[4] simplices share exactly one vertex, and the two simplices sharing the vertex have cleverly been rotated with respect to one another in order to minimize ρ. To test the hypothesis that the positioning of these tetrahedra in the 3-sausage really is optimal, we computed ρ for 10000 7-point sets. Each 7-point set was obtained by taking the union of a regular tetrahedron (4 points) with a random 3-dimensional rotation of itself about one of its vertices. The result was 10000 ρ values. All of these values turned out to lie in the interval $[0.804809, 0.950884]$. Meanwhile the 7-point 3-sausage has $\rho \leq .802859897$. Thus *The 7-point 3-sausage is almost certainly optimal among the 7-point sets consisting of a regular tetrahedron and a rotation of itself about one of its vertices.*

We also looked at the 6-point sets that were subsets of these 10000 7-point sets. The minimal ρ found was 0.811661, not beating propane. Thus *The 6-point 3-sausage is almost certainly optimal among the 6-point sets consisting of a regular tetrahedron and a 3-dimensional rotation of one of its triangular faces about one of its vertices.*

10.4 Searches among "carbon molecules"

Since a regular tetrahedron has 4 faces and a carbon atom has 4 (single) bonds in the same tetrahedral orientation, it is convenient to steal some notation from organic chemistry and refer, for example, to the 6-point set made by gluing together 3 equal regular tetrahedra, as "propane." Tetrahedrons mentally correspond to carbon atoms. We have done this in table 1.

We considered all (≤ 9)-point sets arising as the vertices of all simplicial complexes made of ≤ 6 equal regular tetrahedra glued together at common faces. (The 9-point sets are "hexanes.")

The situation first becomes interesting when one reaches butane, since there are three noncongruent butanes, namely two "chain" butanes and one "tree" butane featuring a 3-valent carbon. (Meanwhile there is only one methane, ethane, and propane.) These three butanes have $\rho \approx 0.802860, 0.812906, 0.828871$ respectively. One may inductively generate the molecules with $c+1$ carbons from those with c by considering every possible way to stick on another tetrahedron. Molecules with c carbons yield sets of $N = c+3$ points.

We computed the ρ value of each such set. We found that: *The N-point 3-sausages uniquely minimize ρ among $(N-3)$-carbon molecules when $N \leq 9$.*

When $N \geq 10$ too many carbon molecules arose for us to search them exhaustively. However, we noticed that the carbon molecules with the smallest ρ values always seem to be "chains." That is, carbon atom c is always attached to carbon atom $c-1$ and there are no (≥ 3)-valent carbons. There are considerably fewer carbon chain molecules than carbon molecules. In fact, one easily sees that that the number of c-carbon chain molecules is $\leq 2 \times 3^{c-4}$, $c \geq 4$. They may be generated inductively by considering the ≤ 3 ways to stick another carbon onto the end of the chain. We generated all c-carbon chain molecules with $c \leq 7$, and upon computing their ρ values, again the sausages were uniquely optimal.

The N-point 3-sausages uniquely minimize ρ among chain $(N-3)$-carbon molecules when $N \leq 10$.

It should be noted that in the searches so far, absolutely nothing prevented the tetrahedra defining the simplicial complex from overlapping, and it was not required that the minimum distance between any two points had to be the same as the length of a tetrahedron edge.

If these constraints are enforced, then the number of

[4] Here, we are saying that two simplices in the d-sausage are "consecutive" if their vertices are sausage points numbers $\{m, m+1, \ldots, m+d\}$ and $\{m+d, m+d+1, \ldots, m+2d\}$ for some integer m.

chains is reduced[5], enabling us to search further. We found:

The N-point 3-sausages uniquely minimize ρ among chain $(N-3)$-carbon molecules with nonoverlap and minimal-distance constraints when $N \le 11$.

10.5 The octahedron and other "molecules"

Since the regular octahedron ($N = 6$ points) has a rather small ρ value ≈ 0.811197, one wonders whether one may produce record low ρ-values by using the vertices of complexes got by gluing regular octahedra and/or regular tetrahedra together at common faces.

There are 256 ways to glue regular tetrahedra onto some subset of the 8 faces of a regular octahedron. (Actually, there are considerably fewer than this if one takes advantage of the order-48 symmetry group of the octahedron.) Fortunately, the ones with a lot of points (which our SMT-computing program takes a long time to solve) all seemed to have large ρ values. We computed exact (or putative, when $N \ge 10$) ρ values, for them all. The best three (besides the octahedron itself) were:

- octahedron with 2 tetrahedra glued on antipodally ($N = 8$) $\rho \approx 0.808696$,
- octahedron with 1 tetrahedron glued on ($N = 7$) $\rho \approx 0.810776$,
- octahedron glued to 3 tetrahedra, 2 adjacent & 1 nonadjacent ($N = 9$) $\rho \approx 0.81236$.

We also tried gluing an ethane to an octahedron ($N = 8$, $\rho \approx 0.806237$), and gluing two ethanes to an octahedron antipodally in such a way that the whole thing was centrally symmetric ($N = 10$, $\rho \approx 0.806167$).

Finally, we tried gluing two octahedra together at a face ($N = 9$, $\rho \approx 0.830142$), and we also tried various unions of two congruent octahedra sharing an edge ($N = 10$) or sharing a vertex ($N = 11$), none of which had particularly small ρ.

Comparing these numbers with those in table 1, it seems clear from this that *Nonrigorous heuristic principle: using octahedra inside complexes of octahedra and/or tetrahedra yields larger ρ values than using tetrahedra alone.*

10.6 Various interesting polyhedra

We tried various polyhedra with triangular and square faces, among them:

polyhedron	N	rho
tetrahedron (methane)	4	0.813052
tri. bipyramid (ethane)	5	0.815470
square pyramid	5	0.826296
octahedron	6	0.811197
triangular prism (TP)	6	0.846410
cube	8	0.885165
edge-midpoints of TP	9	0.874093
icosahedron	12	0.843314
edge-midpoints of cube	12	0.867296

TABLE 2. STEINER RATIOS OF VARIOUS POLYHEDRA.

We tried placing an extra central point inside these polyhedra:

polyhedron & central pt	N	rho
tetrahedron	5	0.995782
tri. bipyramid (ethane)	6	0.971760
octahedron	7	0.958474
triangular prism (TP)	7	0.927134
cube	9	0.894337
edge-midpoints of TP	10	0.870308
icosahedron	13	0.828146
edge-midpoints of cube	13	0.809324

TABLE 3. STEINER RATIOS OF VARIOUS POLYHEDRA WITH AN EXTRA CENTRAL POINT.

We also tried various right equilateral-triangular prisms with *rectangular* faces. Among these, the one which minimizes ρ seems to be the one with square faces.

In no case were the ρ values obtained smaller than the ρ value of the N-point 3-sausage with the same value of N.

10.7 Random point sets

We generated sets of random points in the unit cube $[0,1]^3$ and computed their Steiner ratios. The results were as follows.

```
     ***   4-point sets  ***
#sets generated        136000
minimum rho found      0.827453
[.82(.01).86] populations: 1,17,67,280
     ***   5-point sets  ***
#sets generated        100000
minimum rho found      0.839155
[.83(.01).86] populations: 1,5,56
     ***   6-point sets  ***
#sets generated        350000
minimum rho found      0.844255
[.84(.01).86] populations: 2,23
     ***   7-point sets  ***
#sets generated        87000
minimum rho found      0.861577
[.86(.01).89] populations: 14,77,330
```

To explain the information on "populations" by example: of the 136000 4-point sets we investigated, 17 had

[5] Another interesting subset of carbon molecules are the ones which lead to *convex* point sets. It is also possible to generate these inductively by trying all possible ways to stick on another tetrahedron in such a way that the resulting point set (of tetrahedron vertices) is still convex. However, within the range of our experiments, requiring convexity did not greatly reduce the number of carbon molecules – although asymptotically we suppose the reduction must be enormous.

$0.83 \le \rho < 0.84$. Although random point sets are not likely to have particularly small ρ, they do have the advantage that no assumptions are being made; this is a broad spectrum search. These figures also give one an idea of how good minimum spanning trees are usually going to be "in practice."

10.8 Random helices

Next, we tried N-point sets of the form

$$\vec{p}_m = (\sin(m\theta),\ \cos(m\theta),\ \beta m), \quad m = 1, 2, \ldots N, \qquad (7)$$

where θ and β are fixed. In our experiments, (θ, β) were chosen randomly from a certain distribution in $[0, \pi] \times [0.15, 3.9]$. These "random helix" point sets were inspired by thet fact that when $\theta = \arg(i\sqrt{5}-2) \approx 131.8103°$ and $\beta = \sqrt{10/27} \approx 0.6085806$ these sets are the N-point 3-sausages.

Our results were as follows.

```
     ***   6-point sets  ***
#sets generated        11746
minimum rho found      0.81162
[.81(.01).84] populations: 14,47,59
     ***   7-point sets  ***
#sets generated        5883
minimum rho found      0.80526
[.80(.01).83] populations: 1,10,32
     ***   8-point sets  ***
#sets generated        1147
minimum rho found      0.81368
[.81(.01).84] populations: 3,6,6
```

In all cases the "minimum rho found" set involved θ and β values within 1 part in 30 of the sausage values and having a not-as-small Steiner ratio. *(Nonrigorous) Conclusion: it appears that among all point sets that are uniformly spaced along a helix, the 3-sausage has the minimal Steiner ratio.*

10.9 A numerical multi-dimensional optimizer

We interfaced the general purpose derivative-free multidimensional optimizer "Powell" (taken from [34]) with Prim's MST algorithm. The result was a program which moved points (both N original points and $N-2$ "Steiner" points) around in a crude automated attempt to find the N-point set minimizing ρ, or more precisely the ratio of the MST of the original points plus the Steiner points, divided by the MST of the original points only. Powell's possibly wrong choice of Steiner points and Steiner topologies can lead to overestimates of ρ but never to underestimates.

Powell's method [31] is a derivative free method designed for finding a local minimum of a function $f(\vec{x})$ by successive 1-dimensional searches along a set of conjugate directions. The method should always converge to a local minimum for sufficiently well-behaved functions; also it generally exhibits quasi-quadratic convergence when f behaves quadratically near its minimum. The f in the present problem (ratio of two MST lengths) is "well behaved," but is only piecewise differentiable, and is usually not differentiable at minima. Thus there is no reason that "Powell" should be a particularly efficient optimizer for our purposes, nor is there any reason to think it will find a global optimum. But it at least will find a nearby local minima without supervision.

One may keep 2 of the N non-Steiner points fixed WLOG, viewing this as a $(6N-12)$-dimensional optimization problem. In practice, though, Powell often got up to 3 more decimals of accuracy if one allowed all the points to move.

First, we ran Powell starting from the N-point 3-sausages with $N \le 15$ and their SMTs. Sure enough, Powell was unable to improve upon them, thus "proving" (we do not claim that this is a rigorous proof, but it is certainly pretty convincing) that *Heuristically: the N-point 3-sausages with $N \le 15$ minimize ρ within the class of all sufficiently small perturbations of the point coordinates.*

Second, we tried running Powell starting from pseudorandom N-point sets in the unit cube. The results were as follows. We Powelled 34 pseudorandom 4-point sets. The best one it found had (it claimed) $\rho \approx 0.81533$. Upon re-Powelling[6] this (inadequately optimized) set, this improved to $\rho \approx 0.81305$. Thus Powell is sufficiently powerful to find the regular tetrahedron (which this set was, to high accuracy) starting from essentially nothing.

This inspired us to Powellize 100 pseudorandom 5-point sets. The best one it found had $\rho \approx 0.81945$, which improved upon re-Powelling to $\rho \approx 0.81305$. The point set it found is, to high accuracy, the regular tetrahedron with a duplicated point.

Unfortunately, Powell is a less effective searcher when one tries it with larger numbers of points. We Powelled and re-Powelled 305 pseudorandom 6-point sets. The best two sets it found had $\rho \approx 0.81727$ and $\rho \approx 0.81805$. Although this is a substantial improvement on the best of 350000 un-optimized random 6-point sets (§10.7) at $\rho \approx 0.844255$, it is still nowhere near the 6-point sausage at $\rho \approx 0.808065$. Powelling 149 random 7-point sets, the best it could do was $\rho \approx 0.83198$.

10.10 Point lattices

Since we are conjecturing that the true ρ-minimizing configuration is an infinite point set with an infinite symmetry group, one is led to ask about infinite point lattices, which in fact have even "larger" infinite symmetry groups than the 3-sausage, in the sense that the 3-sausage has a group isomorphic to $2 \times \mathbf{Z}$, while the cubic lattice, for example, has a group $\mathbf{Z} \times \mathbf{Z} \times \mathbf{Z} \times 2 \times 2 \times 2 \times S_3$.

We will now compute the putative Steiner ratios for several interesting lattices. The only cases in which

[6] here and below, "re-Powelling" runs allowed all the points to move, but the original search had fixed two of them; thus, re-Powelling runs optimized more precisely

we have a proof that our ρ value is correct, are the 2-dimensional cases when $\rho = \sqrt{3}/2$.

In the other cases, the ρ value we give is merely an upper bound. We conjecture, with varying amounts of confidence, that these upper bounds are actually tight[7].

Despite any lack of confidence we may feel in our putative ρ values, it still seems very likely to us that none of these lattices beat the 3-sausage. The reason for this belief is basically that these lattices have lots of "unavoidable octahedra," combined with the conclusion of §10.5.

We also remark that our results on *planar* lattices are not hard and were mostly known before. We have included them because they make a good introduction to our "TED-set" methods.

Our results are as follows.

Lattice	rho
equilateral triangle lattice in plane	.866025
kagome nonlattice in plane	.866025
square lattice in plane	<= .910684
octahedron-square tiling in plane	<= .933013
FCC lattice in 3-space	<= .801(.002)
HCP nonlattice in 3-space	<= .801(.002)
BCC lattice in 3-space	<= .845549
simple cubic lattice in 3-space	<= .885165

TABLE 4. PUTATIVE STEINER RATIOS FOR LATTICES.

Terminology. A "treelike set" in a graph (or multigraph) G is a subset S of the vertices of G such that the subgraph (or submultigraph) induced in G by S is a tree. A subset S of the vertices of a graph G is said to be "edge dominating" if every edge of G is incident on at least one vertex in S. A subset S of vertices that is both treelike and edge dominating is called "TED."

A "lattice" is an infinite but nondense set of points closed under vector addition and subtraction. With each lattice we associate its "graph" in which two points are linked by an edge iff they are nearest neighbors.

If G is the graph of a lattice or infinite periodic point set, then "TED sets" in G will be (by fiat) allowed to be forests consisting of of infinite trees, i.e. not trees, if desired.

A useful connection between TED sets and Steiner trees of point lattices is as follows.

Theorem 14 *Let P be a point set that is the vertices of a set of congruent polyhedral tiles T, each of which has edges of unit length only. Define an "adjacency multigraph" G on the polyhedral tiles by associating one node of G to each tile and two such nodes are joined by k edges in G iff the corresponding tiles share k vertices. Then: if G contains a TED set, then $\rho(P) \leq \rho(T)$.*

Proof. Place an SMT (of the vertices of that tile) inside each tile in the TED set to get a (possibly nonminimal) Steiner tree for P. The union of the MSTs of the tiles in the TED set is an MST of P. □

10.10.1 The integer 2D lattice $\mathbf{Z}^2$.

Consider the points are the vertices of a checkerboard. The centers of the red squares form a (larger, 45-degree rotated) $\mathbf{Z}^2$. Find a TED-set in this $\mathbf{Z}^2$. (They exist. See figure 4.)

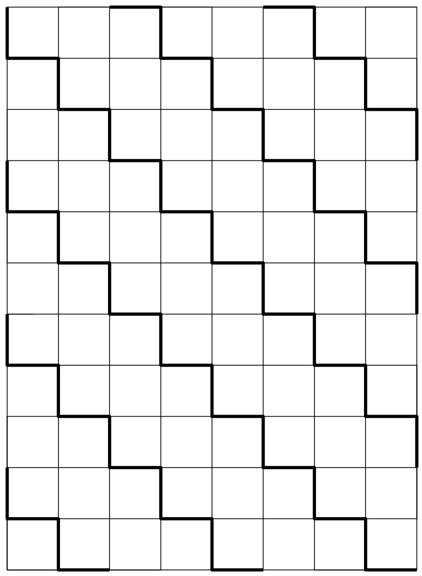

Figure 4: TED set in $\mathbf{Z}^2$

In each red square corresponding to an element of the TED set, place an SMT of its 4 vertices. Result is an SMT (definitely a Steiner tree; minimality, however, is only conjectural) for $\mathbf{Z}^2$ whose steiner ratio $\rho = (1 + \sqrt{3})/3 \approx .91068$.

Thus $\rho(\mathbf{Z}^2) \leq .910684$. Further support for the conjecture that this bound is tight, is provided by computational results in figure 5 of [14]. This conjecture had been made previously in [12], along with a version of the same Steiner tree construction we have described here.

10.10.2 The 2D equilateral triangle lattice A_2.

3-color the triangles blue, black and red so no same color triangles share an edge and each vertex is in 2 triangles of each color. The centers of the red triangles form a regular hexagon tiling graph H. Find a TED set in H. (They exist. See figure 5.) Place SMTs in the red TED triangles.

Result is an SMT with optimal ρ (by the Du-Hwang theorem) $\rho = \sqrt{3}/2 \approx .866025$.

The same sort of result and a similar construction was known previously [29].

[7] Interesting and difficult open problems: 1. find the Steiner ratios of these and other lattices, 2. find the d-dimensional point lattice with minimal Steiner ratio.

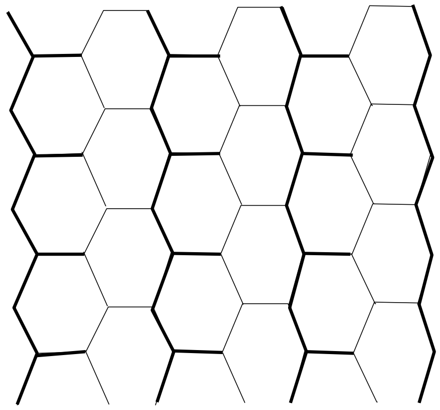

Figure 5: TED set in H

10.10.3 Kagome nonlattice in 2D

The Kagome nonlattice is the tiling of plane by regular hexagons (6) and triangles (3) with 3636 around each vertex in that cyclic order. The centers of the triangles form the graph H of a regular hexagon tiling. Find a TED set in H. Place SMTs in the TED triangles. Again we get $\rho = \sqrt{3}/2 \approx .866025$, which is optimal by the Du-Hwang theorem.

10.10.4 Tiling of plane by regular octagons and squares

Where the cyclic pattern around each vertex is 884. Can get $\rho = (2 + \sqrt{3})/4 \approx .933013$, conjecturally optimal, by placing SMTs in each square and connecting squares by SE-NW diagonal edges.

We've now discussed the most pleasant Archimedean tilings of the plane; now on to 3D.

10.10.5 Simple cubic lattice $\mathbf{Z}^3$.

Color one cube red and then a cube is red iff it shares a vertex, but does not share an edge or a face, with a red cube. The centers of the red cubes form a BCC lattice. Find a TED set in this BCC lattice. (An example of a TED-set in the BCC lattice is the points with coordinates $(4a + c, 4b + c, c)$, $a, b, c \in \mathbf{Z}$ inside the BCC lattice whose points are (x, y, z), $x, y, z \in \mathbf{Z}$, x, y, z all even or all odd.) Put an SMT (length$\approx$ 6.196152) inside each red TED cube. In this way one shows $\rho(\mathbf{Z}^3) \le \rho(\text{cube}) \approx .88516463$.

The fact (proven by computer) that two iso-oriented congruent cubes sharing exactly one vertex, have the same Steiner ratio as a single cube, proves that this SMT is at least minimal to small perturbations.

The fact that 2 abutting cubes have larger ρ ($\approx$ .8862296) than one cube ($\approx$ .88516) and two iso-oriented cubes sharing exactly one edge have $\rho \approx .886839$ suggests that the construction above is optimal.

10.10.6 BCC lattice

The BCC lattice is the points of $\mathbf{Z}^3$ which have all coordinates even or all coordinates odd. It may also be thought of as the vertices of a tiling of 3-space by a certain "squat octahedron" soon to be described.

A layer ("layer 0") of this lattice is isomorphic (up to scaling and rotation) to $\mathbf{Z}^2$. Consider the red squares of the $\mathbf{Z}^2$ checkerboard and erect pyramids on them, thus touching half the points of the next layer of BCC. In fact, erect pyramids in both directions to make a squat octahedron to get half the points in both layer 1 and layer -1. Take the black squares of the BCC layer 2 and erect squat octahedra on them similarly (getting the other half of the layer 1 points) etc.

The centers of these octahedra form alternating layers, each a $\mathbf{Z}^2$ rotated 45 degrees. Find a TED set in these $\mathbf{Z}^2$'s, put in SMTs of the octahedra corresponding to the TED set. Result is $\rho(\text{BCC}) \le \rho(\text{squat octahedron}) \approx .8455485362$. This is probably optimal since various creatures made of two squat octahedra (with common vertex, edge, or face) have $\ge$ this ρ.

10.10.7 FCC lattice and HCP nonlattice.

The FCC lattice is the points of $\mathbf{Z}^3$ which have even sum-of-coordinates. FCC may also be thought of as the vertices of a tiling of 3-space by regular tetrahedra and octahedra of the same edge length.

In FCC, each vertex is shared by 6 octahedra and 8 tetrahedra. Each triangle face is shared by exactly one tetrahedron and one octahedron. Each edge is shared by 2 tetrahedra and 2 octahedra, cyclic order OTOT.

Assuming that certain TED sets exist, one may show that $\rho(\text{FCC}) \le \rho(\text{octahedron}) \approx .811197$, and $\rho(\text{FCC}) \le \rho(\text{tetrahedron}) \approx .813052$. However, one doubts that these bounds are optimal, since, for example, the "acorn" (an 8-point set made of an octahedron with abutting tetrahedra on its north and south faces) has $\rho \approx .808696$ and will tile 3-space to make an FCC lattice. (This does *not* imply $\rho(\text{FCC}) \le \rho(\text{acorn})$ since a suitable TED set does not exist.)

In fact, these doubts are correct. The best Steiner tree we know of for the FCC lattice shows

$$\rho(\text{FCC}) \le \rho(\text{mountain range}) \approx 0.801. \tag{8}$$

Here a "mountain range" is the 3D point set obtained by taking the 2-sausage in the plane, 2-coloring its triangles, and erecting regular tetrahedra on top of the blue triangles. It turns out the points of the FCC lattice, or of the HCP nonlattice, may be partitioned into disjoint mountain ranges, hence the bound.

This is most easily seen by building models of FCC and HCP. Use the tetrahedral "carbons" in molecular modeling kits to make a "diamond" nonlattice. Use both blue and red carbons, where no two same-color carbons are connected by a bond. The blue carbons will then form an FCC lattice, demonstrating how the diamond nonlattice is the union of two FCC lattices. A family of parallel tunnels, of slightly *nonregular* hexagonal cross section, will then be visible. The red carbons on the wall of each such tunnel form a mountain range, and a suitable partitioning is then easily found. A model of HCP may be constructed similarly[8]; one should be warned that the HCP model also has a family of parallel tunnels of *regular* hexagon cross section, which are to be disregarded; the important tunnels are of nonregular hexagonal cross section.

The 1,2, and 3-mountain ranges have $\rho \approx .813052$, .809325, .807163. The "mountain range" (with an infinite number of mountains) has a smaller Steiner ratio than these numbers, of course. Apparently its ρ value is $\approx .801 \pm 0.002$.

10.11 Miscellaneous other point sets

In addition to the point sets mentioned above, we have tried many other point sets, in fruitless attempts to beat the N-point 3-sausages. We mention some of them here.

- Various complexes made by gluing together some of the polyhedra in table 2 at common faces, edges, or vertices.
- All subsets of the vertices of a cube.
- Various subsets of various 3D point lattices.
- 10000 sets consisting of a unit-side regular tetrahedron plus a random point on the sphere of radius 1 about a vertex. The best one found had $\rho = 0.814043$ and the 5th point was very close to the 4th point. This bolsters the conjecture that the min-ρ 5-point set is the regular tetrahedron with a duplicated point.
- We also tried another 10000 5-point sets defined the same way as above, except that the radius of the sphere was 0.5. The minimum ρ found was 0.827562.

11 Conclusion

We have presented a lot of heuristic evidence, including both computer searches and partial proofs, which makes it plausible that the 3-sausage has minimal Steiner ratio among 3D point sets. We think this evidence is fairly convincing. Its greatest weakness is: most of our partial results and all of our computer searches concerned point sets with ≤ 15 points.

Knowledge of the 3-sausage's helical tetrahedronal-chain configuration should be useful in the design of heuristics for the general 3D SMT problem [41].

12 Corrections to W.D.Smith: *How to find SMTs...*

To correct the most serious typographical errors in [43], in line 18 of routine `main()` page 71, the "`j`" should be an `i` and the line 19 the "`+j`" should be "`; j`". In table 1 page 153, top left, the "1 2 3" should have been "12 3".

A version of the SMT-finding C program given in [43] along with additional code to compute the MST, is now available through anonymous FTP from external.nj.nec.com in the file /pub/steinrat.c.

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References

[1] Agarwal, P.K., H. Edelsbrunner, O. Schwarzkopf, E. Welzl: Euclidean Minimum Spanning Trees and bichromatic closest pairs, Discr. and Comput. Geometry 6 (1991) 407-422.

[2] Sanjeev Arora, Carsten Lund, Rajeev Motwani, Madhu Sudan, Mario Szegedy, October 1992. On the intractability of approximation problems, *33rd IEEE Symposium on Foundations of Computer Science* 14-23.

[3] Bern, M. and R. Graham, 1989. "The Shortest-Network Problem," *Scientific American 260* (1), 84–89.

[4] Beasley, J.E., "A Greedy Heuristic for the Euclidean and Rectilinear Steiner Problem," *European Journal of Operational Research.* Beasley also has an improved heuristic in a manuscript submitted to *Networks.*

[5] Bern, M. and Paul Plassman, 1989. "The Steiner problem with edge lengths 1 and 2," *Information Processing Letters* 32, 171-176.

[6] Bondy, J.A. and U.S.R. Murty, Graph Theory with applications, North-Holland 1976.

[7] Booth, R.S. and J.F. Weng: Steiner minimal trees for a class of zigzag lines, *Algorithmica* 7, 231–246.

[8] Chang, S.K., 1972 "The Generation of Minimal Trees with a Steiner Topology," *JACM 19* (4) 699–711.

[9] Cheriton, D. and R. E. Tarjan, 1976. "Finding Minimal Spanning Trees," *Siam J. of Computing 5 (4),* 724–742.

[10] Chung,F.R.K. and F.K. Hwang, 1976, "A Lower Bound for the Steiner Tree Problem," *Siam J. Appl.Math 34(1),* 27–36.

[8] Using a "modified diamond" nonlattice in which every third layer is "twisted" by 120°

[11] Chung, F.R.K. and R.L. Graham, 1978. "Steiner Trees for Ladders," *Annals Of Discrete Mathematics 2,* 173–200.

[12] Chung, F.R.K., M. Gardner, and R.L. Graham, 1989. "Steiner Trees on a checkerboard," *Math. Mag.* 62, 83–96.

[13] Cockayne, E.J. and Z.A. Melzak, 1969. "Euclidean Constructibility in Graph Minimization Problems." *Math.Mag.42,* 206–208.

[14] Cockayne, E.J. and D.E. Hewgill, 1992. "Improved computation of plane Steiner minimal trees," *Algorithmica* 7, 219–232.

[15] Courant, D.R. and H. Robbins, 1941. *What Is Mathematics?* New York: Oxford University Press.

[16] Dixon, L.C.W., 1972. *Nonlinear Optimization.* The English Universities Press, Ltd: St. Paul's House Warwick Lane, London EC4P 4AH.

[17] Du, D-Z., F.K.Hwang, and J.F. Weng, 1983. "Steiner Minimal Trees on Zig-Zag Lines." *Trans. Amer. Math Soc. 278* (1), 149–156.

[18] Du, D-Z. and F.K.Hwang. *Computing and Euclidean Geometry* eds. D.Z. Du and F.K. Hwang. World Scientific 1992.

[19] Du, D-Z. and F.K.Hwang, 1992. "State of the art in Steiner ratio conjectures," pages 163–192 in [18].

[20] Du, D-Z., 1991. Paper in J.M. Smith and P. Winter (ed.), Topological Network Design, *Annals of Operations Research* 33 (1991) 437-451.

[21] Du, D-Z., Y. Zhang, Q. Feng, 1991. "On Better Heuristic for Euclidean Steiner Minimal Trees," *32nd IEEE Sympos. on Foundations of Computer Science,* 431–439.

[22] Du, D-Z, and Warren D. Smith, 1992 "Three disproofs of the Gilbert-Pollak Steiner ratio conjecture in three or more dimensions," Submitted, J. Combinatorial Theory.

[23] Garey, M.R., R.L. Graham and D.S. Johnson, 1977. "The Complexity of Computing Steiner Minimal Trees," *Siam J. Appl. Math 32* (4), 835–859.

[24] Garey, M.R. and D.S. Johnson, 1979. *Computers And Intractability; A Guide To The Theory Of NP-completeness.* (San Francisco:W.H.Freeman and Company.)

[25] Graham, R.L. and F.K. Hwang, 1976, "Remarks on Steiner Minimal Trees." *Bull. Inst. Math. Acad. Sinica 4,* 177–182.

[26] Grünbaum, B., 1967. Convex Polytopes, John Wiley & Sons. Now available from University Microfilms International.

[27] Gilbert, E.N. and H.O. Pollak, 1968, "Steiner Minimal Trees." *Siam J. Appl. Math 16,* 1–29.

[28] Hwang, F. K. and D. Richards, 1992 "Steiner Tree Problems," *Networks* 22, 55-90.

[29] Hwang, F. K. "Steiner Trees on the Chinese checkerboard," manuscript 1992.

[30] Melzak, Z.A., 1961. "On the Problem of Steiner," *Canad. Math Bulletin 4,* 143–148.

[31] Powell, M.J.D., 1964. "An Efficient Method for Finding the Minimum of a Function of Several Variables without Calculating Derivatives." *Computer Journal 7,* 155-162.

[32] Pollard, Harry, and H.G. Diamond. Algebraic Numbers. MAA (Carus Monograph #9) 1975.

[33] Preparata, F. and M.I. Shamos, 1985. *Computational Geometry.* Springer-Verlag.

[34] Press, W.H. et. al., 1986. *Numerical Recipes in Fortran.* Cambridge University Press.

[35] Prim, R.C., 1957. "Shortest Connecting Networks and Some Generalizations." *BSTJ 36* 1389–1401.

[36] Rankin, R.A, 1955. "The Closest Packing of Spherical Caps in N Dimensions," *Proc. Glasgow Math. Assoc. 2,* 145-146.

[37] Rubinstein, J.H., and D.A. Thomas, 1992. Graham's problem for shortest networks for points on a circle, Algorithmica 7 (1992) 193-218.

[38] Smith, J. MacGregor and J.S. Liebman, 1979. "Steiner Trees, Steiner Circuits, and the Interference Problem in Building Design." *Eng Opt 4* (1), 15–36.

[39] Smith, J. MacGregor, Lee, D.T. and J.S. Liebman, 1981. "An O(NlogN) Heuristic for Steiner Minimal Tree Problems on the Euclidean Metric." *Networks 11* (1), 23–39.

[40] Smith, J. MacGregor and P. Winter, 1992. "Computational Geometry and Topological Network Design," pages 287–371 in [18].

[41] Smith, J. MacGregor and R. Weiss, 1992. "An Heuristic for 3-dimensional Steiner Minimal Trees." Manuscript in progress. Will be presented at the Chicago ORSA/TIMS meeting, May 1993.

[42] Smith, Warren D. Studies in Discrete and Computational Geometry, Ph.D. Thesis, Program in Applied and Computational Mathematics, Princeton University, September 1988.

[43] Smith, Warren D., 1992. "How to find Steiner minimal trees in Euclidean d-space," *Algorithmica 7* 137-177.

[44] Vaidya, Pravin M., 1988. "Minimum Spanning Trees in $k-$Dimensional Space" *SIAM J. Comput 17* (3), 572–582.

[45] Winter, P., 1987. "Steiner Problem in Networks: A Survey." *Networks 17*, 129–167.