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The State of Art on the Steiner Ratio Value in R^3

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Abstract Our aim in this work is to make a brief review of the results related to the search of the Infimum and Supremum Values of the Steiner Ratio for point sets in R^3. We show the fundamental achievements which were obtained in a research period of 35 years. We also comment on a recently proposed new upper bound value which is an improvement of Smith and Mac Gregor Smith's bound.

1. Introduction

A Minimal Spanning Tree (MST) is the minimal length network which span a set of points V in a metric space M. If additional points are necessary to get the minimum, the corresponding minimal length tree is the Steiner Minimal Tree (SMT), with these additional points being the Steiner points. There is a set V in the space M such that its MST length (l_{MST}) is the best approximation to the SMT length (l_{SMT}) over all sets in M. This means that there is a number ρ such that $\rho\, l_{MST}$ is the greatest lower bound for $l_{SMT}(V)$.

In this sense, the Steiner Ratio

$$\rho(V) = \inf_{V \in M} \frac{l_{SMT}(V)}{l_{MST}(V)} \tag{1.1}$$

is a measure of the MST length decrease by the introduction of Steiner points.

In the present work, we are interested in the case $M = E^3$, and the corresponding problem is the Euclidean Steiner Problem in $D = 3$ spatial dimensions. The history of this problem is intermingled with that of the Steiner problem for the Euclidean plane, since researchers have used their expertise with the $D = 2$ problem, to solve some cases of the $D = 3$ problem. We include the reference of a very famous paper [9], since it is essential in the understanding of the fundamental characteristics of the Steiner Problem. It has also the tendency of inducing researchers into error. This will be treated in detail in section 2. The third section reports on some tentatives to derive upper and lower bounds for configurations with an infinite number of dimensions. It also gives some inferences from these results for $D = 2$ and $D = 3$.

This has led researchers to think the other way: the possibility of deriving results in dimensions $D \geq 3$ from results already proven in $D = 2$. This was the source of

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wrong results in the literature since some specific properties of the Euclidean plane favour the construction of proofs. These properties are absent in $D = 3$. Section 4 is then the place for deriving a new upper bound of the Euclidean Steiner Ratio in $D = 3$ in a direct modelling approach. In section 5 we introduce some comments and remarks about a conjecture on the existence of a gap between lower and upper bounds for the Steiner Ratio. We also stress the usefulness of the direct approach of section 4 which was inspired by the study of biomacromolecular structure.

2. A Collection of results and the Gilbert-Pollak's paper

The first derived result for a lower bound to the Euclidean Steiner Ratio in any number of spatial dimensions is Moore's [9]. In Figure 1 below, let l_P be the perimeter of the external polygon obtained by the connection of all given points.

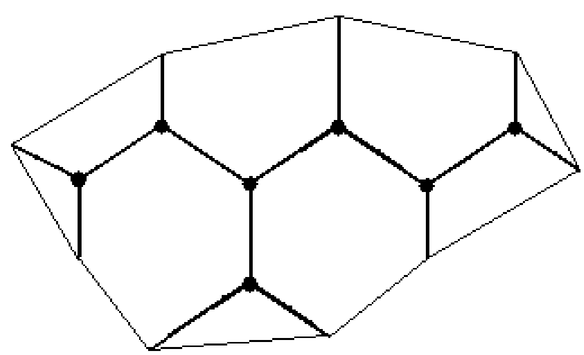

Figure 1: A sketch diagram for deriving the Moore's lower bound.

We can see that $l_{MST} \leq l_P \leq 2l_{SMT}$, which means $\rho \geq 0.5$. Gilbert and Pollak have made two important conjectures. A successful one that the point set $\overline{V}$ in which to realize the infimum defined into (1.1) was given by the vertices of an equilateral triangle with the corresponding value $\rho = \sqrt{3}/2$. This conjecture can be written as $l_{SMT}/l_{MST} \geq \sqrt{3}/2$. The other conjecture is to consider the simplex as the best configuration in which we have to look for an ratio (l_{SMT}/l_{MST}). This second conjecture of Gilbert and Pollak, it was disproved by the work of Smith and Mac Gregor Smith (S - MacG-S) as we show in the fourth section. However, we can consider that this conjecture has motivated 35 years of research work since only recently we have disproved the main conjecture of the work of Smith and MacGregor Smith [11].

Gilbert and Pollak in their breakthrough paper have also made some calculations of upper bounds. In $D = 2$ and $D = 3$ they got $\rho_2 = \sqrt{3}/2 = 0.866026$ and

$\rho_3 = 0.813052$, respectively. For D large, their value was

$$\lim_{D\to\infty} \frac{l_{SMT}}{l_{MST}} \leq \frac{1+\sqrt{3}}{4} = 0.683010\ldots \tag{2.1}$$

The next important results to report came in 1976 [1], [10]. The first work seems to have been done under the direct influence of Gilbert and Pollak simplex conjecture in their search of upper bounds of the Steiner ratio for large D-dimensional configurations. It improves the Gilbert and Pollak's result (2.1) and it is given by

$$\lim_{D\to\infty} \frac{l_{SMT}}{l_{MST}} \leq \frac{\sqrt{3}}{4-\sqrt{2}} = 0.66984\ldots\ . \tag{2.2}$$

The second work derives a lower bound. This was done by an independent geometrical construction which is valid in any number of spatial dimensions. This lower bound can be written as

$$\frac{l_{SMT}}{l_{MST}} \geq \frac{\sqrt{3}}{3} = 0.577\ldots\ . \tag{2.3}$$

This is a valid result in any number D of spatial dimensions. We shall give now the derivation corresponding to the bound above. This is going to be proved for full Steiner Trees with $2n-2 > 4$ vertices (a tree with $n-2$ Steiner points). In terms of the proof to be made, we can also start from a Steiner Tree which is not full, since this can be decomposed into a union of full Steiner Trees and an induction process can be applied.

Let R_{ij} to be the D-dimensional Euclidean distance between points i, j. Let us take the tree to be that represented in Figure 2 below

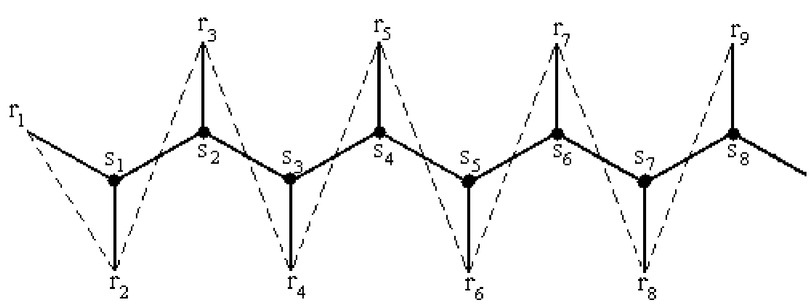

Figure 2: The Steiner Minimal Tree (—-) and the Minimal Spanning Tree (- - -).

The structures corresponding to the minimal spanning tree and Steiner minimal tree are clearly represented in this figure. The external points are given by r_j $(1 \leq j \leq n)$ and Steiner points by s_k $(1 \leq k \leq n-2)$ and we restrict ourselves to full Steiner Trees.

Let us suppose that

$$R_{r_2\,s_1} \geq R_{r_1\,s_1}. \tag{2.4}$$

We shall use the equation

$$(R_{r_1\,s_1} + R_{r_2\,s_1}) \sin\alpha = R_{r_1\,r_2} \cos\beta \tag{2.5}$$

which was obtained from the diagram of Figure 3 below.

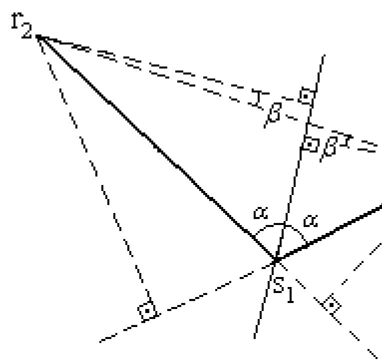

Figure 3: The diagram used in the derivation of equation (2.3).

We consider the angle β to be small and the angle α in the left neighbourhood of $(\pi/3)$ or

$$\beta = \epsilon_1, \qquad \alpha = \frac{\pi}{3} - \epsilon_2, \tag{2.6}$$

where ϵ_1, ϵ_2 are infinitesimal positive numbers.

We have from equation (2.5),

$$(R_{r_1\,s_1} + R_{r_2\,s_1}) \frac{\sqrt{3}}{2} \geq (R_{r_1\,s_1} + R_{r_2\,s_1}) \left(\frac{\sqrt{3}}{2} - \frac{\epsilon_2}{2} \right) \approx R_{r_1\,r_2}. \tag{2.7}$$

By using equation (2.4), we get

$$R_{r_1\,r_2} \leq (R_{r_1\,s_1} + R_{r_2\,s_1}) \frac{\sqrt{3}}{2} \leq R_{r_2\,s_1} \sqrt{3}. \tag{2.8}$$

We now consider the set

$$A_1 = \{r_j\} - \{r_1\}, \quad j = 1, 2, \ldots, n. \tag{2.9}$$

This set corresponds to the tree in Figure 4.

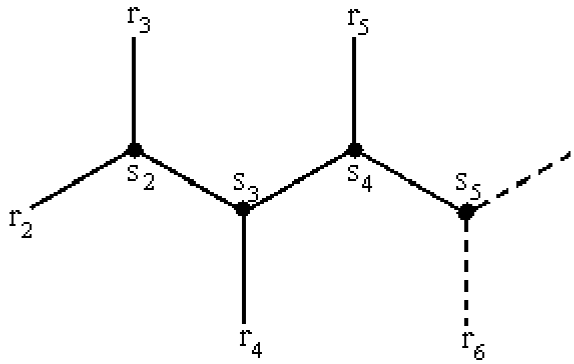

Figure 4: Graphical representation of part of a full Steiner Tree corresponding to set A_1.

We now consider the set $A_2 = A_1 - \{r_2\}$. After an analogous calculation, as was done for set A_1, by using

$$R_{r_2\, r_3} \geq R_{r_3\, s_2}, \tag{2.10}$$

we can have

$$R_{r_2\, r_3} \leq R_{r_3\, s_2}\, \sqrt{3}. \tag{2.11}$$

The induction process is then self-evident and we sum up all the inequalities derived above to obtain

$$R_{r_1\, r_2} + R_{r_2\, r_3} + R_{r_3\, r_4} + \cdots \leq (R_{r_2\, s_1} + R_{r_3\, s_2} + R_{r_4\, s_3} + \cdots)\, \sqrt{3}. \tag{2.12}$$

The left hand side is the length of the minimal spanning tree l_{MST}. The length of the Steiner minimal tree is an upper bound for the right hand side. We can then write,

$$l_{MST} \leq l_{SMT}\, \sqrt{3}. \tag{2.13}$$

This is a proof of the result introduced in equation (2.3).

The same induction process can be used to prove the Moore's bound if we start from the triangle's inequality and equation (2.4),

$$R_{r_1\, r_2} \leq R_{r_1\, s_1} + R_{r_2\, s_1} \leq 2\, R_{r_2\, s_1}. \tag{2.14}$$

We think it is useful to stress that this last proof will depend on the angle α to be in the neighbourhood of $\pi/3$.

D. -Z. Du [4] has improved the lower bound given by equations (2.3), (2.13) to

$$\rho_D = \frac{l_{SMT}}{l_{MST}} \left(V \subset E^D\right) \geq 0.615 \ldots\ . \tag{2.15}$$

The present work is not the right place of deriving this lower bound. We shall do it elsewhere. The improvement of this bound in a generic number of spatial dimensions is still an open problem [7].

3. The History of the $D = 2$ Lower Bound

The two last results of Section 2 could be also written as

$$\rho_2 > \rho_3 > \cdots > \lim_{D\to\infty} \rho_D \geq 0.577\ldots\ , \tag{3.1}$$

$$\rho_2 > \rho_3 > \cdots > \lim_{D\to\infty} \rho_D \geq 0.615\ldots\ , \tag{3.2}$$

since it seems to be a commonly observed effect the reduction of the Euclidean Steiner ratio when the number of spatial dimensions increases.

The works of the references [4] and [10] got the influence of Gilbert and Pollak's paper on its polemical part: the validity of the D-dimensional simplex configuration as the best set point candidate for an infimum of the Steiner Ratio. However, the research towards the greatest lower bound in $D = 2$ has produced some very good pieces of work. They can be summarized by the table below

Authors	**year**	**Value of D=2 lower bound** $\boldsymbol{\rho_2 = l_{SMT}/l_{MST}}$
Chung and Hwang	1978	$\rho_2 \geq 1/3\left(2\sqrt{3}+2-\sqrt{7+2\sqrt{3}}\right) = 0.743\ldots$
Du and Hwang	1983	$\rho_2 \geq 0.8$
Chung and Graham	1983	$\rho_2 \geq 0.8241\ldots$
Du and Hwang	1990	$\rho_2 \geq \sqrt{3}/2 = 0.866\ldots$
Du and Hwang	1992	$\rho_2 \geq \sqrt{3}/2 = 0.866\ldots$

Table 1: Lower bounds for $D = 2$.

The last line on Table 1, corresponds to the value obtained in a full proof of the Gilbert-Pollak's conjecture. It took 22 years of research work to achieve this lower bound. We are now convinced that there is no gap between the lower and an upper bounds for the Euclidean Steiner Ratio in $D = 2$ dimensions. All the authors of the bounds quoted above and published before the work of Du and Hwang knew about the existence of the value $\sqrt{3}/2$ corresponding to the Steiner Ratio for the equilateral triangle. Du and Hwang have derived a new bound, $\rho_2^{(n)} \geq \sqrt{3}/2$ which is valid for an arbitrary n-point configuration. The value of the new bound is exactly the value of the equilateral triangle configuration. The result $\rho_2^{(n)} = \sqrt{3}/2$ then follows from the fact that we also have

$$\mathrm{inf}_{V\in\mathbb{R}^2} \frac{l_{SMT}(V)}{l_{MST}(V)} = \rho(V) \leq \rho_2^{(3)} = \frac{\sqrt{3}}{2}.$$

The value of the Steiner Ratio for a n-point configuration is then given effectively by $\rho_2^{(n)} = \sqrt{3}/2$.

4. The D-Sausage configuration of Smith and Mac Gregor Smith. The improvement of the upper bound for $D = 3$.

The works of Smith and Mac Gregor Smith [15, 16], as well as Du and Smith [8], have disproved the Simplex Gilbert-Pollak conjecture in dimensions $3 \leq D \leq 9$. A D-dimensional point set structure was introduced, the D-sausage. In $D = 3$, it is achieved by the vertices of regular tetrahedra bounded together at common faces in an infinite structure. The D-sausage Steiner Minimal Tree has a topology like that of Figure 2 which the authors have called the "path-topology". The best upper bound value to the Euclidean Steiner Ratio was found to be

$$\rho_3 \leq \frac{1}{10}\left(3\sqrt{3} + \sqrt{7}\right) = 0.784190\ldots \ . \tag{4.1}$$

This should be compared to the reported value of $\rho_3 \leq 0.813052$ by Gilbert and Pollak. In $D = 2$, the 2-sausage structure which is realized by abutting equilateral triangles has also confirmed the successful $D = 2$ Gilbert and Pollak's conjecture.

In some recent works [11, 12, 13, 14], which have been inspired by the observation of biomacromolecular structure, we have adopted the topology of Figure 2 to derive a direct approach to the Steiner Ratio in $D = 3$. All the vertices of the 3-sausage belong to a right circular helix. We can take it with unit radius and write for the position vectors of the vertices,

$$\vec{r}_j = (\cos j\omega, \sin j\omega, \alpha j\omega)\,, \qquad 1 \leq j \leq n, \tag{4.2}$$

where ω is the polar angle, $0 \leq \omega \leq 2\pi$, and $2\pi\alpha$ is the helix pitch.

The Steiner tree point distribution is also along an helix [12] of radius $r\,(\omega, \alpha)$.

$$\vec{s}_k = (r\,(\omega,\alpha)\cos k\omega, r\,(\omega,\alpha)\sin k\omega, \alpha k\omega)\,, \qquad 1 \leq k \leq n-2. \tag{4.3}$$

A tedious but straightforward derivation leads to the expressions for the radius $r\,(\omega, \alpha)$ and the Steiner Ratio for a 3-dimensional infinite set of points ($n \to \infty$)

$$r\,(\omega,\alpha) = \frac{\alpha\omega}{\sqrt{2(1-\cos\omega)(1-2\cos\omega)}}, \tag{4.4}$$

$$\rho\,(\omega,\alpha) = \frac{1 + \alpha\omega\sqrt{\frac{1-2\cos\omega}{2(1-\cos\omega)}}}{\sqrt{\alpha^2\omega^2 + 2(1-\cos\omega)}}, \tag{4.5}$$

where $(\omega,\alpha) \in V,\ V = \{(\omega,\alpha)|(\omega,\alpha) \in R_{++}, \arccos\frac{1}{3} < \omega < 2\pi - \arccos\frac{1}{3}, \alpha \geq 0\}$.

For (ω, α) values taken from the helix whose vertices belong to regular tetrahedra ($\omega = 2.300523\ldots, \alpha = 0.264540\ldots$), we get a coincidence of the values from equation (4.1) and (4.5) up to the 38th decimal place [11, 13]. By cutting the surface $\rho(\omega, \alpha)$ with a plane $\alpha = 0.264540\ldots$, we obtain an example of a new upper bound in a structure formed from irregular chiral tetrahedra [14].

$$\rho_3 \leq 0.776001\ldots \ . \tag{4.6}$$

This value for the new upper bound was proposed as a possible disproof of the conjecture of ref. [16].

However, the lower bound as obtained from equation (4.5) is the trivial Moore's bound $\rho_3 \geq 0.5$. We think that this is due to the poorness of our modelling in spite of its success at reproducing value (4.1). Nevertheless, we should observe that there is some hidden assumption of regularity in the literature related to the D-sausage. Some bias can be also observed towards to favour a modelling which does not violate a Copernican axiom of geometric perfection. From the observation of helical patterns of input points in $D = 3$ as taken from protein databases, we were able to improve the upper bound given into equation (4.1). This was done by keeping the 3-sausage topology but deforming the configuration until a new rigid structure is found.

5. Concluding Remarks

There are two lines of research work which seem to be worthwhile to follow in forthcoming contributions. The first is the search for lower bounds according the development of section 2. The second is to look for the improvement of upper bounds by the direct approach of section 4. The last one depends strongly on modelling and should be based on a deep understanding of biomacromolecular structure.

We believe that the existence of a gap between lower and upper bound values in $D = 3$ is mandatory. It should correspond to the specification of a region which nature has elected for biomacromolecular organization and life emergence. In this sense, the $D = 3$ euclidean problem is essentially different from the 2-dimensional problem in which researchers have obtained the excellency of their works. We stress this point because we think that the Steiner Problem has a fundamental importance for the understanding of biomacromolecular structure. This Was shown in refs. [11, 12, 13, 14, 16] and we have been a engaged in this research program.

Resumo O objetivo do presente trabalho é fazer um breve sumário dos resultados relacionados à pesquisa dos valores Ínfimo e Supremo da Razão de Steiner para conjuntos de pontos em R^3. São mostradas as realizações fundamentais conseguidas em um período de pesquisa de 35 anos. É também comentado um novo valor do limite superior proposto recentemente, que aperfeiçoa o limite superior de Smith e Mac Gregor Smith.

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