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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. A very famous paper has to be quoted, since it has the characteristics of promoting research as well as to induce researchers into error [9]. 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

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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 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. Section 5 closes the paper with comments and remarks to be remembered as useful ones in the improvement of the modelling adopted here.

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 fig. 1 below, let l_P be the perimeter of the external polygon obtained by the connection of all given points.

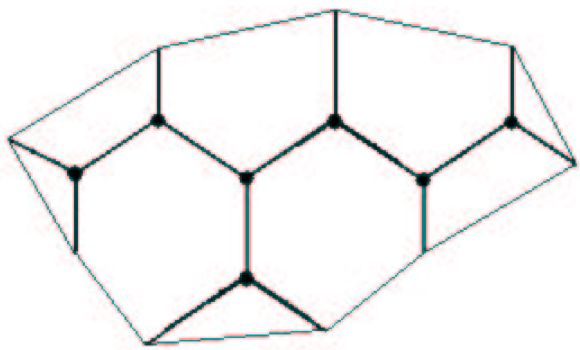

Figure 1: A sketch diagram for deriving the Moore's lower bound.

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}). It was disproved by the work of Smith and Mac Gregor Smith (S - MacG-S) as we show in the fourth section. However, this conjecture has motivated 35 years of research work since only recently we have disproved the main conjecture of (S - MacG-S) [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 fig. 2 below

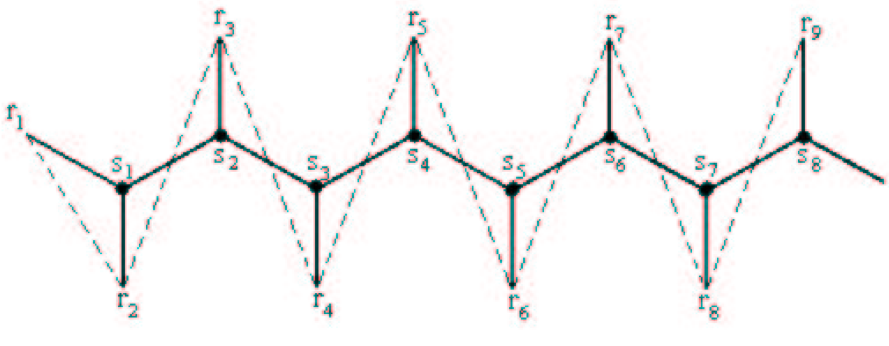

Figure 2: The Steiner Minimal Tree (—-) and the Minimal Spanning Tree (- - -).

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 below

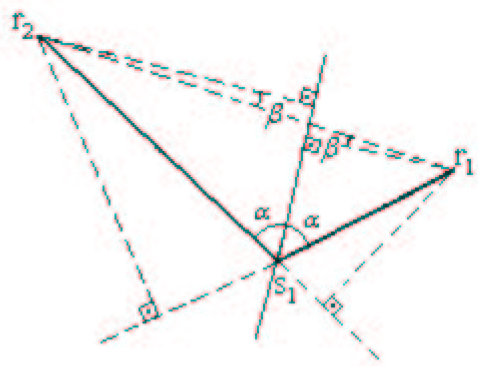

Figure 3: The diagram used in the derivation of eq. (2.3).

We consider the angle β to be small and 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 eq. (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 eq. (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

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

This set corresponds to the tree in fig. 4.

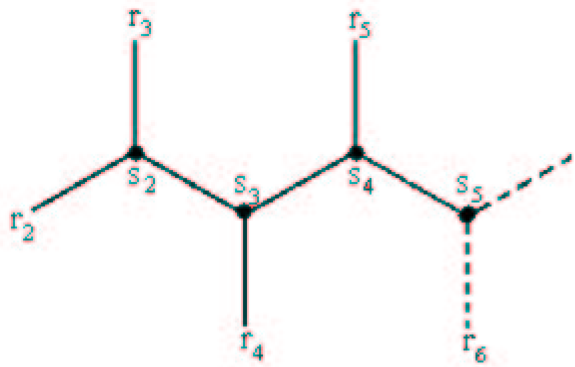

Figure 4: Graphical representation of part of a full Steiner Tree corresponding to set A_1.

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 eq. (2.3).

The same induction process can be used to prove the Moore's bound if we start from the triangle's inequality and eq. (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 note that this last proof will not depend on the angle α as it was already evident from fig. 1.

D. -Z. Du [4] has improved the lower bound given by eqs. (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.

These works 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 $\rho_2 = l_{SMT}/l_{MST}$**
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. The value of this ratio is given effectively by $\rho_2 = \sqrt{3}/2$.

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 fig. 2 which the authors have called the "path-topology". The best upper bound value to the Euclidean Steiner Ratio was found to be

$$\rho_3 \leq \frac{1}{10}\sqrt{34+6\sqrt{21}} = 0.784190\ldots \tag{4.1}$$

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, which have been inspired by the observation of biomacromolecular structure, we have adopted the topology of fig. 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 eq. (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].

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

However, the lower bound as obtained from eq. (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 eq. (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 the gap between lower and upper bounds in $D = 3$ is mandatory. It should correspond to the specification of a region which Nature has elected for biomacromolecular organization and life emergence. It seems that there are two good lessons to be learned here. One about Mathematics and another one about mathematicians: Mathematical truth reflects Nature's laws and there is no truth outside of the reality of natural phenomena. These are then a good source of inspiration for understanding new mathematical structures unveiled from Nature. Moreover, the molecules from which a mathematician is made do not allow him to get a proof of closure of the gap between lower and upper bound values of the Steiner Ratio in $D = 3$ spatial dimensions. It is like a kind of anthropic argument. There is not a solution to this problem because there would be not a living mathematician to ask how it can be solved.

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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