The Study of Steiner Points Associated with the Vertices of Regular Tetrahedra Joined Together at Common Faces

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Abstract
The aim of this contribution is to help the improvement of the knowledge about the Steiner ratio function by showing some recent results related to the uniqueness of a point distribution which have been obtained about this problem. The exposition is almost pedagogical and the choice of a right circular helix input pattern is motivated by its usefulness for working with the geometrical modelling as an approach to the problem of protein folding.

Resumo
O objetivo desta contribuição é melhorar o conhecimento sobre a função razão de Steiner, mostrando alguns resultados recentes relacionados à unicidade de uma distribuição de pontos que foram obtidos estudando o problema. A exposição é quase pedagógica e a escolha de pontos dados como pertencentes a uma hélice construída sobre um cilindro circular é motivada pela utilidade no trabalho de modelagem geométrica como um enfoque do problema de estrutura das moléculas de proteína.

Keywords: Combinatorial Optimization; Applications to Natural Sciences; Protein Folding.

1 Introduction

It is now becoming usual to study the structure of organic molecules with simple methods of elementary differential geometry [1]. As elementary methods are concerned, it is enough to realize that a sequence of regular tetrahedra joined together at common faces forming a necklace are a pattern for input points necessary to model, say, an α helix-structure [2, 3].

The same can be done related to a sequence of regular octahedra and we easily see that their square equators are a good candidate for modelling a β-sheet structure [2, 3]. We plan to give here a summary of our work with the helix pattern and we start from the preliminaries. Working on this approach, we try to motivate our reader to join in this scientific adventure which has very nice promises of putting together the methods of topology and differential geometry for understanding macromolecular structure. In the next section we study the possibility of regular polygons to be inscribed in a helix. In section 3 we presented a numerical approach for the geometrical position of Steiner points associated with a special helix point configuration. A geometrical model to study protein folding is discussed in section 4.

2 Special Helix Point Configuration

Our starting point is to consider the input points as given on a right circular helix of unit radius whose cartesian coordinates are given by

$$x^{(1)} = \cos\omega \;\;;\quad x^{(2)} = \sin\omega \;\;;\quad x^{(3)} = \alpha\omega \;\;;\quad 0 \leq \omega \leq 2\pi \tag{1}$$

where ω is the angular parameter of evenly input points along the helix and α is the pitch of it (actually, the pitch is usually denoted by $2\pi\alpha$).

The coordinates of the j-th input points can then be written

$$x_j^{(1)} = \cos j\omega \;\;;\quad x_j^{(2)} = \sin j\omega \;\;;\quad x_j^{(3)} = \alpha j\omega \;\;;\quad 0 \leq j \leq p-1 \tag{2}$$

for p input points.

We turn now to the enunciation of our problem:

By following the helix pattern, eq. (1), we would like to pile up regular polyhedra such that all of their vertices are points of the helix like that given by eq. (2). The solution will depend on the possibility of inscribing regular polygons in the helix. Let a be the side length of the polygons, p their side number, we shall have for the equations which describe that possibility, see [6],

$$\alpha^2\omega^2 = 2F_p(\omega) \tag{3}$$

$$a^2 = 2\left(1 - \cos\frac{2\pi}{p}\right)^{-1}(1-\cos\omega)^2 \tag{4}$$

$$\cos(p-1)\omega = p(p-2)F_p(\omega) + \cos\omega \tag{5}$$

$$\cos(p-2)\omega \;=\; p(p-4)F_p(\omega) + \cos 2\omega \tag{6}$$

where

$$F_p(\omega) = \left(1 - \cos\frac{2\pi}{p}\right)^{-1} (1-\cos\omega)^2 \left(\cos\frac{2\pi}{p} - \cos\omega\right) \quad ; \quad p \neq 1 \tag{7}$$

The non-trivial solutions ($\alpha \neq 0$) should be bound by

$$\frac{2(p-1)\pi}{p} > \omega > \frac{2\pi}{p} \tag{8}$$

Equations (5) and (6) give some additional information in the sense that they help to understand the solutions in a systematic way. It should be observed that the values $\omega = 2\pi/p$ and $\omega = 2(p-1)\pi/p$ are solutions for every $p \geq 2$. They correspond to inscribe the polygons of $p \geq 2$ sides in a circle according to (3), or $\alpha = 0$. It should also be noted that the value $p = 2$ is a triviality, since it leads to $\alpha = 0$, and $\omega = \pi$, $a = 2$ from (3) and (4) and we have two points separated by a diameter of circle of unit radius. For ω-values which satisfy (8) and $p = 3$, all equations (3)-(6) above become identities and we get the unique solution that only equilateral triangles can be inscribed in a helix defined by (1). The angular coordinates of the second vertex these triangles are in the region

$$\frac{4\pi}{3} > \omega > \frac{2\pi}{3} \tag{9}$$

and we go back to eqs. (3), (4) to determine the pitch of the helix and the side lengths of these triangles.

To construct a tetrahedron, we consider a fourth point

$$x_3^{(1)} = \cos 3\omega \quad ; \quad x_3^{(2)} = \sin 3\omega \quad ; \quad x_3^{(3)} = 3\alpha\omega \quad , \tag{10}$$

by connecting it to the point $(1, 0, 0)$.

After using eqs. (3) - (6), we get:

$$(1-\cos\omega)^2(2+3\cos\omega) = 0 \tag{11}$$

The non trivial roots ($1 - \cos\omega \neq 0$) are given by $\omega = \pi \pm \arccos(2/3)$. We can then consider the uniqueness of the solution found since the two resulting tetrahedra will be mirror images. We have for the solution

$$\omega = 2.30052398302\,, \quad \alpha = 0.26454000216\,, \quad a = 1.92450089730 \tag{12}$$

The coordinates of the other points of the structure are shown to be given by the relation, see [1],

$$x_n^{(s)} = \frac{2}{3}\left(x_{n-1}^{(s)} + x_{n-2}^{(s)} + x_{n-3}^{(s)}\right) - x_{n-4}^{(s)} \quad ; \quad s = 1, 2, 3 \tag{13}$$

3 The Euclidean Steiner Problem in 3-Dimensions

In [4] the Euclidean Steiner problem in 3-dimensions is well defined and a conjecture for the Steiner ratio in 3-dimensions is proposed. Given n points in R^d, let $l(MST)$ be the length of the minimal spanning tree connecting this n points in a complete graph K_n in which each edge is associated with the Euclidean distance between its terminal nodes. Let $l(SMT)$ be the length of the Steiner minimal tree connecting this same n points, we know that $l(MST) \geq l(SMT)$ and the ratio we will be consider is $\rho = \frac{l(SMT)}{l(MST)}$.

Suppose that $X \subset R^d$ is a set of an enumerated number of points, $MST(X)$ and $SMT(X)$ the minimal spanning tree length and Steiner minimal tree length to connect the points of X.

The Steiner ratio can be defined as follows:

$\rho_d = \text{infimum}_X \{\frac{SMT(X)}{MST(X)}\}$, where X was defined above.

Just for $d = 2$ we have the value of $\rho_d = \rho_2 = \frac{\sqrt{3}}{2}$, when the points of X are the vertices of an equilateral triangle, see [7]. We define by $X_n = \{x_1, x_2, ..., x_n\}$ the set of the first n points generated by (13) for which x_1, x_2, x_3, x_4 are the vertices of a tetrahedron as showed before. In [4] it is conjectured that

$$\rho_3 = \lim_{n\to\infty} \frac{SMT(X_n)}{MST(X_n)} = 0.78419037337... \tag{14}$$

The Steiner minimum tree for X_n has $2n-2$ nodes (n associated with the given points and $n-2$ with the Steiner points) and it is conjectured also in [4] that this tree have a special configuration called in [5] a "fishbone" configuration. We would like to know about the geometrical position of these Steiner points.

In order to proceed with our modelling scheme, we have tried to fit the Steiner points, using classical softwares, in a generic 2-dimensional conoid surface which is described in parametric form by

$$x^{(1)} = r\cos\omega \ ; \quad x^{(2)} = r\sin\omega \ ; \quad x^{(3)} = z(\omega) \tag{15}$$

where r, ω are the radial and angular coordinates respectively. The results are shown in Figure 1.

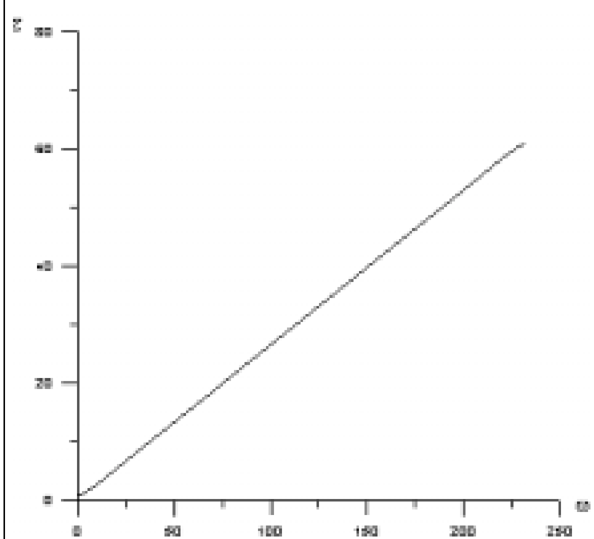

Fig. 1

We have a polynomial ω-dependence for the function $z(\omega)$. By working with $p = 102$ input points, this polynomial is given by

$$\begin{aligned} z(\omega) \;\; = \;\; & -3.87432 \times 10^{-18}\,\omega^9 + 4.05095 \times 10^{-15}\,\omega^8 - 1.78493 \times 10^{-12}\,\omega^7 \\ & +4.30955 \times 10^{-10}\,\omega^6 - 6.20721 \times 10^{-8}\,\omega^5 + 5.44106 \times 10^{-6}\,\omega^4 \\ & -0.000283663\,\omega^3 + 0.00819696\,\omega^2 + 0.15176\,\omega + 0.508884 \end{aligned} \tag{16}$$

The smallness of the coefficients above with the exception of those which correspond to the linear approximation has motivated to obtain the fit with a straight line. In Figure 2 we have shown this best fitted straight line as well as the straight line obtained by getting rid of some points of lower and higher z-values of coordinates.

These results show that there is a strong tendency for the Steiner points to belong to a helicoidal surface. Actually, Figure 2b points to the conclusion that the best fit can be considered to be a helix. We have worked with $p = 102$ input points. The straight lines of Figures 2a, 2b, are given by

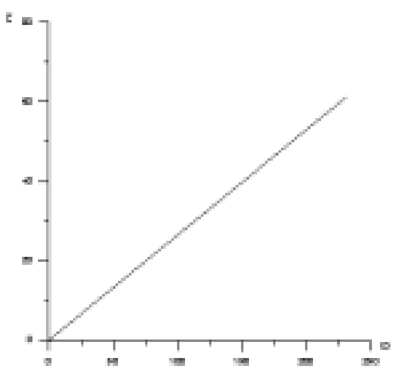

Fig. 2a

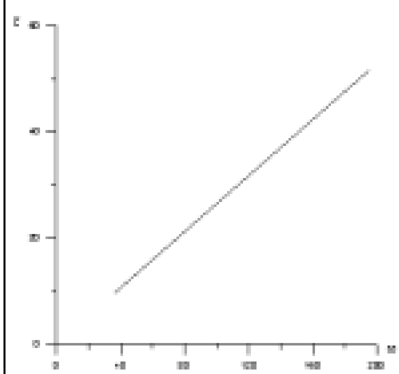

Fig. 2b

$$z(\omega) = 0.264343\,\omega + 0.0229275 \tag{17}$$

$$z(\omega) = 0.26454\,\omega + 5.8647 \times 10^{-6} \tag{18}$$

As a confirmation of the conclusions written above of this elementary example of Steiner point modelling we have also done the work of fitting the Steiner point distribution on a surface of revolution, or

$$x^{(1)} = r(z)\cos\omega \;\; ; \quad x^{(2)} = r(z)\sin\omega \;\; ; \quad x^{(3)} = z \tag{19}$$

In Figure 3 we show our best fit associated to $p = 102$ input points.

It is to be observed the existence of a helix structure for the calculated distribution of Steiner points. The average radius of this distribution is found to be $r_{av} = 0.217217424$ for an input point configuration on a helix of unit radius. Further work with greater number of input points, after getting rid of the almost constant number of lower and higher z-values points will reinforce this conclusion.

4 Characterization of Protein Structure

It was observed in [9] that the backbone structures of most proteins are Euclidean Steiner minimal trees. The backbone or network structure of a protein is a linked together sequence of rigid peptide groups. Examining the structure of two proteins, Actin and Fibroin, illustrated in [9], we think to model their backbone structure, it is enough to consider some linked $2n-2$ points as a "fishbone" tree with n points on a right circular helix of radius c and the other $n-2$ points on another right circular helix of radius $r_{av}c$ as proposed in [1].

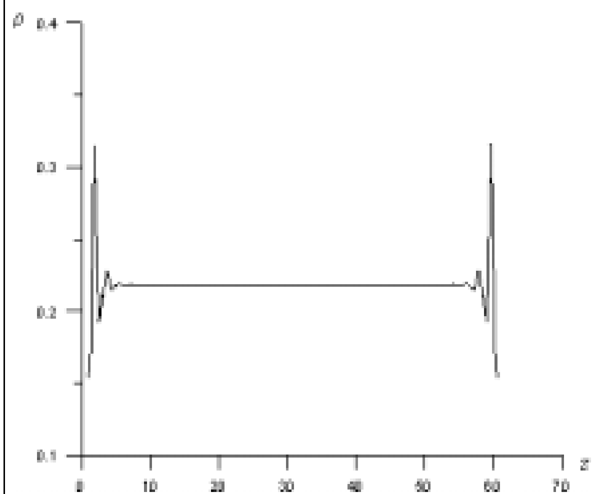

Fig. 3

5 Conclusion

Using the results presented in [6], we have summarized the possibility of inscribing regular polygons in the helix: only regular tetrahedra can be inscribed in a helix. A chain of tetrahedra illustrated in [4] was constructed by another technique. The Steiner points for tetrahedron chain vertices have a very strong tendency to belong to another helix of smaller radius.

Acknowledgment

We feel indebted to F. Montenegro for some useful suggestions. This work has been supported by PRONEX-MCT and CNPq.

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