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An analytical method for derivation of the Steiner Ratio of 3D euclidean Steiner trees

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Abstract We stress the convenience of some analytical methods which have been introduced recently [Mondaini, R. P.: In: Nonconvex Optimization and its Applications series, pp. 373–390. Kluwer Acad. (2003); Mondaini, R. P.: In: BIOMAT 2005, International Symposium on Mathematical and Computational Biology, pp. 327–342. World Scientific Co Ltd (2006)] for calculating the Steiner Ratio of finite sets of points in $\mathbb{R}^3$. These methods are good enough at reproducing the results obtained by reduction of the search space of numerical algorithms and can be easily extended to any number of dimensions.

Keywords Steiner ratio · Analytical method · Euclidean Steiner trees

1 Introduction

The scientific literature of mathematical modelling of macromolecular structure as well as the biochemical and biological literature is full of helical models, helicoidal strips, helices and other similar graphical representations in the textbooks [1]. Even the literature of Discrete Mathematics contains assumptions of helical conformation of point sets as the basis for the introduction of still unproved conjectures. If the search for Steiner minimal trees corresponds to the search for minimal energy configurations of those structures, we can start to doubt of the faithfulness of these representations. We can imagine that they are unnecessary since any family of smooth and continuously differentiable curves will play the same role in a modelling process. It now follow a summary of the present contribution: in Sect. 2, we introduce the treatment of evenly spaced points in 3D Euclidean Space. We also make a digression about sets of points which are simultaneously even spaced along continuous and differentiable curves. We think that it would be worthwhile to use these observations in the construction of successful models and we hope to contribute with useful information as a valid track in the

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search of the uniqueness of helical representations of biomolecular structures. The third section is aimed to develop the systematic description of spanning and Steiner trees. This section also emphasizes that the arbitrary character of an intrinsic function of the modelling could be taken as a new variable in a new two-dimensional problem of unconstrained optimization. Section 4 contains the extension of this analytical treatment to a new form of associating subsequences of evenly spaced points. These structures are analogous to protein structures of α-helices and β-sheets connected by coils. We stress that in spite of the fact that all the subsequences have been taken with the same connection topology, their free association can create all the different structures with different connection topologies and the method introduced is general enough. In Sect. 5, we use the Nelder–Mead search method to look for the global minimum of the objective Steiner Ratio function introduced in Sect. 4. The robustness and generality of the techniques used here can be verified by the coincidence of numerical values with that obtained by working with this search method. We close the paper with some comments on the generality of the present formulation, its extension to higher number of dimensions and the application to the modelling of molecular chirality.

2 Sequences of evenly spaced points along a smooth and continuously differentiable curve

Let $\vec{r} = (x(\lambda), y(\lambda), z(\lambda))$ to be a 3D curve parameterized by λ. The position vector of a point on this curve will be given by $\vec{r}_j = (x_j(\lambda), y_j(\lambda), z_j(\lambda)) = (x(\lambda_j), y(\lambda_j), z(\lambda_j))$. The arc length between points of position vectors $\vec{r}_{j+k}$ and $\vec{r}_j$ is

$$s_{j+k} - s_j = \int_{\lambda_j}^{\lambda_{j+k}} \sqrt{x'^2 + y'^2 + z'^2}\, \mathrm{d}\lambda, \tag{1}$$

where $(') = d/d\lambda$.

If the points are evenly spaced along the curve, we have,

$$s_{j+k} - s_j = k(s_{j+1} - s_j). \tag{2}$$

The parameter value can always be taken as evenly spaced, or

$$\lambda_{j+k} - \lambda_j = k(\lambda_{j+1} - \lambda_j). \tag{3}$$

The solution of these difference equation can be written as

$$s_j = jS, \tag{4}$$

$$\lambda_j = j\Lambda, \tag{5}$$

where S and Λ are new parameters.

From Eq. 1, we can see that the family of curves which satisfy Eq. 2 is given by

$$x'^2 + y'^2 + z'^2 = a^2, \tag{6}$$

where a is a constant.

Two elementary solutions of Eq. 6 are a straight line and a right circular helix

$$\vec{r} = \left(k_1 z, \sqrt{a^2 - 1 - k_1^2}\, z, z\right), \tag{7}$$

$$\vec{r} = \left(\sqrt{a^2 - \alpha^2}\cos(z/\alpha), \sqrt{a^2 - \alpha^2}\sin(z/\alpha), z\right), \tag{8}$$

with z as a parameter and $2\pi\alpha$ the pitch of the helix.

If we choose the parameter as z satisfying a difference equation like (1) or (2), we can write for the z-coordinate of the jth point

$$z_j = jZ, \tag{9}$$

and Z is a new parameter.

The corresponding position vectors of Eqs. 7, 8 will satisfy the relations

$$\vec{r}_{j+k} - \vec{r}_j = k(\vec{r}_{j+1} - \vec{r}_j), \tag{10}$$

$$\left\|\vec{r}_{j+2} - \vec{r}_{j+1}\right\| = \left\|\vec{r}_{j+1} - \vec{r}_j\right\|, \tag{11}$$

where $\|\cdot\|$ stands for the Euclidean norm.

A fortiori, the vectors of Eq.10 will satisfy also Eq. 11.

From Eqs. 8, 9 and 11 we can see that consecutive evenly spaced points along a right circular helix are also consecutive evenly spaced in $\mathbb{R}^3$. This is an expected property of the right circular helix. However, this property is not necessary in the search of the minimum length of a Steiner tree as will be shown in the next section. We can use then, instead a right circular helix, any smooth and continuously differentiable curve, but the essential step of the modelling is the consideration of evenly spaced points and not a particular curve to pass by all of them.

The position vectors of the points in the curve are

$$\vec{r}_j = \left(\sqrt{x_j^2 + y_j^2}\cos\left(\arctan\frac{y_j}{x_j}\right), \sqrt{x_j^2 + y_j^2}\sin\left(\arctan\frac{y_j}{x_j}\right), jZ\right). \tag{12}$$

The conditions to be satisfied for evenly spaced points in $\mathbb{R}^3$ are:

$$x_j^2 + y_j^2 = r^2(\varphi), \quad \forall j, \tag{13}$$

$$\arctan\frac{y_j}{x_j} = \varphi_j = j\phi, \tag{14}$$

where we have taken another parameter $\lambda = \phi$ to describe the curve. This parameter satisfy Eqs. 3 and 14 with ϕ a new parameter.

We then write the position vectors for n consecutive points on the curve and evenly spaced in $\mathbb{R}^3$:

$$\vec{r}_j(\phi) = \left(r(\phi)\cos(j\phi), r(\phi)\sin(j\phi), jZ(\phi)\right), \quad 0 \le j \le n-1. \tag{15}$$

Analogously, the position vectors of the $(n-2)$ consecutive Steiner points along their curve and also evenly spaced in $\mathbb{R}^3$ should be written as

$$\vec{r}_{S_k}(\phi) = \left(r_S(\phi)\cos(k\phi), r_S(\phi)\sin(k\phi), kZ_S(\phi)\right), \quad 1 \le k \le n-2. \tag{16}$$

3 The organization of Steiner trees

We choose a fishbone or path-topology [2] for the Steiner tree. The point $\vec{r}_{S_1}$ is connected to the points $\vec{r}_0$ and $\vec{r}_1$; the point $\vec{r}_{S_{n-1}}$ is connected to $\vec{r}_{n-2}$ and $\vec{r}_{n-1}$. The points $\vec{r}_{S_k}$ are connected consecutively as well as the intermediate couples of points $\vec{r}_j, \vec{r}_{S_k}$ such that $j = k$.

From the coordinates of the fixed and Steiner points given by Eqs. 15 and 16, we can calculate the consequences of the requirement of edges meeting at Steiner points with angles of $(2\pi/3)$. This will lead to

$$Z_S(\phi) = Z(\phi), \tag{17}$$

$$Z_S^2(\phi) = r_S^2(\phi) A_1 (A_1 + 1), \tag{18}$$

where

$$A_1 = 1 - 2\,\cos(\phi) \tag{19}$$

and

$$\frac{r_S(\phi)}{r(\phi)} = \frac{F(\phi)}{\sqrt{A_1(A_1+1)}}, \tag{20}$$

$$F(\phi) = \frac{Z(\phi)}{r(\phi)}. \tag{21}$$

If only full Steiner trees with $(n-2)$ points are to be considered, there is an additional requirement to be imposed on the spanning trees: the smallest angle θ_1 between consecutive edges of a spanning tree whose vertices have position vectors $\vec{r}_j$ should be lesser than $2\pi/3$. This requirement can be expressed by:

$$-\frac{1}{2} < \cos\theta_1 = -1 + \frac{(A_1+1)^2}{2(F^2 + A_1 + 1)}. \tag{22}$$

Equation 22 can be also written as

$$\cos\theta_1 = \max\left(-\frac{1}{2},\ -1 + \frac{(A_1+1)^2}{2(F^2 + A_1 + 1)}\right). \tag{23}$$

This kind of modelling is dependent of the function $F(\phi)$. If $F(\phi) = \alpha\phi$, the curves given by Eqs. 15 and 16 are right circular helices and $2\pi\alpha$ is their pitch.

The representation of the position vectors of the fixed and Steiner points can be generalized to represent surfaces. We now have, instead Eqs. 15, 16

$$\vec{r}_j(\phi, Z) = (r(\phi, Z)\cos(j\phi), r(\phi, Z)\sin(j\phi), jZ), \quad 0 \le j \le n-1, \tag{24}$$

$$\vec{r}_{S_k}(\phi, Z) = (r_S(\phi, Z)\cos(k\phi), r_S(\phi, Z)\sin(k\phi), kZ_S), \quad 1 \le k \le n-2. \tag{25}$$

The organization of the full Steiner tree is the same as described above, but we now have instead Eqs. 17, 18

$$Z_S = Z, \tag{26}$$

$$Z_S^2 = r_S^2 A_1(A_1 + 1) \tag{27}$$

and $r_S(\phi, z)$ is a surface given by

$$\frac{r_S(\phi, Z)}{r(\phi, Z)} = \frac{F(\phi, Z)}{\sqrt{A_1(A_1+1)}}, \tag{28}$$

where

$$F(\phi, Z) = \frac{Z}{r(\phi, Z)}. \tag{29}$$

This modelling is independent of the functional form of $F(\phi, Z)$.

A candidate for a spanning tree will be formed by connecting all the points with position vectors given by Eq. 24. Its Euclidean length is

$$l_{S_{P_1}} = r(\phi, F)(n-1)\sqrt{F^2 + A_1 + 1}. \tag{30}$$

A fishbone topology as described above is adopted for writing the Euclidean length of the candidate for a Steiner tree. We have after using Eqs. 26, 27,

$$l_{S_{T_1}} = r(\phi, F)\left[n - 2 + ((n-3)A_1 - 1)\frac{F}{\sqrt{A_1(A_1+1)}} + 2\sqrt{1 + (A_1 - 1)\frac{F}{\sqrt{A_1(A_1+1)}} + (A_1^2 + A_1 + 1)\frac{F^2}{A_1(A_1+1)}}\right]. \tag{31}$$

We now define $l_1 = l_{S_{P_1}}/r(\phi, F)$ and $L_1 = l_{S_{T_1}}/r(\phi, F)$. We have for a large set of points, $n \gg 1$,

$$l_1 = n\sqrt{F^2 + A_1 + 1}, \tag{32}$$

$$L_1 = n\left(1 + F\sqrt{\frac{A_1}{A_1+1}}\right). \tag{33}$$

There is a problem with formulae (30), (31) or (32), (33). These formulae do not contain all the length values of a minimal spanning tree or Steiner minimal tree for $0 \le \phi \le \pi$. We have to improve the present method by taking into consideration other possibilities of writing formulae for the spanning and Steiner trees. This will be done by generalizing the sequences of points from those given by Eqs. 24, 25. As a shortcoming of the present formulation as well as a motivation to improve it, we announce that the ratios $l_{S_{T_1}}/l_{S_{P_1}}$ and l_1/L_1 do not correspond to a Steiner Ratio Function. These ratios are the convex envelope functions of the corresponding Steiner Ratio functions. This will be shown explicitly in the next section for $n \gg 1$.

4 Generic sequences of points and Steiner ratio function

In this section we will introduce sequences of evenly spaced but non-consecutive points [3] which can be formed from the sequences given by Eqs. 24 and 25. These subsequences can be written as

$$(P_j)_{m,\, l_{P\max}} : \vec{r}_j, \vec{r}_{j+m}, \vec{r}_{j+2m}, \ldots, \vec{r}_{j+l_P m}, \ldots, \vec{r}_{j+l_{P\max} m}, \quad 0 \le j \le m-1, \tag{34}$$

$$(S_k)_{m,\, l_{S\max}} : \vec{S}_k, \vec{S}_{k+m}, \vec{S}_{k+2m}, \ldots, \vec{S}_{k+l_P m}, \ldots, \vec{S}_{k+l_{P\max} m}, \quad 1 \le k \le m, \tag{35}$$

where $(m-1)$ is the of skipped points necessary to form the subsequence.

The values $l_{P\max}$, $l_{S\max}$ can be calculated from the following restrictions on the integer generic index of the position vectors above, we have

$$j + l_P m \le n-1, \quad 0 \le l_P \le l_{P\max} \tag{36}$$

$$k + l_S m \le n-2, \quad 0 \le l_S \le l_{S\max} \tag{37}$$

From these equations, we can write

$$l_{P\max} = \left[\frac{n-j-1}{m}\right], \quad 0 \le j \le m-1, \tag{38}$$

$$l_{S\max} = \left[\frac{n-k-2}{m}\right], \quad 1 \le k \le m, \tag{39}$$

where the square brackets above $[x]$ stand for the greatest integer value $\le x$.

There are m subsequences of the form given by Eqs. 34 and 35. Each of them has $(l_{P\max}+1)$ and $(l_{S\max}+1)$ points, respectively. We then propose to define sequences of n and $n-2$ points by

$$\mathbb{P}_m = \bigcup_{j=0}^{m-1} (P_j)_{m,\, l_{P\max}}, \tag{40}$$

$$\mathbb{S}_m = \bigcup_{k=1}^{m} (S_k)_{m,\, l_{S\max}}, \tag{41}$$

respectively.

The number of points of these sequences can be elementarily checked by using Eqs. 38 and 39, we get

$$\sum_{j=0}^{m-1} (l_{P\max}+1) = m + \sum_{j=0}^{m-1} \left[\frac{n-j-1}{m}\right] = m + n - m = n, \tag{42}$$

$$\sum_{k=1}^{m} (l_{S\max}+1) = m + \sum_{k=1}^{m} \left[\frac{n-k-2}{m}\right] = m + n - m - 2 = n-2. \tag{43}$$

The original sequences of Eqs. 24 and 25 are trivially included in the scheme given by Eqs. 40 and 41. They are $\mathbb{P}_1 = (P_0)_{1,\,n-1}$ and $\mathbb{S}_1 = (S_1)_{1,\,n-1}$, respectively.

The coordinates of the points of the subsequences can be written analogously to Eqs. 26 and 27. We have,

$$\vec{r}_{j+l_P m} = (r(\phi, Z)\cos(j + l_P m)\phi, r(\phi, Z)\sin(j + l_P m)\phi, jZ), 0 \le j \le m-1, \quad (44)$$

$$\vec{S}_{k+l_S m} = \left(r_{S_m}(\phi, Z)\cos(k + l_S m)\phi, r_{S_m}(\phi, Z)\sin(k + l_S m)\phi, kZ_{S_m}\right), \quad 1 \le k \le m. \quad (45)$$

A fishbone topology will be adopted for the organization of the Steiner tree for a couple of subsequences $(P_j)_{m,\,l_{P\max}}$ and $(S_k)_{m,\,l_{S\max}}$ given by Eqs. 44 and 45, respectively. The first point $\vec{S}_{k+m}$ will be connected to the two first points $\vec{r}_j$ and $\vec{r}_{j+m}$. The last point $\vec{S}_{k+l_{S\max}m}$ will be connected to the two last points, $\vec{r}_{j+(l_{P\max}-1)m}$ and $\vec{r}_{j+l_{P\max}m}$. The points $\vec{S}_{k+l_S m}$ are connected consecutively as well as all the intermediate couples of points $\vec{r}_{j+l_P m}$, $\vec{S}_{k+l_S m}$ with $j = k, l_P = l_S$. It is worthwhile to notice that the Steiner trees to be formed from the subsequences above with fishbone topology could be associated in order to have a generic connection topology for the resulting Steiner tree. The Euclidean length of the resulting Steiner tree does not depend on the special combination of the subsequences with fishbone topology. On each sub-Steiner tree formed by the subsequences $(P_j)_{m,\,l_{P\max}}$ and $(S_k)_{m,\,l_{S\max}}$ as explained before, we introduce the requirement of edges meeting at each Steiner point with angles of $2\pi/3$. From Eqs. 44 and 45, the introduction of this requirement will lead to

$$Z_{S_m} = Z, \quad (46)$$

$$m^2 Z_{S_m}^2 = r_{S_m}^2 A_m(A_m + 1), \quad (47)$$

where

$$A_m = 1 - 2\cos(m\phi) \quad (48)$$

and r_{S_m} is a surface $r_{S_m}(\phi, Z)$ given by

$$\frac{r_{S_m}(\phi, Z)}{r(\phi, Z)} = \frac{mF(\phi, Z)}{\sqrt{A_m(A_m + 1)}}, \quad (49)$$

where

$$F(\phi, Z) = \frac{Z}{r(\phi, Z)}. \quad (50)$$

The additional requirement of full sub-Steiner trees with $(n - 2)$ Steiner points gives for the angle θ_m between consecutive edges of a spanning tree formed with the points of position vectors $\vec{r}_{j+l_P m}$

$$-\frac{1}{2}\cos\theta_m = -1 + \frac{(A_m + 1)^2}{2(m^2F^2 + A_m + 1)}, \quad (51)$$

or

$$\cos\theta_m = \max\left(-\frac{1}{2}, \; -1 + \frac{(A_m + 1)^2}{2(m^2F^2 + A_m + 1)}\right). \quad (52)$$

The Euclidean length of the candidate for a spanning corresponding to the union of the subsequences $(P_j)_{m, l_{P\max}}$ is now given by

$$l_{SP_m} = r(\phi, F)\left[(n-m)\sqrt{m^2F^2 + A_m + 1} + (m-1)\sqrt{F^2 + A_1 + 1}\right], \tag{53}$$

$(m-1)$ is the number of skipped points to form each subsequence and is also the number of coils necessary to connect these subsequences.

Since the fishbone topology is adopted for each sub-tree formed by a couple of subsequences $(P_j)_{m, l_{\max}}$, $(S_k)_{m, l_{S\max}}$, we will have for the Euclidean length of the candidate of a Steiner tree corresponding to the union of the subsequences $(S_k)_{m, l_{S\max}}$,

$$l_{ST_m} = r(\phi, F)\left[n - 2 + ((n-m-2)A_m - m)\frac{mF}{\sqrt{A_m(A_m+1)}}\right.$$
$$\left. +2\sqrt{1 + (A_m - 1)\frac{mF}{\sqrt{A_m(A_m+1)}} + (A_m^2 + A_m + 1)\frac{m^2F^2}{A_m(A_m+1)}}\,\right], \tag{54}$$

The straightforward but tedious derivation of Eqs. 53 and 54 has been done by using the mathematical identities of Eqs. 42, 43.

We can now define $l_m = l_{SP_m}/r(\phi, F)$; $L_m = l_{ST_m}/r(\phi, F)$ for a large set of points, $n \gg 1$. We have,

$$l_m = n\sqrt{m^2F^2 + A_1 + 1}, \tag{55}$$

$$L_m = n\left(1 + mF\sqrt{\frac{A_m}{A_m + 1}}\right). \tag{56}$$

The Eqs. 52–54 above correspond to the generalization of formulae (23), (30), (31) given in the last section.

By using the usual prescription for a Steiner Ratio [2,4], we can have for $n \gg 1$,

$$\rho(\phi, F) = \frac{\min_{(m)}(l_m)}{\min_{(m)}(L_m)}. \tag{57}$$

We now collect some facts about the surfaces given into Eqs. 52–54.

1. The surfaces L_1, L_2, L_3 intersect on a point, its coordinates in the interval $0 \le \phi \le \pi$ are given by

$$\phi = \pi - \arccos\left(\frac{2}{3}\right); \quad F = \frac{\sqrt{30}}{9}, \quad L_1 = L_2 = L_3 = L = \frac{10\sqrt{3}}{9}. \tag{58}$$

2. There is not a common intersection of m surfaces $L_1, L_2, \ldots, L_m$ for $m \ge 4$ unless the trivial one $\phi = 0$, $F = 0$.

3. All the other triads of surfaces which intersect on a point have a lesser value for the third coordinate as can be seen from Table 1 below, where we can see the coordinates of the intersection points of these triads amongst the surfaces $L_1, \ldots, L_7$.

4. From Eq. 52, the set of favoured surfaces l_m and L_m which participate in the minimization process of Eq. 57 could be taken as the triads l_1, l_2, l_3 and L_1, L_2, L_3. The others correspond to degenerated Steiner trees in the most part of the interval $0 \le \phi \le \pi$ and should be discarded. The Fig. 1 below shows the surfaces $\cos\theta_m(\phi, F)$ for $m = 1, \ldots, 5$ and the restriction to full Steiner trees imposed by the plane $\cos\theta_m = -1/2$.

Table 1 Coordinates of the intersection points for triads of surfaces L_m

	x	F	L
L_1, L_5, L_6	1.116654868	0.1648758578	1.072288269
L_1, L_4, L_5	1.351143469	0.2367361174	1.272895251
L_1, L_3, L_4	1.705939270	0.3637117036	1.549758080
L_3, L_4, L_7	1.782228977	0.1419984623	0.9981221038
L_1, L_2, L_3	2.300523983	0.6085806198	1.924500897
L_2, L_3, L_5	2.475644465	0.2664972618	1.345665351
L_2, L_5, L_7	2.656751591	0.1337959340	0.9697845029

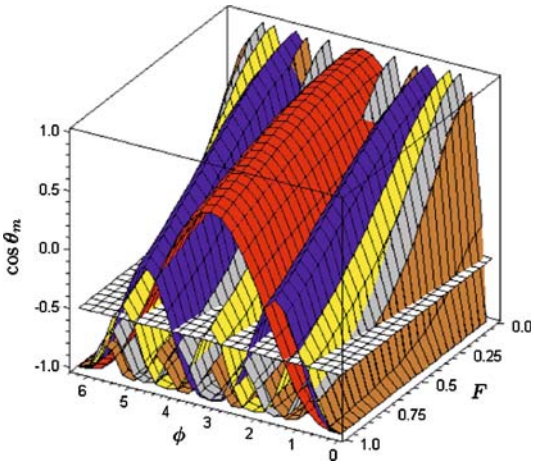


Fig. 1 The surfaces $\cos\theta_m(\phi, F)$ for $m = 1, \ldots, 5$ and the plane $\cos\theta_m = -1/2$

5. For surfaces l_m of the numerator of Eq. 57, there are no triads of surfaces intersecting at a point. There are couples of surfaces intersecting along straight lines parallel to F-axis. The intersection straight lines with the lowest values of the third coordinate are given by $l_1 = l_2$ and $l_1 = l_3$. We can restrict the search for a minimum of Eq. 57 with this information and a detailed analysis of the intersections of the surfaces ρ_{12}, ρ_{13} and ρ_1 which are given by

$$\rho_{13} = \frac{\min(l_1, l_3)}{\min(L_1, L_2, L_3)}, \tag{59}$$

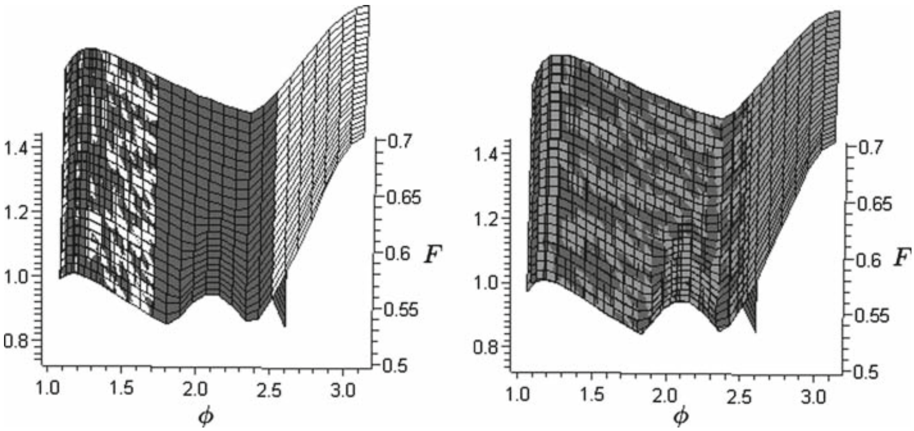
$$\rho_{12} = \frac{\min(l_1, l_2)}{\min(L_1, L_2, L_3)}, \tag{60}$$

$$\rho_1 = \frac{l_1}{\min(L_1, L_2, L_3)}. \tag{61}$$

In Table 2 below we show the regions in the interval $0 \le \phi \le \pi$ of the predominance of surfaces given by Eqs. 59–61 in a minimization process. The Fig. 2 shows the relative position of these surfaces and helps to corroborate our conclusions.

Table 2 Regions of predominance of the surfaces of first column

	ϕ
ρ_{13}	[0, 0.1745329252]
	[2.443460953, 2.459930995]
	[2.617993878, π]
ρ_{12}	[0, 1.732472954]
	[1.745329252, 2.443460953]
	[2.459930995, 2.617993878]
ρ_1	[0, 1.732472954]
	[1.745329252, 2.443460953]
	[2.459930995, 2.555907110]
	[2.617993878, π]



(a) ρ_{13} (light gray) and ρ_{12} (dark gray) **(b)** ρ_{12} (dark gray) and ρ_1 (light gray)

Fig. 2 Surfaces ρ_{13}, ρ_{12}, ρ_1 for the ϕ-interval [1, 5]. The mixed part means the superposition of the surfaces in the corresponding region

The coordinates of the global minimum are given by

$$\phi = \pi - \arccos\left(\frac{2}{3}\right); \quad F = \frac{\sqrt{30}}{9}, \quad \rho_1 = \rho_{12} = \frac{1}{10}(3\sqrt{3} + \sqrt{7}). \tag{62}$$

In Fig. 3 we present the surface ρ_1 and the restriction imposed by the planes $\rho_1 = 1$, and $\rho_1 = 0.615$ (Du's lowest bound) [6].

5 The global minimum of the Steiner ratio function

It is easy to define a compact dominium in the plane ϕ, F and to give a proof of the uniqueness of the minimum of Eq. 62 by the Weierstrass theorem [3,7]. We prefer to give a computational emphasis on the conclusions of the present work.

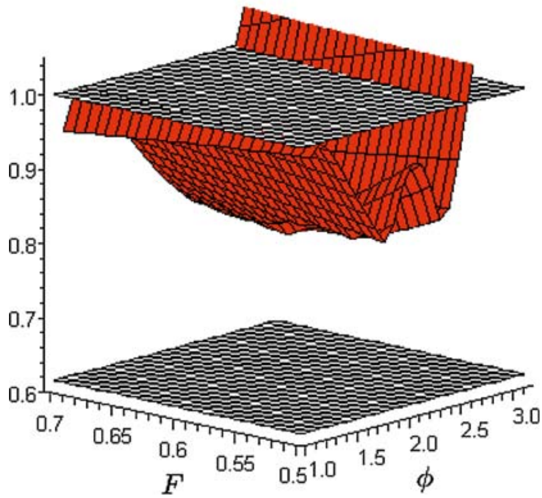


Fig. 3 The surface $\rho_1(\phi, F)$ and the planes $\rho_1 = 1$ and $\rho_1 = 0.615$

The Nelder–Mead method [8] is an unconstrained non-linear optimization method without derivatives. It is very adequate for non-differentiable objective functions with a small number of variables like functions $\rho_{13}, \rho_{12}, \rho_1$. We give the result of application of this method to the function $\rho_1(\phi, F)$. For this problem of two variables, the coordinates of the initial simplex (triangle) can be chosen from Eq. 61 and Tables 1 and 2, as

$$(2.2, 0.59); \quad (2.2, 0.58); \quad (2.3, 0.57)$$
$$\phi_{\min} = 1.745329252, \quad \phi_{\max} = 2.443460953$$
$$F_{\min} = 0.5000000000, \quad F_{\max} = 0.7000000000$$

and we get for the coordinates of the minimum:

$$\phi_M = 2.300523983; \quad F_M = 0.6085806194, \quad \rho_{1_M} = 0.7841903733. \tag{63}$$

We can compare this result with that obtained with the analytical method of this work, Eq. 62. They are the same within the 10-digits approximation used in the calculation with the Nelder–Mead method. Actually, Eq. 62 is the correct result for any number of digits.

6 Concluding remarks

The analytical method which was presented in this work can be easily extended to any number of dimensions. The essential 3D result here is that we recover the best upper value usually proposed for the 3D Euclidean Steiner Ratio by starting from a generic cylindrical distribution. This formulation is also adequate for deriving useful expressions of the geometric chirality function [6] as well as for unveiling the true nature of the molecular processes which have driven the formation of biomacromolecules. Research along these lines is now in progress and will be published elsewhere.

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