A Generalised Flatness Index for a Simplex Hypersolid

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Paper 2013-1032
2013 September

Abstract
The sequential simplex method is an efficient algorithm for setting experimental plans for evolutionary optimization. The variable step size algorithm embeds a self-tuning feature, adapting, at each step, the span of exploration of the domain. One of the weak points of this algorithm is cohypoplanarity, reducing the ability of simplex to explore the domain. To maintain a high efficiency it is crucial to detect collapsing of a simplex in an early stage to avoid waste of tests or calculation resources. In the present paper, this problem will be addressed through the introduction of a flatness index; application cases will be presented where such index is benchmarked against the standard cohypoplanarity index.

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Introduction

The sequential simplex method represents an efficient way to implement evolutionary optimization and is easily applicable to a wide variety of problems. The algorithm is very flexible as it is not limited by the number of input variables. It can be applied to non-continuous domains and can be extended to multi-output optimization problems through definition of desirability functions. Sequential simplex is particularly effective when the problem contains many input variables, as the minimum number of experiments required for the initiation of the optimization is significantly smaller compared to an orthogonal experimental plan, even if fractional. As there is no limitation in the span between initial experiments, it is possible in application to start the optimization with small changes in initial values of the parameters, thus avoiding the disruption of process settings. Evolutionary methods are intended to provide progressive optimization at each step, and the optimization process can be stopped at any step when a satisfactory value for the output function is reached.

During the subsequent iterations, the simplex method may lose its ability to explore the domain in which the problem is defined and get stopped in a limited subspace. In this case, the sequential simplex has to be restarted. This issue is commonly known as cohypoplanarity and is related to collapsing of the simplex. As cohypoplanarity is a result of iterations, it is crucial to detect the arising of this problem in an early stage, so that sequential simplex could be restarted promptly, saving test or calculation iterations.

The subject of this paper is the introduction of an index based on simplex topology used to evaluate and detect the tendency to collapse for each iteration. Some application cases will be discussed in which such index is compared to the standard cohypoplanarity index introduced in [1].

Sequential Simplex Method

The sequential simplex method provides a path for iterative optimization by seeking the local steepest ascent (maximization problem) or descent (minimization problem) direction. When n is the number of input factors for the phenomenon or function to be optimized, a simplex is defined as s of $n+1$ points (namely vertices) in the n-dimensional domain under study. At each iteration of the algorithm, the vertices are ranked according to the associated output value. Out of the whole set, three significant vertices are identified:

- – B (Best) – Vertex with best output;
- – W (Worst) – Vertex with worst output;
- – N (Next to worst) – Vertex with the closest but still better value than W.

Out of these three significant vertices, a new trial vertex is computed for the next experiment. When $n>2$ there are more than 3 vertices for the simplex, only the three mentioned significant vertices will be used to compute a new vertex. All the vertices of the simplex from the previous step, except for the W, will be vertices of a new simplex together with the newly computed point. Such next simplex is the basis for a new optimization step. There are two variants of the algorithm for the sequential simplex, namely Fixed Size Simplex and Variable Size Simplex.

The Fixed Step Size algorithm constrains the position of the new vertex (R) to a fixed distance from the W vertex for each step. In Figure 1 [2] the principle is shown for the bi-dimensional domain (n=2).

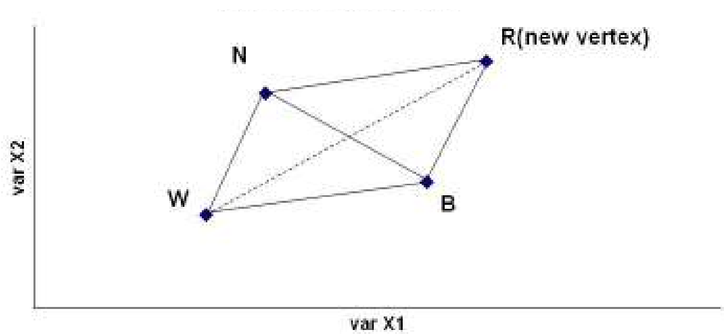

Figure 1 [2] – Fixed step simplex for k=2

In the Variable Step Size variant, the distance between the worst point (W) and the new optimized point can vary at each step of the optimization. The step size, i.e. the distance from the new point and the W vertex can have four different values, as shown in Figure 2 [2] for the bi-dimensional case (n=2). The new point is selected among the four options according to the criteria summarized in the table in Figure 3 [2]. The algorithms leading to the position of the new vertex for both variants are described in detail in [1].

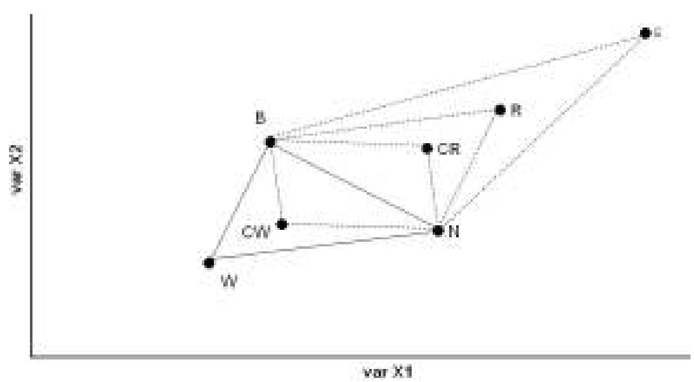

Figure 2 – Vertices in variable step size simplex

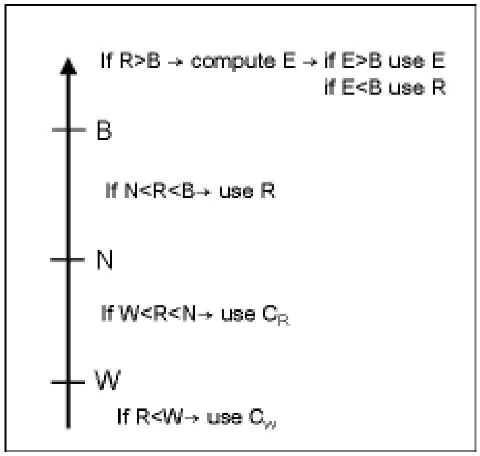

Figure 3 [2] – Criteria for selection of new retained vertex in variable step size simplex in maximization problem

Cohypoplanarity of a Simplex

As explained previously, at each iteration, a new move is defined from the current simplex from previous step. Therefore the ability of the algorithm to explore the domain depends on the current simplex. The basic condition for exploring the whole hyperspace is the maintenance of the simplex's *n* dimensions. When the number of dimensions of such hyperspace is less than *n*, the vertices of the simplex become cohypoplanar and the sequential simplex optimization will not be able to explore the full domain, but only a *n-1*-dimensional subspace.

In a 3-dimensional domain, the four vertices are cohypoplanar if they lay on a plane. In a 2-dimensional domain, three cohypoplanar vertices lay on a line. In Figure 4, the cohypoplanarity is shown for a 2-dimensional case.

Normally cohypoplanarity is approached progressively, i.e. it takes a number of steps with subsequent compressions on the worst side (C_w moves) for the simplex to collapse. In Figure 5, the collapsing is shown for a 2-dimensional case, being C_w',C_w'', C_w''' three subsequent optimization steps. When simplex collapses, it needs to be restarted by creating a new simplex around the collapse area, a re-starting method is explained in [2]. It is therefore of high importance to be able to detect this tendency as early as possible to avoid wasting experiments.

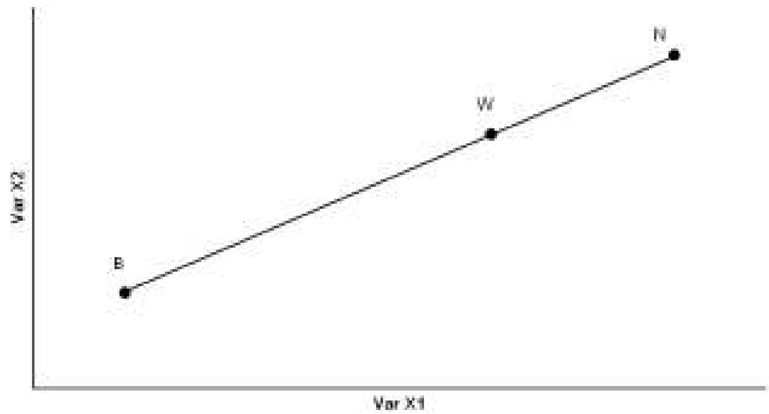

Figure 4 – Cohypoplanarity in a 2-dimensional simplex

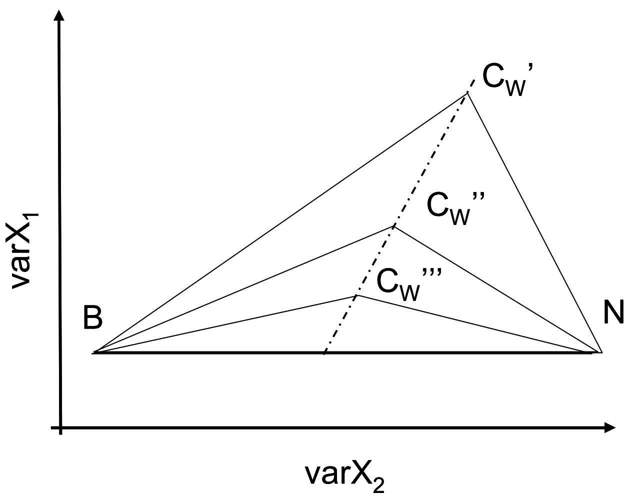

Figure 5 – Collapsing simplex in a 2-dimensional case

Flatness of a Simplex

A simplex can be represented by a matrix having *n+1* rows and *n* column; each row containing the values of the *n* coordinates for the *n*-th vertex of the simples, as shown below, where superscript relates to vertex and subscript to coordinate:

$$V_{new} = \begin{bmatrix} x_1^1 & x_2^1 & x_3^1 & \dots & x_n^1 \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_n^2 \\ \dots & \dots & \dots & \dots & \dots \\ x_1^{n+1} & x_2^{n+1} & \dots & \dots & x_n^{n+1} \end{bmatrix} \quad (1)$$

The cohypoplanar status of a simplex is detected through a *cohypoplanarity index.*
Such index can be constructed as follows [1]:

1. Subtract the coordinates of one vertex from the coordinates of all other vertices. As a result, the simplex is translated to the origin of the coordinate axis.
2. The remaining vertices will form a square *n x n* matrix
3. The determinant of such matrix is the cohypoplanarity index. If it is zero, then the simplex is cohypoplanar, i.e. it exists in an *n-1*-dimensional subspace.

By tracking the value of the cohypoplanarity index, it is possible to monitor the evolution of the simplex and detect tendency for collapsing. Considering the simplex expressed as per (1), and considering as a reference for the shift the n+1-th vertex, the square matrix in point 2 of previous procedure is as follows:

$$V_{new} = \begin{bmatrix} x_1^1 - x_1^{n+1} & x_2^1 - x_2^{n+1} & x_3^1 - x_3^{n+1} & \dots & x_n^1 - x_n^{n+1} \\ x_1^2 - x_1^{n+1} & x_2^2 - x_2^{n+1} & x_3^2 - x_3^{n+1} & \dots & x_n^2 - x_n^{n+1} \\ \dots & \dots & \dots & \dots & \dots \\ x_1^n - x_1^{n+1} & x_2^n - x_2^{n+1} & \dots & \dots & x_n^n - x_n^{n+1} \end{bmatrix} \quad (2)$$

The determinant of such matrix is therefore dependent on the distance between vertices, i.e. the length of edges. Thus, the progressive reduction of its value may be related either to actual cohypoplanarity, or to progressive reduction of the size of the simplex, or both. While the zero value of cohypoplanarity index corresponds to the total cohypoplanarity, the reduction of cohypoplanarity index to small values may be not sufficient to detect tendency to collapse, at least unless the repetition of C_w moves is observed too.

The definition of a flatness index is aimed at identifying a relevant indicator for the *aspect ratio* of the simplex, insensitive to any extent to its "overall" size.

Multiple approaches are possible to define such aspect ratio in an *n*-dimensional space. The actual volume of the simplex may be referred to an ideal volume computed out of the size of the length of all edges. The definition of such reference volume is not straightforward.

A first hypothesis could be the volume of inscribed sphere, i.e. the biggest *n*-dimensional hyper-sphere wholly contained inside the simplex and touching all faces. The difference in volume could give an indication of the flatness of the simplex, as showed for the 2-dimensional example in Figure 6. The formula linking the simplex volume (area of triangle in 2-dimensional case) and the area of inscribed circumference is given by the following expression:

$$\frac{A_c}{A_t} = \frac{1}{p}\sqrt{\frac{(p-a)(p-b)(p-c)}{p}} \quad (3)$$

where:

- A_c= area of inscribed circumference
- A_t= area of triangle
- *a,b,c* length of triangle edges
- $p = (a+b+c)/2$

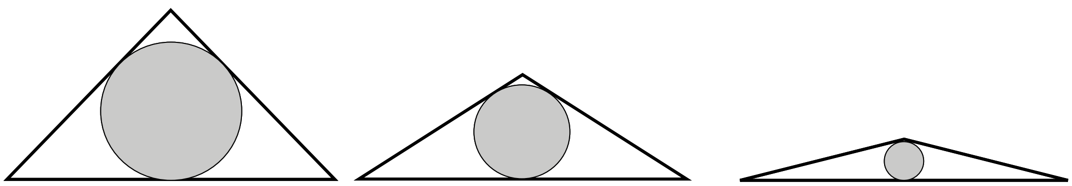

Figure 6 – Comparison between area of 2-dimensional simplex and circumscribed circumference

In Table 1, the value for (3) is computed for four cases with decreasing aspect ratio. It can be observed that the value of this ratio is decreasing with flatness. All regular polyhedra have a unique inscribed sphere, but most irregular polyhedra do not have all faces touching on an inscribed sphere. The concept of an inscribed sphere is then shifted on the largest hypersphere contained inside the simplex. [3]

inscribed circle				
a	10	17	1	0.5
b	10	25	10	10
c	10	28	10.5	10.2
p	15	35	10.75	10.35
r	2.886751	6	0.412381	0.223526
At	43.30127	210	4.433096	2.313492
Ac	26.17994	113.0973	0.534253	0.156966
Ac/At	0.6046	0.538559	0.120515	0.067848

Table 1 – Value of triangle area to inscribed circumference area

Alternatively, the reference volume for the simplex flatness could be the volume of circumscribed hypersphere, i.e. the sphere containing the simplex and touching all simplex vertices.

A comparison can be made again with the 2-dimensional case. The radius R_{cs} the circumference circumscribed around a triangle is computed as follows:

$$R_{cs} = \frac{abc}{4A_t}$$

In this case, the closer the area of triangle is to the area of circumscribed circumference, the lower is the flatness (See Figure 7). The ratio between the area of the triangle and the area of circumscribing circumference shown in table 2 for the four bi-dimensional cases as per previous example:

circumscribed circle				
a	10	17	1	0.5
b	10	25	10	10
c	10	28	10.5	10.2
p	15	35	10.75	10.35
At	43.30127	210	4.433096	2.313492
R	5.773503	14.16667	5.921369	5.51115
Ac	104.7198	630.5002	110.1524	95.41889
Ac/At	0.413497	0.333069	0.040245	0.024246

Table 2 – Value of triangle area to circumscribing circumference area

All regular polyhedra have circumscribed spheres, but most irregular polyhedra do not have one. Since, in general, not all vertices lie on a common sphere. It is possible to define the smallest containing sphere for such shapes. [4].

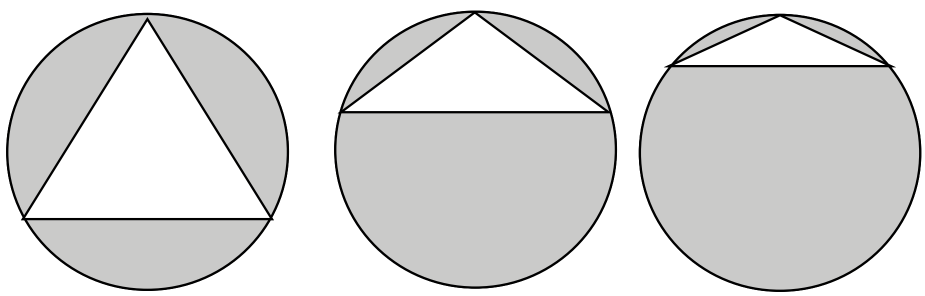

Figure 7 – Comparison between area of 2-dimensional simplex and circumscribed circumference

The two abovementioned methods are easily applicable for $n < 3$, but for higher number of dimensions, they have less significance as the hyperspheres are not uniquely defined in a closed formula for all simplices. Moreover, the calculation of the radii (inscribed or circumscribed) would require a numerical iterative solution.

A third possible approach would be the generalization of the law of sines to hypersolids. Let us consider a simplex in *n*-dimensional space; the *n+1* vertices will be connected to each other by *n-1-dimensional* hyperfaces. Such hyperfaces will be delimiting the volume occupied by the simplex.

In the 2-dimensional case, the simplex is the triangle, delimited by 3 vertices connected by 3 mono-dimensional edges. Analogously, in 3-dimensional space, a simplex is a tetrahedron delimited by four triangles. The *n-1*-dimensional hyperfaces are called subvolumes, and the size is called content. The law of sines for *n* dimensions can be expressed as follows ([5] – Corollary 2.2):

$$\frac{F_1}{\sin\alpha_1} = \frac{F_2}{\sin\alpha_2} = \ldots = \frac{F_{n+1}}{\sin\alpha_{n+1}} \quad (4)$$

For each *i-th* vertex:

- F_i = content of the *i-th* subvolume opposite to the *i-th* vertex, i.e. the volume of the subvolume formed by all vertices but the *i-th*
- α_i = solid angle correspondent to *i-th* vertex

If the vertices are known, all sub-volume contents are known and solid angles α_i can be computed by inverting (4). The values of solid angles could then be combined to identify simplex flatness. The main drawback of this method will be the need for solving (4) by the angles α_i, i.e. solving a non-linear system (sines).

Flatness Index

In the present section, an alternative flatness index will be proposed, still defined on the sub-volume contents. F_i sub-volume contents have been defined previously as size indicator of each hyperface connecting *n+1* vertices of an *n* simplex. Let's consider the array of *n+1* sub-volume contents sorted ascending $\{F\}^s$, the *n+1-th* element of such array will be the size of the biggest subvolume.

The flatness index is defined as the sum of all subvolume contents but the biggest, divided by the biggest. Defined F_i^s the *i-th* element of $\{F\}^s$, the flatness index FI is defined as follows:

$$FI = \frac{\sum_{i=1}^{n} F_i^s}{F_{n+1}^s} \quad (5)$$

The meaning of FI can be clearly identified through a 2-dimensional and a 3-dimensional example.

In a 2-dimensional case, the simplex is a triangle. Its three edges are *n+1 mono-dimensional* sub-volumes, and the length of each the volume will be a subvolume content. Considering the two triangles in Figure 8, having respectively as sides *a,b,c* and *a',b',c'*, the sorted subvolume content arrays, as defined in (5), sorted, will be:

$$\{F\}^s_{abc} = \{b, a, c\}$$
$$\{F\}^s_{a'b'c'} = \{b', a', c'\}$$

And the flatness index FI will be as follows:

$$FI_{abc} = \frac{c}{a+b}$$
$$FI_{a'b'c'} = \frac{c'}{a'+b'}$$

In a 3-dimensional case, a simplex is a tetrahedron and its volume is delimited by *n+1* faces (bi-dimensional), the area of each face is again one of the *n+1* subvolume contents.

Let's consider the two simplices in Figure 9.

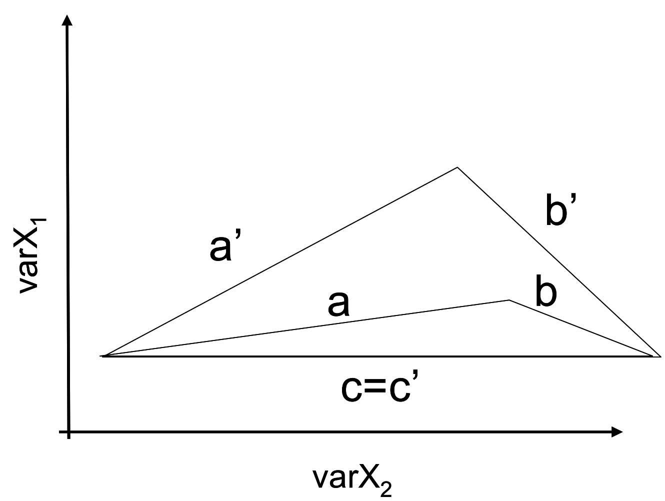

Figure 8 – Simplices in 2-dimensional space

For simplicity, both will have three out of the four faces contained in a reference plane. A first simplex has faces A, B and C contained respectively in the varX1varX2, varX1varX3 and VarX2varX3 planes, and the fourth face D. The second, bigger simplex, will have faces A', B' and C' contained respectively in the varX1varX2, varX1varX3 and VarX2varX3 planes, and the fourth face D.
The two sorted subvolume content arrays will be:

$$\{F\}^s_{ABCD} = \{B, C, A, D\}$$
$$\{F\}^s_{a'b'c'} = \{B', C', A', D'\}$$

And the flatness index FI will be as follows:

$$FI_{abc} = \frac{D}{A+B+C}$$
$$FI_{a'b'c'} = \frac{D'}{A'+B'+C'}$$

It can be observed that the FI has values bigger than one, and the closer the simplex is to flatness, the closer the FI value gets to 1. It can also be observed that the FI refers to a concept of "aspect ratio" which is quite intuitive and usual when considering 2-dimensional or 3-dimensinal solids. It can easily be extended to *n*-dimensional cases by considering that all subvolumes will have same dimensions, and therefore the area of hyperfaces can be summed.

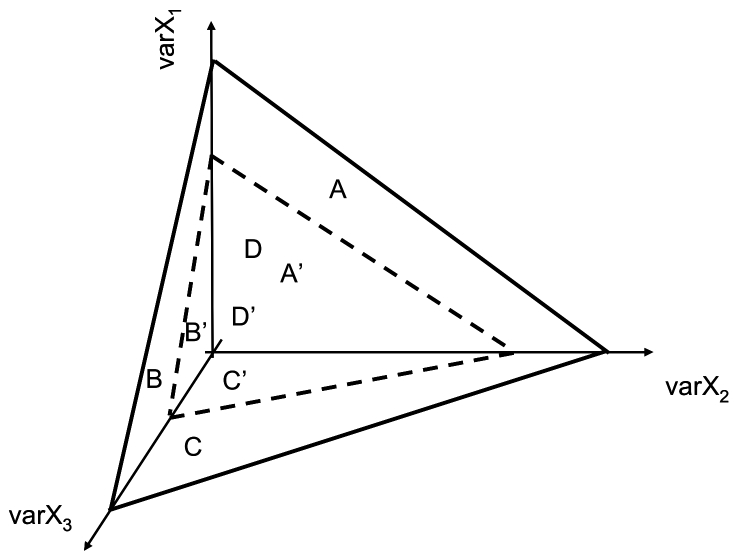

Figure 9 - Simplices in 3-dimensional space

Implementation

In order to compute the FI given by expression (5), subvolumes contents have to be computed. As a general simplex will have same number of vertices and subvolumes (*n+1*), and each subvolume is defined through the *n* vertices it connects, it is possible to define a one to one correspondence between each subvolume and the *opposite* vertex not contained in such subvolume.

The volume of a simplex can be computed through the Cailey-Menger determinant [6]. The Cailey-Menger matrix for a general simplex is expressed as follows:

$$\overline{B} = \begin{bmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & |v_1 - v_1|^2 & |v_1 - v_2|^2 & \dots & |v_1 - v_{n+1}|^2 \\ 1 & |v_2 - v_1|^2 & |v_2 - v_2|^2 & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ 1 & |v_{n+1} - v_1|^2 & \dots & \dots & |v_{n+1} - v_{n+1}|^2 \end{bmatrix} \quad (6)$$

Where $|v_i - v_j|^2$ is the square of the distance between the *i-th* and *j-th* vertex in the *n-dimensional* space, thus by definition the Cailey Menger matrix is symmetrical and all elements on the diagonal are zeros.

The square of the volume content of the simplex is then given by the following expression:

$$V^2 = \frac{(-1)^{n+1}}{2^n (n!)^2} \det\left(\overline{B}\right) \quad (7)$$

To compute the *n+1* subvolume contents of the simplex, it is sufficient therefore to create the Cailey Menger matrix (6) for each subset of vertices by removing one at a time and computing the contents by formula (7). Operatively, for each sub-volume identified through the *j-th* opposite vertex, this equals to removing the *j-th* row and the *j-th* column from the Cailey Menger matrix for the general simplex.

Application case 1 - Single 3-dimensional simplex

In this section, the value of the FI and the standard cohypoplanarity index will be compared for different types of 3-dimensional simplices (tethraedra). Let's consider a simplex as per Figure 10, i.e. with three faces contained in the three reference planes. The edges connecting v_1 with v_3 and v_1 with v_4 will have the same length in all cases, such length will be the reference length and will define in different sub-cases the general size of the simplex. The edge connecting v_1 and v_2 will be varied within different cases freely, therefore defining different values of the simplex flatness (see Figure 11).

Four sizes will be considered with reference edge length respectively equal to two units, one unit, half a unit and a tenth of unit.

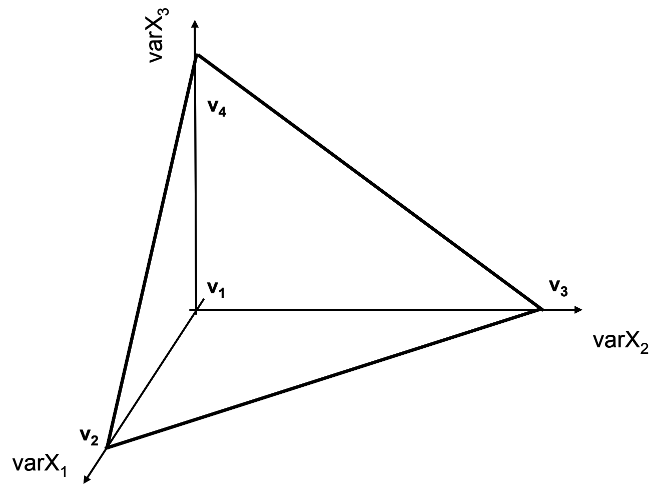

Figure 10 – Reference simplex for application

For each size the flatness will be varied, expressed by the ratio of the length the shortest edge (connecting v_1 and v_2) on the length of the reference edges. In Table 3, the simplex types are summarized. The cases are designed to span through different sizes and flatness values to highlight properties of the flatness index. For each case, the FI and cohypoplanarity index have been computed via a routine compiled in Python 2.7. In Figure 12, the values of FI and cohypoplanarity index are plotted versus the size index (length of reference edge), for all values of ratio shortest edge to reference edge for the size 2, same plot is repeated for the sizes 1, 0.5 and 0.1 respectively in Figure. 13, 14 and 15.

It can be observed that, for all flatness cases, the value of the FI is independent from the size of the simplex (reference edge length) while the cohypoplanarity index is sensitive to it.

As the simplex size is likely to change significantly in variable step evop sequence, any flatness check threshold based on cohypoplanarity index should be set relative to the initial simplex size and be checked against actual simplex size. It can also be observed that, depending on the simplex size, the range of values for FI and cohypoplanarity index may be distinct or overlap.

Table 4 summarizes the values for FI for the different value of the ratio of the length the shortest edge (connecting v_1 and v_2) on the length of the reference edges; the FI value ranges from 1.73 to 1.0002, being much easier to judge and compare than the range of the cohypoplanarity index.

Reference length (size)	Ratio shortest edge/reference edge	Vertices
2	1	0 0 0 2 0 0 0 2 0 0 0 2
1	1	0 0 0 1 0 0 0 1 0 0 0 2
0.5	1	0 0 0 0.5 0 0 0 0.5 0 0 0 0.5
0.1	1	0 0 0 0.1 0 0 0 0.1 0 0 0 0.1
2	0.1	0 0 0 0.2 0 0 0 2 0 0 0 2
1	0.1	0 0 0 0.1 0 0 0 1 0 0 0 1
0.5	0.1	0 0 0 0.05 0 0 0 0.5 0 0 0 0.5
0.1	0.1	0 0 0 0.01 0 0 0 0.1 0 0 0 0.1
2	0.01	0 0 0 0.02 0 0 0 2 0 0 0 2
1	0.01	0 0 0 0.01 0 0 0 1 0 0 0 1
0.5	0.01	0 0 0 0.5 0 0 0 0.005 0 0 0 0.005
0.1	0.01	0 0 0 0.1 0 0 0 0.001 0 0 0 0.001

Table 3 – Summary of reference simplices for application cases

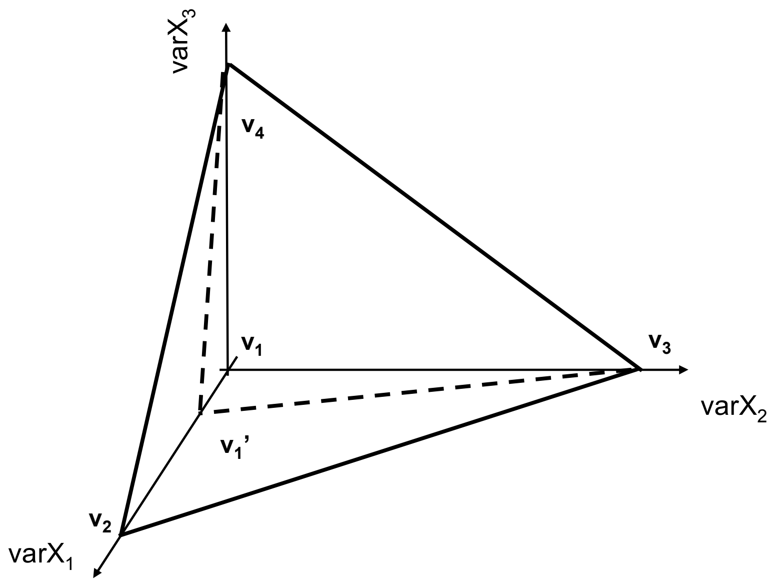

Figure 11 – Two reference simplices with different flatness reference simplices

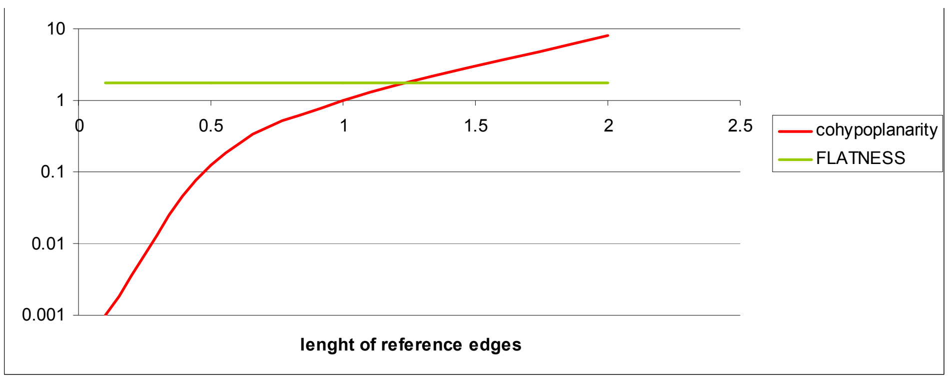

Figure 12 – FI and cohypoplanarity index versus simplex size, aspect ratio 1

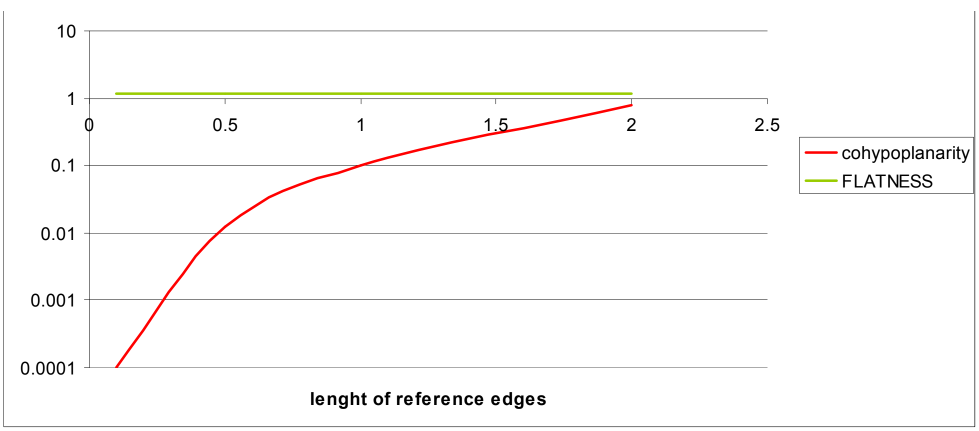

Figure 13 – FI and cohypoplanarity index versus simplex size, aspect ratio 0.1

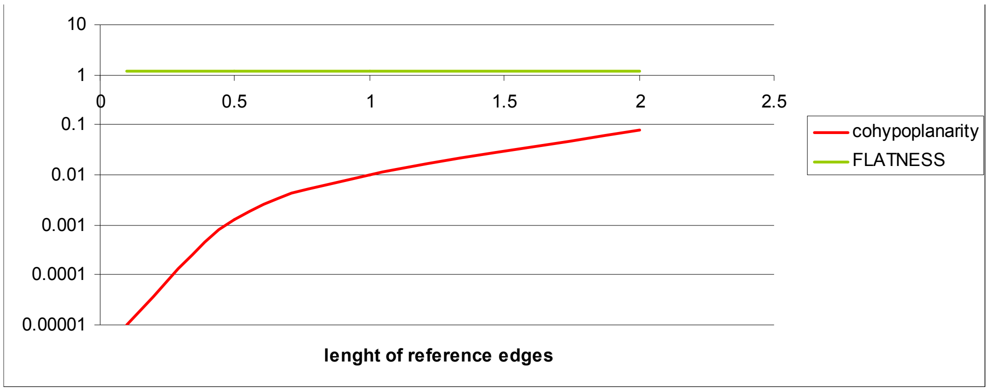

Figure 14 – FI and cohypoplanarity index versus simplex size, aspect ratio 0.01

Ratio shortest edge to reference edges	FI
1	1.732
0.1	1.188
0.01	1.002

Table 4 – Value of FI vs. ratio shortest edge to reference edges for 3-dimensional case

Application Case 2 – Generalized 4-Variables Rosenbrock Function Minimization

In the present chapter, a sequential simplex optimization will be applied to a reference function, and FI and cohypoplanarity index will be compared through the optimization path. The simplex optimization and the computation of FI and cohyplanarity index at each step are obtained through a Python 2.7 script.

Rosenbrock's function is a 2-variable 4th-order non-convex polynomial function, its equation is given by the expression:

$$f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1{}^2)^2$$

The Rosenbrock function can be generalized for *n*-dimensional space as follows:

$$f(x_1, \ldots, x_n) = \sum_{t=1}^{n-1} 100\left(x_i^2 - x_{i+1}\right) + \left(x_i - 1\right)^2$$

For this study, a sequential simplex optimization has been performed on the 4-variable from of the generalised Rosenbrock function. The optimisation space was set as:

$$-5 < x_1 < 10$$
$$-4 < x_2 < 8$$
$$-6 < x_3 < 11$$
$$-7 < x_4 < 12$$

With the following initial simplex:

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{bmatrix} = \begin{bmatrix} -5 & -4 & -6 & -7 \\ 10 & -4 & -6 & -7 \\ -5 & 8 & -6 & -7 \\ -5 & -4 & 11 & -7 \\ -5 & -4 & -6 & 12 \end{bmatrix}$$

Thresholds for cohypoplanarity index and FI were set respectively at 10E-04 and 1.05. In Figure 15, the values of alarms are plotted against optimization step number for the first 150 steps.

It can be observed that the cohypoplanarity index, from step 85, is constantly below the alarm value, although optimization proceeds with reflection and expansions up even in the following steps. Stopping iteration after 90 steps would not have been efficient in this case. FI, on the other hand, detects flatness tendency around step 120. After step 130, the flatness threshold is below the threshold, but by proceeding up to 300 steps, the optimization would still proceed without simplex collapsing. In this case though, the simplex gets very small, and thus its ability to move is limited. At Step 300, the FI would still have a value of about 1.36, comparable in a *2*-dimensional case with an isosceles triangle having the two smaller angles at about 42.5 degrees.

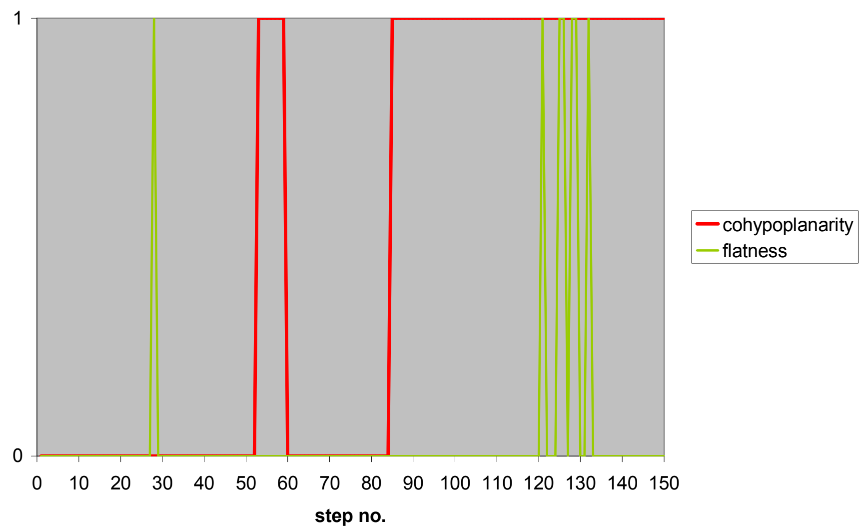

Figure 15 – Comparison cohypoplanarity index vs FI

Conclusions

In the present article, a collapsing of simplices has been discussed. A formulation for a flatness index has been proposed and compared to the standard cophypoplanarity index and other possible approaches. The FI is defined as a ratio between the sum of all subvolumes contents but the biggest, and the biggest subvolume content. The main advantage of the proposed flatness index, with respect to the cohypoplanarity index, as discussed in the "Flatness Index" section, is that FI values only depends on the shape of the simplex, or aspect ratio, and not to the overall size of the simplex.

The subvolumes can be computed through the Cailey-Menger matrix, a number of $n+1$ matrices are built for the $n+1$ subvolumes defined by removing each time one vertex, and the value of FI has a unique value identified through a closed formula. The formulation is simple and can be intuitively related to the flatness of a triangle (2-dimensional simplex). In application case no. 2, the FI has been applied to a simplex optimisation for a 4-variable Rosenbrock function. Results highlight how FI captures the aspect ratio of the simplex and is not sensitive to simplex size.

Alternative approaches for the definition of a flatness index may be considered. A first possibility is to compare the volume of the simplex to the volume of the inscribed n-dimensional hypersphere. A second, complementary, approach could be to compare the simplex volume with the volume of circumscribed n-dimensional hypersphere. In both cases, if $n>3$, the radius is not uniquely defined unless the simplex is regular; otherwise, it has to be determined by minimization. This is disadvantageous with respect to the defined FI. A third approach applies the generalized Law of Sines, linking subvolume contents to the value of sine of the opposite n-dimensional solid angle. The extraction of solid angles value, though, requires the inversion of a trigonometric formula, thus again a numerical solution.

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