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# The Most Chiral Disphenoid*

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**Abstract**

We calculate the analytical expression of the chiral index of the disphenoids and we show that this chiral index has a maximum value. It is reached when the disphenoids have their four triangular faces congruent to a triangle with squared sidelengths ratios $1:3\text{-}\sqrt{2}/2:3$. To our knowledge it is the first time that a maximal chirality three dimensional set is characterized in the non labeled case.

## 1 Introduction

There were many attempts to quantify the geometric degree of chirality of a conformer or of a set of points since more than a century (see [1] for a review). Although it is clearly understood that the minimal degree of chirality corresponds to achirality, it is unclear what could be the maximal degree of chirality, as noticed by Fowler [2]. We point out that we do not look for maximizing physical quantities related to circular dichroism or optical rotatory power, these latter having no simple relation with a geometric degree of chirality, in some mathematical sense. Since several chirality measures exist, several maximally chiral sets are potentially expected. This is exemplified by the case of triangles (i.e. sets of three non labeled points in the plane), for which several maximally chiral triangles were proposed [3–8].

To overcome this difficulty, we considered a chirality measure which operates both on discrete sets and on continuous sets, with or without weights. Only one chirality measure offering these properties was available in the literature: the chiral index [9], which is

*Dedicated to the memory of Professor André S. Dreiding (1919-2013)* formally issued from a more general concept of shape dissimilarity [10], applied to the case of mirror images. It is emphasized that, in the non labeled case, the chiral index is an asymmetry coefficient which applies to probability distributions, these latter being discrete or continuous, as desired. We do not consider anymore the labeled case for which the points are labeled due to colors, or, for conformers, due to the molecular graph (e.g., in the bromochlorofluoromethane, all five points at which the atomics centers are located, are labeled because the atoms are of different natures). In the labeled case, extremal chirality objects are known for set of colored points [9, 11] and for conformers [12].

In the case of multivariate probability distributions (what we called the non labeled case), the chiral index is an asymmetry coefficient. As for the labeled case, it is is zero if and only if the distribution is indirect symmetric, i.e. achiral. Few results are available in this case: the maximally chiral triangle is known [7], and only a conjecture is available for general planar sets [13]. Due to the fundamental role of the tetrahedron in organic chemistry, we would like to identify the most chiral tetrahedra. Alas, it is still an open problem, and it is why we considered a subclass of the set of tetrahedra, the disphenoids, for which the analytical treatment of our optimization problem remains feasible.

A disphenoid is a tetrahedron whose four faces are congruent triangles. It is also called an isosceles tetrahedron [14] or an equifacial tetrahedron [15], and has several remarkable geometric properties [14, 16]. Let $\alpha$, $\beta$, $\gamma$ be the face sidelengths. These latter define an acute triangle, and no disphenoid can be built from an obtuse triangle [14]. The limiting case of a right triangle corresponds to a degenerated tetrahedron whose edges are those of a rectangle with its two diagonals. The disphenoid is achiral (i.e. it has mirror symmetry) when the triangle ($\alpha$, $\beta$, $\gamma$) is isosceles or has a right triangle. For an acute scalene triangle, the disphenoid is chiral. Thus we look for the most chiral disphenoid, in the sense of the upper bound of the chiral index in the space of the distributions of the four vertices.

According to [9], the chiral index $\chi$ of a $d$-dimensional multivariate distribution $\mathcal{P}$ is defined as the squared Wasserstein distance [17] between $\mathcal{P}$ and its mirror inverted image $\bar{\mathcal{P}}$, minimized for all rotations and translations of $\bar{\mathcal{P}}$, and divided by $4T/d$, $T$ being the inertia of $\mathcal{P}$, i.e. the trace of its covariance matrix. The Wasserstein metric was introduced by the Russian mathematician Wasserstein (originally written Vasershtein) [18]. This metric is intimately related to the Monge-Kantorovitch transportation problem [19]. The

Wasserstein distance between two distributions $\mathcal{P}_1$ and $\mathcal{P}_2$ can be interpreted as the cost to transform $\mathcal{P}_1$ into $\mathcal{P}_2$. In our context, the cost is quadratic, so that we refer implicitely to the $L^2$-Wasserstein metric. Thus, $\chi$ is an asymmetry coefficient taking values in $[0;1]$. It is insensitive to isometries and scaling of $\mathcal{P}$, and it is null if and only if $\mathcal{P}$ is achiral (i.e., if $\mathcal{P}$ has indirect symmetry). The optimal translation being null when the expectation of $\mathcal{P}$ is null, we will further assume only null expectation distributions.

# 2 Notations

Let $P$ be a $n$-by-$n$ permutation matrix, $R$ a $d$-by-$d$ rotation matrix and $Q$ a negative determinant $d$-by-$d$ orthogonal matrix. Let $X$ be the $n$-by-$d$ matrix of the $n$ equiprobable observations, or, in other words, the $n$ lines of $X$ contain the cartesian coordinates of the $n$ input data points. We set $V = X'PX$ and we denote transposed matrices or vectors by a quote. The trace of the covariance matrix is $T = Tr(X'X)$. $Min_{\{R,P\}}$ and $Max_{\{R,P\}}$ denote respectively the minimum (resp. the maximum) of a quantity over the space of all rotations $R$ and permutations $P$. According to [11]

$$\chi = \frac{d}{4T} Min_{\{R,P\}} D^2 \tag{2.1}$$

$$D^2 = Tr[(X - PXQ'R')'(X - PXQ'R')] \tag{2.2}$$

$$\chi = \frac{d}{2T}(T - Max_{\{R,P\}} Tr((V + V')Q'R') \tag{2.3}$$

Given $P$, the optimal solution $R$ in equation 2.3 is known for any $d$ value [20]. However, for $d = 3$ there is a simpler expression of this solution if we set $Q = -I$ and we use the unit quaternion $q$ representing the rotation $R$ [9,11]. We denote by $I$ the identity matrix (any size). The quaternion is $q = \begin{pmatrix} p \\ u \end{pmatrix}$, $p$ being the real part of $q$ (conventionnally set non negative) and $u$ being its vector part. The optimal quaternion in 2.3 is the eigenvector associated to the largest eigenvalue in equation 2.5 and the minimized squared $D$ value is

$$D^2 = 2T + 2Tr(V) - 2L_1 \tag{2.4}$$

$$Bq = L_1 q \tag{2.5}$$

$$B = \left(\begin{array}{c|c} 0 & \xi' \\ \hline \xi & Tr(V+V')I-(V+V') \end{array}\right) \tag{2.6}$$

$$\xi' = \left(\begin{array}{c|c|c} V_{2,3}-V_{3,2} & V_{3,1}-V_{1,3} & V_{1,2}-V_{2,1} \end{array}\right) \tag{2.7}$$

Remark: equation 2.5 can be rewritten $(JBJ)(-Jq) = L_1(-Jq)$, where the 4-by-4 matrix $J = \begin{pmatrix} -1 & 0 \\ 0 & I \end{pmatrix}$, thus the eigenvalues solutions of equation 2.5 are the same for $P$ and $P'$.

# 3 The chiral index of the disphenoid

The coordinates of the disphenoid vertices are parametrized according to [21]. Let $a \geq b \geq c$ be non negative reals, and $\Delta = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix}$, then $X = Y\Delta$, where $Y$ contains the canonical coordinates of the regular tetrahedron

$$Y' = \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

The triangle squared sidelengths are $\alpha^2 = 4(b^2+c^2)$, $\beta^2 = 4(a^2+c^2)$, $\gamma^2 = 4(a^2+b^2)$. They unambiguously define the shape of the disphenoid.

**Theorem 1** (Main Theorem)**.** *The chiral index of the disphenoid is*

$$\chi = \frac{3}{2(a^2+b^2+c^2)} Min\{2c^2; (a-b)^2; (b-c)^2\}$$

*It is associated to at least one symmetric permutation, i.e., there is at least one symmetric permutation matrix solving eq. 2.1 when the optimal rotation is given in eqns. 2.4-2.7.*

*Proof.* $V = \Delta Y' P Y \Delta$ and there are 24 permutations, which are classified according to their cycles:

1. The identity permutation $P = I$

2. 6 symmetric permutations $P_{i,j}$, $1 \leq i < j \leq 4$, with 1 cycle of length 2 and 2 invariant elements. $P_{i,j}$ permutes rows $i$ and $j$ of $X$.

3. 3 symmetric permutations $P_{i,j;k,l}$, with 2 disjoint cycles of length 2 and no invariant element: $P_{i,j;k,l} = P_{i,j}P_{k,l} = P_{k,l}P_{i,j}$.

4. 4 circular permutations $P_{i,j,k}$ over 3 elements with 1 invariant element, plus their 4 transposed permutations. $P_{i,j,k}$ is such that rows $(j,k,i)$ of $X$ are respectively in rows $(i,j,k)$ of $P_{i,j,k}X$.

5. 3 circular permutations $P_{i,j,k,l}$ over 4 distincts elements, i.e. 1 cycle of length 4 and no invariant element, plus their 3 transposed permutations. $P_{i,j,k,l}$ is such that rows $(i,j,k,l)$ of $X$ are respectively in rows $(1,2,3,4)$ of $P_{i,j,k,l}X$.

For each class, we calculate the eigenvalues of $B$.

1. $P = I$, $\xi$ is null, $V = 4I$ is diagonal. The eigenvalues of $B$ are:

   $8(a^2+b^2)$, $8(a^2+c^2)$, $8(b^2+c^2)$, 0.
   Then, $T = 4(a^2+b^2+c^2)$, $L_1 = 8(a^2+b^2)$ and $D^2 = 16c^2$.

2. $P = P'$, $V = V'$, $\xi$ is null. Moreover, $V$ (and thus $B$) has only 4 non null elements: two identical diagonal values, and two identical ones out of the diagonal.

   For $P_{1,2}$ and $P_{3,4}$, they are $8a^2$ (diagonal) and $8bc$ (out of diagonal).

   For $P_{1,3}$ and $P_{2,4}$, they are $8b^2$ (diagonal) and $8ac$ (out of diagonal).

   For $P_{1,4}$ and $P_{2,3}$, they are $8c^2$ (diagonal) and $8ab$ (out of diagonal).
   For these three cases the four eigenvalues are respectively:

   $8(a^2+bc)$, $8(a^2-bc)$, 0, 0,

   $8(b^2+ac)$, $8(b^2-ac)$ (may be negative), 0, 0,

   $8(c^2+ab)$, 0, 0, $8(c^2-ab)$.
   The respective values of $D^2$ in these three cases are $8(a-b)^2$, $8(a-c)^2$, $8(b-c)^2$.

3. $P = P'$, $V = V'$, $\xi$ is null. $V$ is diagonal. The four tuples of eigenvalues of $B$ associated to $P_{1,2;3,4}$, $P_{1,3;2,4}$, $P_{1,4;2,3}$, are respectively

   $8(a^2-c^2)$, $8(a^2-b^2)$, 0, $8(-b^2-c^2)$,

   $8(b^2-c^2)$, 0, $8(-a^2+b^2)$, $8(-a^2-c^2)$,

   0, $8(-b^2+c^2)$, $8(-a^2+c^2)$, $8(-a^2-b^2)$.
   The values of $D^2$ in these three cases are all $16c^2$.

4. For $P_{3,4,2}$, $P_{3,4,1}$, $P_{2,4,1}$, $P_{2,3,1}$ the respective $V$ matrices are

$$4\begin{pmatrix} 0 & ab & 0 \\ 0 & 0 & bc \\ ac & 0 & 0 \end{pmatrix}, 4\begin{pmatrix} 0 & 0 & -ac \\ -ab & 0 & 0 \\ 0 & bc & 0 \end{pmatrix},$$

$$4\begin{pmatrix} 0 & -ab & 0 \\ 0 & 0 & -bc \\ ac & 0 & 0 \end{pmatrix}, 4\begin{pmatrix} 0 & 0 & -ac \\ ab & 0 & 0 \\ 0 & -bc & 0 \end{pmatrix}$$

We denote $\mathbf{1}' = (1, 1, 1, 1)'$. The eigenvectors of the first and the third $B$ matrices are proportional to $J\mathbf{1}$ and to the columns of $JX$. The eigenvectors of the second and the fourth $B$ matrices are proportional to $\mathbf{1}$ and to the columns of $X$. The four $B$ matrices have the same set of eigenvalues:

$4(ab + ac - bc)$, $4(ab - ac + bc)$, $4(-ab + ac + bc)$, $4(-ab - ac - bc)$.

$Tr(V) = 0$ and $D^2 = 8(a^2 + b^2 + c^2 - ab - ac + bc)$ in all cases.

5. For $P_{2,3,4,1}$, $P_{3,4,2,1}$, $P_{2,4,1,3}$ the respective $V$ matrices are

$$4\begin{pmatrix} 0 & 0 & -ac \\ 0 & -b^2 & 0 \\ ac & 0 & 0 \end{pmatrix}, 4\begin{pmatrix} -a^2 & 0 & 0 \\ 0 & 0 & -bc \\ 0 & bc & 0 \end{pmatrix}, 4\begin{pmatrix} 0 & -ab & 0 \\ ab & 0 & 0 \\ 0 & 0 & -c^2 \end{pmatrix}$$

The matrices $V + V'$ are diagonal with only one non null element. The vectors $\xi$ have only one non null element. The eigenvalues of the respective matrices $B$ are:

$8ac$, $-8b^2$, $-8b^2$, $-8ac$ (can be greater than $-8b^2$),

$8bc$, $-8bc$, $-8a^2$, $-8a^2$,

$8ab$, $-8c^2$, $-8c^2$, $-8ab$.

The values of $D^2$ in these three cases are respectively $8(a - c)^2$, $8(b - c)^2$, $8(a - b)^2$.

The smallest $D^2$ value in each class are:

$16c^2$, $Min\{8(a - b)^2; 8(b - c)^2\}$, $16c^2$, $8(a^2 + b^2 + c^2 - ab - ac + bc)$, $8(b - c)^2$. The value for class 4 cannot be smaller than the half sum of $8(a - b)^2$ and $8(a - c)^2$, which in turn cannot be smaller than the value in class 2, thus completing the proof. $\square$

**Corollary 2.** *The disphenoid is achiral if and only if, either the triangle is isosceles or it has a right angle.*

*Proof.* From Theorem (1), $\chi = 0$ either

(i) when $c = 0$, meaning that $\gamma^2 = \alpha^2 + \beta^2$, i.e. the triangle is right and the disphenoid is flat, or

(ii) when $a = b$, meaning that $\alpha = \beta$, i.e. the triangle is isosceles, or

(iii) when $b = c$, meaning that $\beta = \gamma$, i.e. the triangle is isosceles. $\square$

**Theorem 3.** *The most chiral disphenoids exist and have a chiral index* $\chi = 3(13 - 6\sqrt{2})/97$ *(*$\chi = 0.139630...$*). The faces are congruent to triangles whose squared sidelengths are in ratios* $1 : 3\text{-}\sqrt{2}/2 : 3$.

*Proof.* Setting $\hat{b} = b/a$ and $\hat{c} = c/a$, from Theorem (1), $\chi$ is a function of $(\hat{b}, \hat{c})$ which is the minimum over $E = \{0 < \hat{c} \leq \hat{b} \leq 1\}$ of the following three functions: $f_1(\hat{b}, \hat{c}) = 3c^2/(1+\hat{b}^2+\hat{c}^2)$, $f_2(\hat{b}, \hat{c}) = 3(1-\hat{b})^2/2(1+\hat{b}^2+\hat{c}^2)$, and $f_3(\hat{b}, \hat{c}) = 3(\hat{b}-\hat{c})^2/2(1+\hat{b}^2+\hat{c}^2)$. All partial derivatives of $f1$, $f2$, $f3$ are monotonic over $E$: $\partial f_1/\partial \hat{b} < 0$, $\partial f_1/\partial \hat{c} > 0$, $\partial f_2/\partial \hat{b} \leq 0$, $\partial f_2/\partial \hat{c} \leq 0$, $\partial f_3/\partial \hat{b} \geq 0$, $\partial f_3/\partial \hat{c} \leq 0$. The partial derivatives of $f_2$ are null iff $\hat{b} = 1$ and the ones of $f_3$ are null iff $\hat{b} = \hat{c}$. The boundaries for $f_1 = f_2$, $f_1 = f_3$ and $f_2 = f_3$, are respectively at $\hat{c} = (1-\hat{b})\sqrt{2}/2$, $\hat{c} = \hat{b}(\sqrt{2}-1)$ and $\hat{c} = (2\hat{b}-1)$. Then we deduce from the signs of the partial derivatives that $\chi$ is maximized at the intersection of these boundaries (see Figure 1), located at $\hat{b} = (3+\sqrt{2})/7$ and $\hat{c} = (2\sqrt{2}-1)/7$. In other words, the maximal $\chi$ is reached when the three quantities $2c^2$, $(a-b)^2$ and $(b-c)^2$ are equal. Then we get $b = (a+c)/2$, $\frac{a}{c} = 1+2\sqrt{2}$ and $\frac{b}{c} = 1+\sqrt{2}$. The maximal chiral index and the ratios of the sidelengths are deduced from these values. $\square$

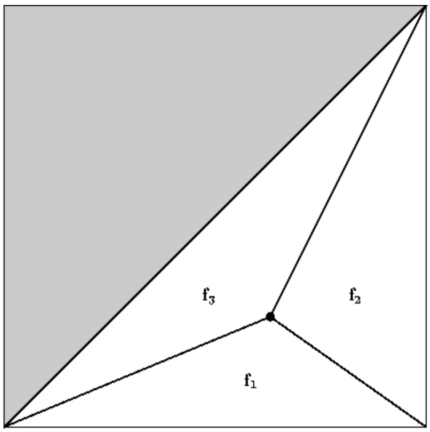


Figure 1: The areas where $f_1$, $f_2$ and $f_3$ are respectively retained to calculate the chiral index. Abscissas: $0 < \hat{b} \leq 1$, ordinates: $0 < \hat{c} \leq 1$.

Theorem 3 was also checked via generating more than $2 \cdot 10^9$ random disphenoids: the highest observed chiral index was lower than the maximal one, the difference being smaller than $10^{-5}$.

# 4 Conclusion

In this paper we insist that the four vertices of a tetrahedron are modeled by a finite discrete distribution rather than by a set of four points in the 3D space, despite that the geometric approach is used for solving analytically our optimization problem. It was shown in the past that modelers missed the following crucial point: the probabilistic model is better than the geometric one because it handles both geometry and mass and charges distributions, discrete or continuous [9, 10]. However, the full mathematical description of this probabilistic model is already published and it is outside the scope of this paper.

Few attempts to exhibit maximal chirality sets or maximally asymmetric distributions appeared in the literaure [1]. Moreover, despite that the tetrahedron is a 3D shape basic for chemistry and stereoisomerism, no analytical result was available about maximally asymmetric tetrahedra, and it is why this paper focussed on isosceles tetrahedra. A maximally chiral triangle based on the chirality measure as used in this paper was found in [7]. In addition to a geometric property that it shares with the most direct dissymetric triangle [11], we observe from the coordinates of its vertices $(-\sqrt{2}\,|\,0)$, $((\sqrt{2}+k)/2\,|\,k/2)$, $((\sqrt{2}-k)/2\,|\,-k/2)$, where $K=k^2$ is root of $K^2-24K+9=0$, that the acute angles side-median are $\theta_1=\pi/4$, $\theta_2=\pi/4$, and $\cos 2\theta_3=3/5$. It seems the scalene triangle of the most chiral disphenoid does not offer such properties. These two triangles are displayed in Figure 2.

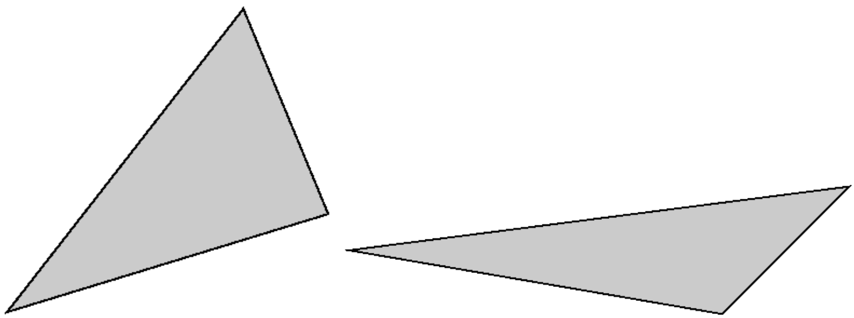

Figure 2: The triangular face of the maximally chiral disphenoid (on the left), and the maximally chiral triangle (on the right), from ref. [7].

Some open problems are: find the most chiral $d$-simplex, $d \geq 3$, and find the upper bound of the chiral index for any set of $n$ points in dimension $d \geq 2$ [22]. This latter bound is known to lie in the interval $[1/2; 1]$ [23]. A narrower interval, $[1 - 1/\pi; 1 - 1/2\pi]$, is known in the planar case [13]. Despite that these problems seem to be non trivial ones, at least the case of the tetrahedron should be investigated because the geometry of the tetrahedron still raises interest, not only in the recent mathematical literature [24–26], but also in the very recent chemistry literature [27]. Random tetrahedra were generated, indicating that the most chiral tetrahedron should have a chiral index greater than 0.194.

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