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THE α, β, γ-HULL AND THE T-HULL OF A POINT SET: TOOLS FOR THE ANALYSIS OF SHAPES AND RELATIVE ORIENTATIONS OF OBJECTS IN 3D-SPACE

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Abstract

Two new generalizations of the concept of convexity are introduced, suitable for detailed shape characterizations of point sets. The generalizations are also applicable for direct shape comparisons between point sets and for discrimination based on relative orientations. The methods of α, β, γ-hull and T-hull are applicable for the description of molecular shapes in external electromagnetic fields or within enzyme cavities. These methods are suggested for the study of the similarity of shapes of interacting molecules, and for the analysis of certain biochemical interactions.

1. Introduction

The analysis of the shape of a continuum or a discrete set of points in two, three or higher dimensions is of fundamental importance in many branches of mathematics and the natural sciences. Convexity is a natural concept which is involved in various ways with such analyses, often leading to polyhedral models [1,2]. Here, we shall present two new generalizations of convexity that are suitable for more detailed shape characterizations of point sets than ordinary convexity. The new approach is also applicable for the study of certain embedding properties of the point set within a space, that is, for the study of shape properties compared to some external references: to reference directions and to the shapes of reference objects.

Our approach is motivated by prospective applications to a family of important problems of molecular physics and chemistry. One of these problems is the description of molecular shapes and similarity in external electromagnetic fields; related problems arise in the study of the similarity of shapes of interacting molecules, and in the analysis of biochemical interactions within enzyme cavities [3–7]. For simplicity, we shall focus our discussion on three-dimensional problems, although it is clear that all the new concepts and methods have straightforward generalizations to arbitrary finite dimensions.

An earlier approach has been based on the concepts of global and local relative convexity and oriented relative convexity [8]. In a Euclidean space E^n, a point set

S is convex in the ordinary sense if and only if for any two points x and y of S the entire straight line segment interconnecting x and y also falls within S. Global relative convexity has been defined [8] by replacing straight line segments with curved line segments of some specified curvature b; we say that a set S fulfilling the modified condition is convex relative to curvature b. Local convexity has been defined along the boundary surfaces of continuous point sets, where one tests the local canonical curvatures at each point of the boundary surface against a tangent plane, or against a tangent sphere of some specified curvature b. Informally, a region of a twice differentiable boundary surface is locally convex relative to the tangent object T if at each point of the region the surface of object T osculates to the boundary surface from the "outside". The region is locally concave relative to tangent object T if the surface of T osculates to the boundary surface region from the inside, and the region is locally of the saddle type if the surface of T intersects the boundary surface at points different from the point of tangent p within any small open neighborhood of p. A zero curvature value b corresponds to a tangent plane, a positive b value corresponds to a tangent sphere of radius $1/b$ placed on the interior side of the boundary surface, and a negative b value corresponds to a tangent sphere of radius $-1/b$ placed on the exterior side of the boundary surface.

If the tangent sphere is replaced by a tangent ellipsoid, oriented in some specified way, then one obtains the concept of oriented local relative convexity [8]. If the axes of the ellipsoid are aligned with some external directions, e.g. with those of an external electromagnetic field, or with characteristic features of enzyme cavities, or with the axes of inertia of the same or another interacting molecule, then the shape characterization based on oriented relative local convexity conveys both shape and physically important embedding and orientation properties of the molecule. By scaling both the object and the ellipsoid along the directions of the ellipsoid axes so that the ellipsoid is converted into a sphere, the oriented local relative convexity problem of the original object can be converted into a non-oriented, local relative convexity problem of the scaled object. The inverse scaling applied to this latter problem allows one to obtain the oriented case relative to an ellipsoid by actually carrying out the analysis for the simpler, spherical, non-oriented case.

Further generalization has been introduced by replacing the tangent ellipsoid by a more general test surface T, for example, by a contour surface of another, oriented molecule [8]; in this case one obtains an oriented, local convexity classification of surface domains of the first molecule relative to the oriented test surface T. By contrast to ellipsoids, for a general test surface T no linear scaling transformation can in general convert the oriented relative convexity problem into a non-oriented relative convexity problem of a scaled object.

The new concepts and method proposed in this work are based on a different approach, having roots in the concept of α-hull, introduced by Edelsbrunner, Kirkpatrick, and Seidel [9]. The α-hull is a natural generalization of a common definition of the convex hull of a point set in the plane. An illustration of the α-hull concept in given in fig. 1.

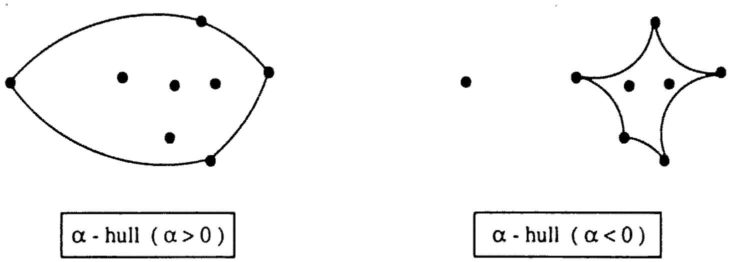

Fig. 1. An illustration of the concept of the α-hull of a point set S, for both positive and negative α values. The *α-hull* $\langle S \rangle_\alpha$ of S is the intersection of all closed generalized discs of radius $1/\alpha$ which contain point set S. Note that the isolated point on the right-hand side is contained in the α-hull of the point set for the given negative α value.

For a set S of n points of the plane, the *convex hull* of S, denoted by $\langle S \rangle$, can be defined as the intersection of all closed halfplanes which contain S. The α-hull of S is obtained by replacing the halfplanes with discs.

Following ref. [9], one may define a *generalized disc of radius* $1/\alpha$ as a disc of radius $1/\alpha$ if $\alpha > 0$, the complement of a disc of radius $-1/\alpha$ if $\alpha < 0$, and a half-plane if $\alpha = 0$.

The α-hull $\langle S \rangle_\alpha$ of S is the intersection of all closed generalized discs of radius $1/\alpha$ which contain S. Clearly, if $\alpha = 0$, then the α-hull $\langle S \rangle_\alpha$ of S becomes the ordinary convex hull $\langle S \rangle$ of S. If one adopts the convention that the empty intersection is the entire space, then for any set S the α-hull exists for any α value. For a sufficiently small value of α, the α-hull is the finite point set S itself.

The following, natural generalization to three-dimensional finite point sets has been briefly outlined in [9]. Here, we give a complete definition.

A *generalized ball of radius* $1/\alpha$ is a ball of radius $1/\alpha$ if $\alpha > 0$, the complement of a ball of radius $-1/\alpha$ if $\alpha < 0$, and a half space if $\alpha = 0$.

If S is a finite point set in a 3D Euclidean space, then the *α-hull* $\langle S \rangle_\alpha$ of S is the intersection of all closed generalized balls of radius $1/\alpha$ which contain S.

The definition of α-hull can be generalized to continua; however, if one considers a continuum S of points instead of a finite point set, then one must deal with the intersection of infinitely many closed balls.

2. The α, β, γ-hull of a point set

One of our goals is to introduce orientational constraints in order to describe some of the embedding properties of a point set S with respect to external references, for example, with respect to three coordinate axes. For this purpose, we shall consider oriented, solid ellipsoids of half axes of lengths $1/\alpha$, $1/\beta$, and $1/\gamma$, which may be restricted to be aligned with three, mutually orthogonal directions of

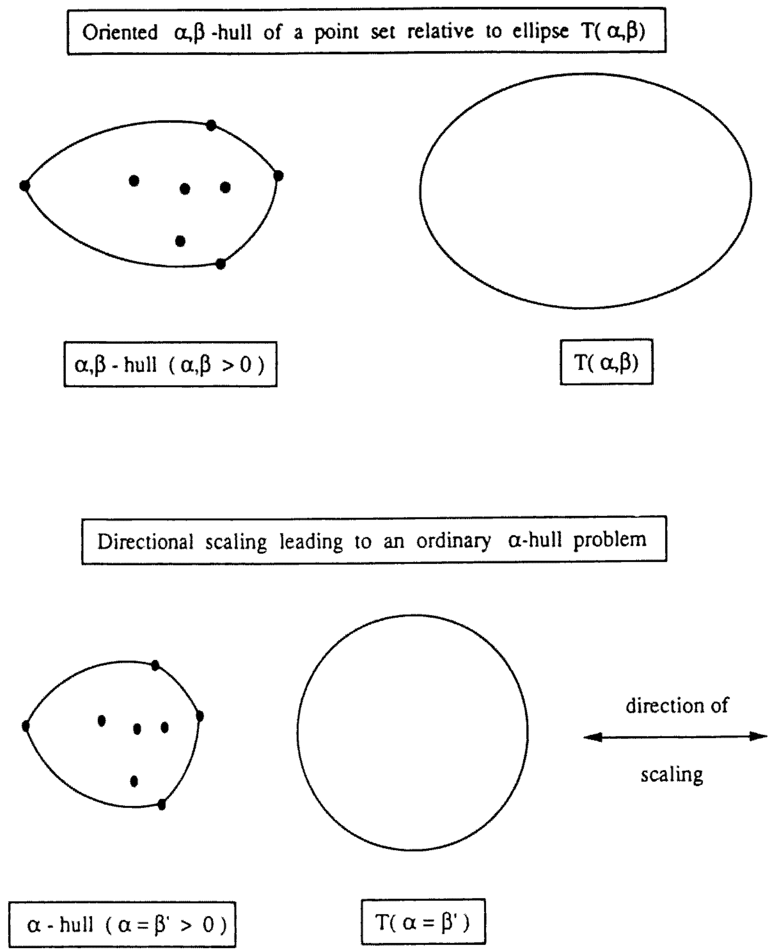

Fig. 2. A two-dimensional illustration of the concept of oriented α, β, γ-hull (actually, an oriented α, β-hull) of a point set S. The oriented α, β, γ-hull $\langle S \rangle_{\alpha, \beta, \gamma, o}$ of a point set S is the intersection of all closed generalized ellipsoids $E(\alpha, \beta, \gamma)$ of orientation o which contain S. A linear scaling can be used to convert the oriented α, β, γ-hull problem into a simple α-hull problem.

the 3D Euclidean space. The concept of the α, β, γ-hull of a point set S is illustrated in fig. 2.

A *generalized solid ellipsoid* $E(\alpha, \beta, \gamma)$ of half axes of lengths $1/\alpha$, $1/\beta$, and $1/\gamma$ is

(i) the solid ellipsoid of half axes of lengths $1/\alpha$, $1/\beta$, and $1/\gamma$ if $\alpha > 0$, $\beta > 0$, and $\gamma > 0$;

(ii) the complement of the solid ellipsoid of half axes of lengths $1/\alpha$, $1/\beta$, and $1/\gamma$ if $\alpha < 0$, $\beta < 0$, and $\gamma < 0$;

(iii) a half space if $\alpha = 0$, $\beta = 0$, and $\gamma = 0$.

Note that here we are concerned only with those second-order surfaces which give rise to bounded regions of the three-dimensional space. A more general scheme, involving all second-order surfaces, and which requires a modification of the terminology, is described in the appendix.

First we consider the case *without orientation constraints.*

The *α,β,γ-hull* $\langle S\rangle_{\alpha,\beta,\gamma}$ of a point set S is the intersection of all closed generalized ellipsoids $E(\alpha,\beta,\gamma)$ which contain S.

The *orientation constraints* can be introduced by considering ellipsoids $E(\alpha,\beta,\gamma)$ of a fixed orientation of their principal axes. The ellipsoids may undergo arbitrary translations but no rotations when testing the containment of set S within the ellipsoids.

The *oriented α,β,γ-hull* $\langle S\rangle_{\alpha,\beta,\gamma,o}$ of a point set S is the intersection of all closed generalized ellipsoids $E(\alpha,\beta,\gamma)$ of orientation o which contain S. The orientation $o = o(a,b,c)$ is specified by the a, b, c angles between the α, β, and γ axes of the ellipsoids $E(\alpha,\beta,\gamma)$ and the x, y, and z Cartesian axes, respectively, of a reference coordinate system.

As a consequence of the restrictions to cases (i), (ii), and (iii), no generalized solid ellipsoid exists for some sign combinations of α, β, and γ. Furthermore, for a given allowed combination of α, β, and γ values (and if specified, an orientation), a given point set S may have no α,β,γ-hull or oriented α,β,γ-hull. However, by considering all second-order surfaces, including those which give rise to no bounded regions of the three-dimensional space, the more general scheme described in the appendix is applicable to all sign combinations of α, β, and γ.

Note that, similarly to the case of oriented local convexity relative to ellipsoids, one may scale both the object and the ellipsoid along the directions of the ellipsoid axes by some transformation t so that the ellipsoid is converted into a sphere of some radius $1/\alpha'$. If one denotes the ordinary α'-hull of the scaled point set tS by $\langle tS\rangle_{\alpha'}$, then the oriented α,β,γ-hull $\langle S\rangle_{\alpha,\beta,\gamma,o}$ of the original point set S can be obtained by the inverse scaling t^{-1} of the α'-hull of the scaled point set tS,

$$\langle S\rangle_{\alpha,\beta,\gamma,o} = t^{-1}\langle tS\rangle_{\alpha'}. \tag{1}$$

That is, the oriented α,β,γ-hull problem of the original point set S is converted into an ordinary α-hull problem of a scaled point set tS.

3. The T-hull of a point set

One may further generalize the concept of convexity by replacing ellipsoids with more general test objects, denoted by T. The concept of the T-hull of a point set is illustrated by two-dimensional examples in fig. 3.

Consider a closed, but otherwise arbitrary three-dimensional set T. For the sake of simplicity in the notation, we shall write T' for the closure of the complement of T, that is, $T' = \mathrm{clos}(E^3 \setminus T)$. Then the set T' can also be chosen as a test object.

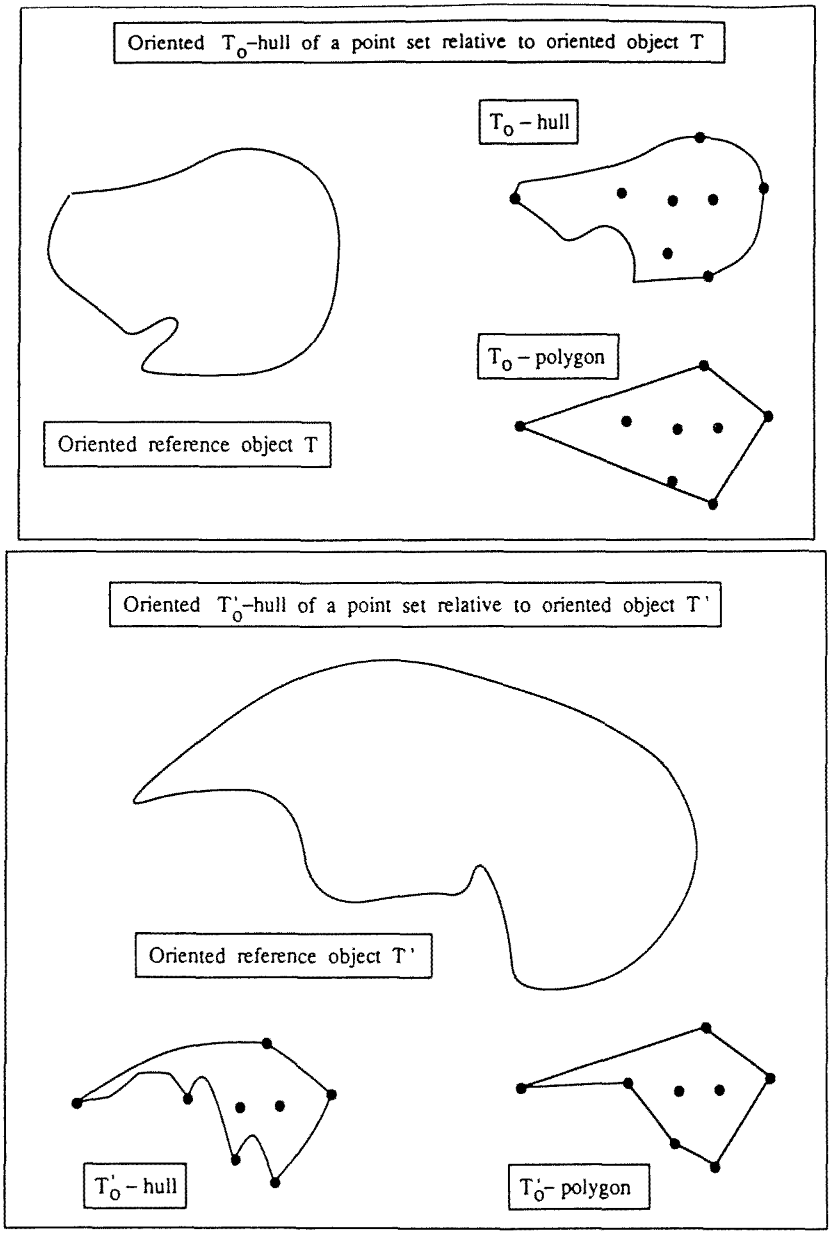

Fig. 3. Two-dimensional examples for oriented T-hull $\langle S\rangle_{T,o}$ and the corresponding T_o-polyhedra $P(S, T_o)$ (actually, T_o-polygons $P(S, T_o)$) of a point set S. The two choices for reference object lead to different T_o-hulls and to different T_o-polygons. In the second example, neither the T_o-hull nor the T_o-polygon is a convex set.

A set obtained by translation and rotation of T will be called a *version* of T. If T is subject to orientation constraints, then a version of T is a set obtained from T by translation.

First we shall test the containment of set S in all possible rotated and translated versions of T.

The *T-hull* $\langle S\rangle_T$ of a point set S is the intersection of all rotated and translated versions of T which contain S.

Consider now a set T of some fixed orientation with respect to some Cartesian axes of the three-dimensional Euclidean space.

The *oriented T-hull* $\langle S\rangle_{T,o}$ of a point set S is the intersection of all translated versions of the oriented set T which contain S.

Note that a T-hull $\langle S\rangle_T$ or an oriented T-hull $\langle S\rangle_{T,o}$ of a point set S is not necessarily connected, even for a connected reference set T. The numbers $k(\langle S\rangle_T)$ and $k(\langle S\rangle_{T,o})$ of maximum connected components of $\langle S\rangle_T$ and $\langle S\rangle_{T,o}$, respectively, are providing information on the shape compatibility of sets S and T.

An ellipsoid is achiral; hence, by allowing reflection of an ellipsoid in addition to translation and rotation in the three-dimensional space, one does not obtain a different condition for the α,β,γ-hull $\langle S\rangle_{\alpha,\beta,\gamma}$ of a point set S. This is no longer necessarily the case for a more general test object T, which may be chiral; hence, by allowing reflection, in addition to rotation and translation, a new convexity concept is obtained:

The T,T^*-hull $\langle S\rangle_{T,T^*}$ of a point set S is the intersection of all rotated, translated, and reflected versions of T which contain S.

Evidently, the following relations hold for the set S, its T,T^*-hull, T-hull, and oriented T-hull:

$$S \subset \langle S\rangle_{T,T^*} \subset \langle S\rangle_T \subset \langle S\rangle_{T,o}. \tag{2}$$

4. The T-front of a point set S

In the following definitions, we shall consider the most general reference objects, denoted by T. It is understood that in the special (and for practical purposes, often most important) case of ellipsoids, the symbol T is replaced with the corresponding symbol $E(\alpha,\beta,\gamma)$ of ellipsoids in all the notations of the forthcoming definitions.

A point p of S is a *T-extreme point in S* if there exists a version of set T such that p lies on its boundary and it contains S. Such a point p is also called a *T-frontal point of S*.

A point p of S is a *T_o-extreme point in S* if there exists a version of the oriented set T_o of a specified orientation o such that p lies on its boundary and it contains S. Such a point p is also called a *T_o-frontal point of S*.

If for three T-extreme points (T_o-extreme points) p,p', and p'' there exists a version of set T (oriented set T_o of a specified orientation o) which has all three points on its boundary and which contains set S, then p, p', and p'' are said to form a *T-frontal triple of S* (a *T_o-frontal triple of S*, respectively).

Note that for a given mutual arrangement of S and T (T_o) there may exist more than three frontal points, and in the case of a continuum set S, there may exist even a continuum of frontal points which fall on the boundary of T (T_o, respectively). However, the case of three points is the most common.

Consider all arrangements of versions of set T (oriented set T_o of a specified orientation o) with respect to set S. The set of all frontal points form the *T-front of S* (the *T_o-front of S*, respectively).

The T-front of S (T_o-front of S) represents the essential shape information (oriented shape information) on set S, as measured by test object T (T_o, respectively). In the typical case, the T-front (T_o-front) is a finite set of at most two-dimensional objects; hence, the shape characterization of a three-dimensional object S is given in terms of a finite set of lower-dimensional objects, the T-front of S (T_o-front of S, respectively).

Below we shall focus on a special case, where the T-front (T_o-front) of S is a finite set of isolated points. This is certainly the case if S itself is a finite set of points, but this is also a common case for some pairs of continua S and T, as illustrated in fig. 4.

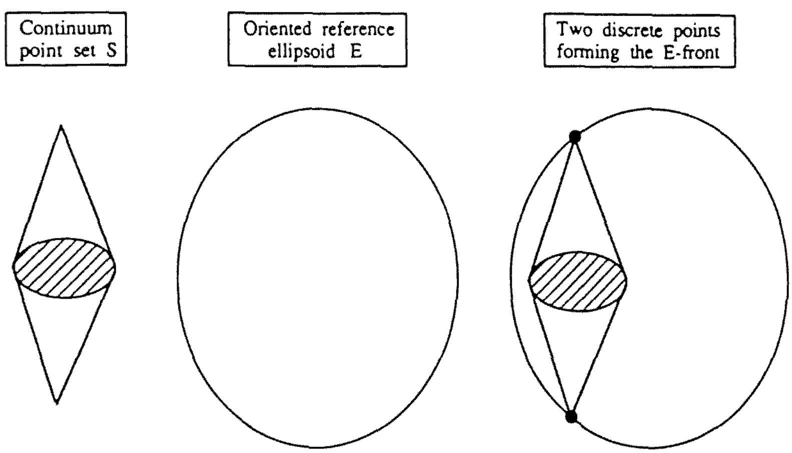

Fig. 4. A continuum point set S with a T-front containing only a finite number of points.

5. Discrete T-fronts and polyhedral T-shapes of point sets S

Let us assume that the T-front (T_o-front) of S is a finite set and no four frontal points of S fall on any one of the sets T (T_o). Then each T-frontal triple (T_o-frontal triple) p, p', and p'' of S defines a triangle, called a *T-frontal triangle* (*T_o-frontal*

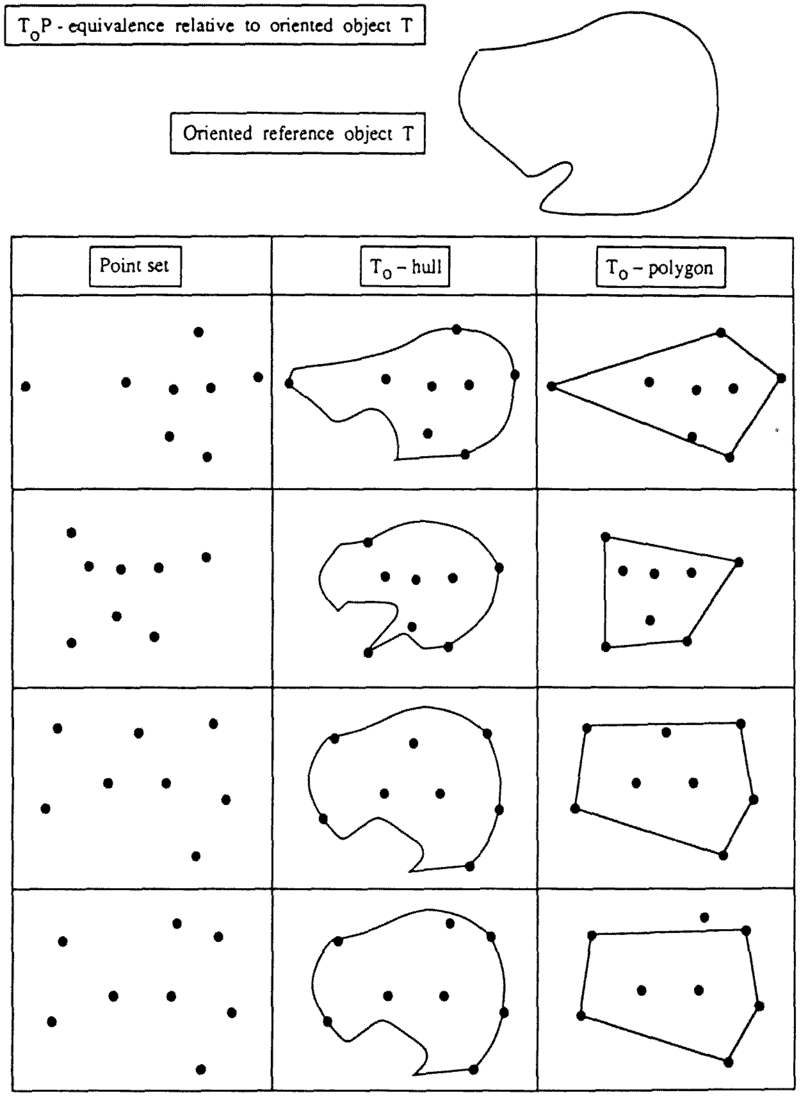

Fig. 5. Two-dimensional illustrations of the concept of T_oP-similarity of point sets. Whereas the first two point sets are T_oP-similar, having quadrilaterals as T_o-polygons, the T_o-polygons of the third and fourth point sets are pentagons; hence, these point sets belong to a different T_oP-shape class. Also note that the ordinary convex hull of the last point set is actually a hexagon, and as illustrated by this example, the T_o-polygon of a set S does not necessarily contain all points of S.

triangle, respectively). If these triangles fulfill certain conditions, then they may be used to construct a polyhedral representation of the shape of set S, called a frontal polyhedron. For simplicity, we shall use the term "frontal polyhedron" in a generalized sense: in some cases, a frontal polyhedron may be a collection of several disjoint polyhedra.

We say that set S has a *T-frontal polyhedron* (*T_o-frontal polyhedron*) if there exists a family of T-frontal triangles (T_o-frontal triangles) with the following properties:

(i) this family of triangles forms a finite number of continuous, closed surfaces which partition the three-dimensional Euclidean space into subsets;

(ii) it is possible to assign the labels i (interior) and e (exterior) to these subsets so that no two subsets separated by one surface have the same label, and each point of S falls either within or on the boundary of a subset labelled by i.

The T-frontal polyhedron (T_o-frontal polyhedron) is not necessarily unique. A T-frontal polyhedron (T_o-frontal polyhedron) of minimum volume is called a *T-polyhedron $P(S,T)$* of S (*T_o-polyhedron $P(S,T_o)$* of S, respectively). The concept of the T-polyhedron of a point set is illustrated by two-dimensional examples in fig. 3, where 3D polyhedra are replaced by polygons.

Two sets S_1 and S_2 are said to be *TP-similar* (*T_oP-similar*) if both have T-polyhedra (T_o-polyhedra) and if the polyhedra $P(S_1, T)$ and $P(S_2, T)$ ($P(S_1, T_o)$ and $P(S_2, T_o)$, respectively) are of the same combinatorial type. If a set S has no T-polyhedron $P(S, T)$ (T_o-polyhedron $P(S, T_o)$), then we say that S is not TP-representable (not T_oP-representable, respectively). If either one of sets S_1 and S_2 is not TP-representable (not T_oP-representable), then we say that these sets are not TP-comparable (not T_oP-comparable, respectively). In fig. 5, the concept of T_oP-similarity of point sets is illustrated by two-dimensional examples.

Clearly, TP-similarity (T_oP-similarity) is an equivalence relation. The corresponding equivalence classes are defined by polyhedral shape representations of set S with respect to the test object T (oriented test object T_o); hence, we may refer to them as the TP-shape classes (T_oP-shape classes, respectively). By regarding the non-TP-representable (non-T_oP-representable) sets as belonging to a special equivalence class, the above similarity classification is applicable to all point sets S. For a given set S, non-TP-representability (non-T_oP-representability) is simply an indication that the test object T (oriented test object T_o) is not a suitable criterion for a simple, polyhedral description of the shape of S.

6. Comments on extensions and applications

Note that, similarly to the simple α-hull concept, all the new convexity concepts introduced in this study refer not only to shape properties but also to size properties of a general point set S. By introducing relative size measures, for example, the relative volumes of a continuum S and a test ellipsoid $E(\alpha, \beta, \gamma)$, the shape and size properties of S can be treated separately.

Simple polyhedral shape representations are advantageous in computer applications, for example, in computer-based molecular modeling and similarity analysis. The present method of polyhedral shape representation is applicable for arbitrary molecular surfaces, such as continua of isodensity contours, fused sphere Van der Waals surfaces, or simple dot representations, yet the freedom in the choice of the test object T (or T_o) allows for the incorporation of additional physical information (e.g. on the shape of an enzyme cavity), as well as orientation constraints.

Appendix

Ellipsoids are only one class of quadratic surfaces which are of special importance in shape analysis. What makes ellipsoids special in this context is their boundedness, a property no longer enjoyed by bodies defined by hyperboloids, cylinders or planes. However, in some applications these latter, second-order surfaces are more relevant, and below we shall present a more general discussion of generalized convexity conditions based on them. In principle, all these cases are covered by the general concepts of *T-hull* $\langle S \rangle_T$ and the *oriented T-hull* $\langle S \rangle_{T,o}$ of a point set S. However, the special scaling properties of second-order surfaces warrant a more detailed exposition.

Take the canonical form of a general second-order surface in three-dimensions as

$$Ax^2 + By^2 + Cz^2 + D = 0, \tag{3}$$

where the usual convention $A > 0$ is followed. Then, the signs of constants B, C, and D define the type of the second-order surface; for example, $B > 0$, $C > 0$, $D < 0$ corresponds to an ellipsoid, $B > 0$, $C < 0$, $D = 0$ to an elliptic cone, $B > 0$, $C = 0$, $D < 0$ to an elliptic cylinder, and $B > 0$, $C < 0$ and $D < 0$ to a single sheet hyperboloid. Some sign choices correspond to degenerate and/or imaginary objects.

We are interested in closed, solid bodies with boundaries defined by second-order surfaces. We shall use the following convention: the defining equation for the second-order surface providing the boundary for a *generalized second-order body* $B(A,B,C,D)$ will be written as

$$|A| x^2 + By^2 + Cz^2 + D = 0, \tag{4}$$

where A may take both positive and negative values. The second-order surface partitions the three-dimensional space into two or three subsets. If A is positive, then we regard the subset(s) containing the focal points (if any) of the surface as the solid body (or pair of bodies). If A is negative, then we regard the subset(s) not containing the focal points as the solid object(s). For example, in the case of the double-sheet hyperboloid, characterized by $B < 0$, $C < 0$, $D < 0$, a positive value $A > 0$ corresponds to regarding the pair of (ordinary) convex regions obtained as the solid object, whereas a negative value $A < 0$ corresponds to regarding the remaining (simply connected) part of the three-dimensional space as the solid object. For an ellipsoid ($B > 0$, $C > 0$, $D < 0$), a positive A value represents the choice of the bounded, closed interior as the solid body, whereas a negative A value corresponds to taking the unbound remainder of the space as the solid object.

With these conventions, one may define generalized second-order convexity as follows:

The *A,B,C,D-hull* $\langle S \rangle_{A,B,C,D}$ of a point set S is the intersection of all second-order bodies $B(A,B,C,D)$ which contain S.

By analogy with the case of ellipsoids, one may consider orientation constraints:

The *oriented A,B,C,D-hull* $\langle S \rangle_{A,B,C,C,o}$ of a point set S is the intersection of all oriented second-order bodies $B(A,B,C,D)_o$ which contain S, where o refers to an orientation specified with respect to the Cartesian coordinate axes of the three-dimensional Euclidean space.

The orientation $o = o(a,b,c)$ is specified by the a, b, c angles between the axes of the second-order bodies $B(A,B,C,D)_o$ and the x, y, and z Cartesian axes, respectively, of a reference coordinate system.

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