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The T-hull approach to transformations of discrete point sets to continua and shape transformations between discontinuous objects using alpha-hulls

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In molecular shape analysis and in the analysis of various molecular functions used in modeling chemical reactions and biochemical interactions, it is often useful to generate transformations that interconvert various molecular models into one another. Some of these models are continua whereas some others have disconnected parts or even separated discrete points. The interconversion between such very different descriptors is a nontrivial task. The associated mathematical and computational problems are even more complex if relations and possible interconversions between models describing *different* molecules are considered. In this contribution two conceptually simple techniques are described. These approaches are based on alpha-hulls and T-hulls, leading to shape transformations between discontinuous objects and transformations between discrete point sets and continua. Applications of these methods are not restricted to chemistry, however, some of the special features discussed are designed for molecular modeling applications.

1. Introduction

Transformations of shapes are often perceived in the context of comparisons to various "standard" shapes, for example, with reference to cubes or spheres. In some instances, more complex reference shapes are used, for example, in comparing faces and general appearances in a police lineup, the reference is either to a "standard" human form, or to the shape of a description of a suspect. Within the chemical context, reference shapes may involve the shape of an enzyme cavity or the catalytic cavity of a zeolite.

In this contribution a rather general technique will be described that is applicable within the context of the simple reference shape of spheres of various radii, and also with respect to arbitrary reference shapes defined by some closed surface, such as a molecular isodensity surface, MIDCO. Below a short review of the elementary tools used, alpha-hulls and T-hulls, is given, followed in the next sections by the description of the actual shape transforms.

1.1. Alpha-hulls

Alpha-hulls, as generalizations of the convex hull, were defined by Edelsbrunner et al. [1], with respect to a variety of two-dimensional problems. The introduction of two-dimensional α-hulls was based on the concept of *generalized disc* $D(1/\alpha)$ *of radius* $1/\alpha$. Generalized disk $D(1/\alpha)$ was defined as

$$D\left(\frac{1}{\alpha}\right) = \begin{cases} \text{a disc of radius } \dfrac{1}{\alpha} & \text{if } \alpha > 0, \\ \text{a halfplane} & \text{if } \alpha = 0, \\ \text{the complement of a disc of radius } -\dfrac{1}{\alpha} & \text{if } \alpha < 0. \end{cases} \tag{1}$$

Based on this definition, the *α-hull* $\langle S\rangle_\alpha$ of a point set S in the plane was defined as the intersection of all closed generalized discs $D(1/\alpha)$ of radius $1/\alpha$ which contain S.

As described in detail in [2,3], the chemically more relevant three-dimensional case is entirely analogous. A *generalized ball* $B(1/\alpha)$ *of radius* $1/\alpha$ was defined as

$$B\left(\frac{1}{\alpha}\right) = \begin{cases} \text{a ball of radius } \dfrac{1}{\alpha} & \text{if } \alpha > 0, \\ \text{a halfspace} & \text{if } \alpha = 0, \\ \text{the complement of a ball of radius } -\dfrac{1}{\alpha} & \text{if } \alpha < 0. \end{cases} \tag{2}$$

Based on this definition, the *α-hull* $\langle S\rangle_\alpha$ of a point set S in a 3D Euclidean space was defined as the intersection of all closed generalized balls $B(1/\alpha)$ of radius $1/\alpha$ which contain S.

If $\alpha = 0$, then the *α-hull* $\langle S\rangle_\alpha$ becomes the ordinary convex hull of the object S, whereas in general, the α-hull $\langle S\rangle_\alpha$ of S is a "curvature-biased" shape representation of the object S, with reference to the specific curvature value α. The concept of α-hull is applicable to both discrete point sets and to continua, and to any combination of these; for example, to a finite point set S such as the collection of nuclei of a molecule, taken as points in a specific configuration. In the latter case, for any sufficiently small negative value of curvature α, the α-hull $\langle S\rangle_\alpha$ of S becomes the finite point set S itself. Note that, according to the usual convention, the empty intersection is regarded as the entire space. This fact ensures that the α-hull of any set S exists for any value of α.

1.2. T-hulls

In the case of α-hulls, the shapes of objects S are characterized with reference to various spherical shapes of various radii. However, a further generalization of the convex hull is possible by replacing spheres with arbitrary shapes. This idea was the basis for the introduction of T-hulls.

The concept of T-hull, applicable to both discrete point sets and continua, was introduced [2] as a generalization of the convex hull with respect to a (finite, bounded) reference object T.

According to the original definition [2], for a given reference object T the ordinary T-hull $\langle S\rangle_T$ of an object S is the intersection of all rotated and translated versions of T which contain S. Several fundamental properties of T-hulls were described in [2–4].

If there exists no version T_{v} of T that contains S then the T-hull of S is the empty intersection, interpreted as the full space. This implies that the T-hull $\langle S\rangle_T$ exists for every set S and for every reference object T. Of course, the T-hull of a set S depends on the shapes of both objects S and T.

In the context of molecular modeling and molecular shape analysis, it is often useful to characterize the shape of the electron density cloud of a molecule A in terms of the electron density of another molecule B. Such a "B-biased" shape representation and shape characterization of the molecular electronic density of molecule A is obtained in terms of its T-hull defined by an electronic density contour of another molecule B, providing also a direct shape comparison of molecules A and B.

In the context of modeling molecular interactions, T-hulls have been proposed for modeling *solvent contact surfaces* as tools in the shape analysis of solvent–solute interactions [4]. In such cases, the solvent molecules are often much smaller than the solute molecules, and it is useful to consider the complements of the solvent molecules when generating T-hulls. In these applications, the notation $-T$ is used for the closure of the complement of an object T:

$$-T = \mathrm{clos}\big(E^3\backslash T\big). \tag{3}$$

Specifically, the T-hull $\langle S\rangle_T$ of a solute electron density level set S is generated with respect to a reference object T where $-T$ is taken as an electron density level set of the solvent molecule.

Assume that objects $-T$ and $-T'$ represent some electron density level sets of two different solvent molecules. Then, the T-hulls and T'-hulls of various objects, such as $\langle S\rangle_T$ and $\langle S\rangle_{T'}$ of the solute molecule S, are the intersections of all those versions of the complements $-(-T) = T$ and $-(-T') = T'$ of the solvent molecules $-T$ and $-T'$ which contain the solute molecule S. Evidently, each version of T that contains S corresponds to an arrangement of solvent molecule $-T$ and solute molecule S where the solvent $-T$ and solute S do not overlap. The intersections of all these arrangements generate the corresponding T-hull $\langle S\rangle_T$. Specifically, the T'-hull $\langle T\rangle_{T'}$ of $-(-T) = T$ is the intersection of all those versions of the complement $-(-T') = T'$ of the second solvent molecule $-T'$ which contain the complement $-(-T) = T$ of the first solvent molecule $-T$. This provides a relation between two different solvent contact surfaces.

If T and T' are two reference objects satisfying the relation

$$\langle T\rangle_{T'} = T, \tag{4}$$

then for the respective T-hull and T'-hull of any object S the relation

$$\langle S\rangle_T \supset \langle S\rangle_{T'} \tag{5}$$

must hold.

2. Alpha-hull shape transforms

For any bounded set A exists a largest α' value such that the α'-hull $\langle A\rangle_{\alpha'}$ is still A:

$$\alpha' = \max\{\alpha\colon\ \langle A\rangle_\alpha = A\}. \tag{6}$$

This α' value may be negative, and the set A may be disconnected, even a discrete point set.

Define α'' as the the reciprocal of the radius of the smallest sphere

$$S(A) = S\left(A, \frac{1}{\alpha''_A}\right) \tag{7}$$

that can enclose A. Then

$$\langle A\rangle_{\alpha''} = S(A). \tag{8}$$

Define a function $A(\alpha)$ as

$$A(\alpha) = \langle A\rangle_\alpha, \quad \alpha' \leqslant \alpha \leqslant \alpha'', \tag{9}$$

then

$$A(\alpha') = \langle A\rangle_{\alpha'} = A \tag{10}$$

and

$$A(\alpha'') = \langle A\rangle_{\alpha''} = S(A), \tag{11}$$

and $A(\alpha)$ transforms A into $S(A)$. If A is connected, then this transformation is continuous, otherwise it is only piecewise continuous.

Consider another bounded object B and the associated transformation $B(\alpha)$. Furthemore, consider a continuous function $R(r)$ changing the radius for a continuum of spheres $S(r)$ from the radius $r_A = 1/\alpha''_A$ of sphere $S(A, 1/\alpha''_A)$ to the radius $r_B = 1/\alpha''_B$ of sphere $S(B, 1/\alpha''_B)$:

$$R(r) = S(r), \tag{12}$$

where $1/\alpha''_A \leqslant r \leqslant 1/\alpha''_B$ if $1/\alpha''_A \leqslant 1/\alpha''_B$ and $1/\alpha''_B \leqslant r \leqslant 1/\alpha''_A$ otherwise.

A shape transformation by alpha-hulls, STAH(A, B, t) is defined as follows:

$$\text{STAH}(A,B,t) = \begin{cases} A\bigl(\alpha'_A + w_\alpha t\bigr) & \text{if } 0 \leqslant t \leqslant t_A, \\ S\left(\dfrac{1}{\alpha''_A - \operatorname{sign}(\alpha''_A - \alpha''_B) w_\alpha (t - t_A)}\right) & \text{if } t_A \leqslant t \leqslant t_B, \\ A\bigl(\alpha'_B + w_\alpha(1-t)\bigr) & \text{if } t_B \leqslant t \leqslant 1, \end{cases} \tag{13}$$

where

$$w_\alpha = \alpha''_A - \alpha'_A + \left|\alpha''_A - \alpha''_B\right| + \alpha''_B - \alpha'_B, \tag{14}$$

$$t_A = \frac{\alpha''_A - \alpha'_A}{w_\alpha}, \tag{15}$$

and

$$t_B = t_A + \frac{|\alpha''_A - \alpha''_B|}{w_\alpha}. \tag{16}$$

For small values of the parameter t (if $0 \leqslant t \leqslant t_A$), this transformation STAH(A, B, t) generates the α-hulls $\langle A\rangle_\alpha$ of object A with

$$\alpha = \alpha'_A + w_\alpha t, \tag{17}$$

turning the object A into the sphere $S(A)$ at $t = t_A$. For intermediate values of parameter t, various spheres are obtained which continuously interpolate between the spheres $S(A)$ and $S(B)$, that is, a sphere $S(r)$ of radius

$$r = \frac{1}{\alpha''_A - \operatorname{sign}(\alpha''_A - \alpha''_B) w_\alpha (t - t_A)} \tag{18}$$

is generated if $t_A \leqslant t \leqslant t_B$. For large values of the parameter t, the transformation STAH(A, B, t) turns the sphere $S(B)$ at $t = t_B$ through a series of α-hulls $\langle B\rangle_\alpha$ of object B into object B, that is, the α-hulls $\langle B\rangle_\alpha$ of object B with

$$\alpha = \alpha'_B + w_\alpha(1-t) \tag{19}$$

is obtained if $t_B \leqslant t \leqslant 1$.

Note that this transformation applies in any finite dimension n with the analogous definition of alpha hull with respect to hyperballs of the appropriate dimensions. Furthermore, a formal “dimension jumping” between objects is also possible, by adding an extra intermediate step at the spherical stage that “flattens out” some dimensions of the hypersphere that are unnecessary in one of the objects, say, object B.

3. T-hull shape transforms

For any bounded object T, the object $T(\alpha)$ is defined as

$$T(\alpha) = \begin{cases} T \text{ scaled by the factor } \dfrac{1}{\alpha} & \text{if } \alpha > 0, \\ \text{a half-space} & \text{if } \alpha = 0, \\ \text{the complement of } T \text{ scaled by the factor } -\dfrac{1}{\alpha} & \text{if } \alpha < 0. \end{cases} \tag{20}$$

Note that for sake of a more direct analogy with the alpha hull approach, the scaling is defined in terms of $1/\alpha$.

If T is a spherical ball, then the discussion in this section and the introduction of the T-hull shape transform based on it become equivalent to those of the alpha hull shape transforms described in the previous section.

For any bounded set A exists a largest α' value such that the $T(\alpha')$-hull $\langle A\rangle_{T(\alpha')}$ of object A is still A:

$$\alpha' = \max\bigl\{\alpha\colon \langle A\rangle_{T(\alpha')} = A\bigr\}. \tag{21}$$

As in the case of alpha-hulls, this α' value may be negative. The set A may be connected or disconnected, and possibly a discrete point set.

Define α'' as the alpha value of the smallest object $T(\alpha)$ that can enclose A. Evidently,

$$\langle A\rangle_{T(\alpha'')} = T\bigl(\alpha''\bigr). \tag{22}$$

Define a function $A_T(\alpha)$ as

$$A_T(\alpha) = \langle A\rangle_{T(\alpha)}, \quad \alpha' \leqslant \alpha \leqslant \alpha'', \tag{23}$$

then

$$A_T\bigl(\alpha'\bigr) = \langle A\rangle_{T(\alpha')} = A \tag{24}$$

and

$$A_T\bigl(\alpha''\bigr) = \langle A\rangle_{T(\alpha'')} = T\bigl(\alpha''\bigr). \tag{25}$$

The function $A_T(\alpha)$ transforms object A into a scaled version $T(\alpha'')$ of the reference object T. If object A is connected, then this transformation is continuous, otherwise $A_T(\alpha)$ is only piecewise continuous.

Take another bounded object B and the associated transformation $B_T(\alpha)$. Furthemore, consider a continuous function $R_T(\alpha)$ scaling the reference object T by a factor $1/\alpha$, transforming $T(\alpha''_A)$ to $T(\alpha''_B)$, where $\alpha''_A \leqslant \alpha \leqslant \alpha''_B$ if $\alpha''_A \leqslant \alpha''_B$ and $\alpha''_B \leqslant \alpha \leqslant \alpha''_A$ otherwise.

A shape transformation by T-hulls, STTH(A, B, t) is defined as follows:

$$\mathrm{STTH}(A,B,t) = \begin{cases} A_T\bigl(\alpha'_A + w_\alpha t\bigr) & \text{if } 0 \leqslant t \leqslant t_A, \\ R_T\bigl(\alpha''_A - \mathrm{sign}\bigl(\alpha''_A - \alpha''_B\bigr)w_\alpha(t - t_A)\bigr) & \text{if } t_A \leqslant t \leqslant t_B, \\ B_T\bigl(\alpha'_B + w_\alpha(1-t)\bigr) & \text{if } t_B \leqslant t \leqslant 1. \end{cases} \tag{26}$$

Here

$$w_\alpha = \alpha''_A - \alpha'_A + \left|\alpha''_A - \alpha''_B\right| + \alpha''_B - \alpha'_B, \tag{27}$$

$$t_A = \frac{\alpha''_A - \alpha'_A}{w_\alpha}, \tag{28}$$

and

$$t_B = t_A + \frac{|\alpha''_A - \alpha''_B|}{w_\alpha}. \tag{29}$$

The range of parameter is $0 \leqslant t \leqslant 1$. For small values of the parameter t (if $0 \leqslant t \leqslant t_A$), the transformation STTH(A, B, t) generates the $T(\alpha)$-hulls $\langle A\rangle_{T(\alpha)}$ of object A with reciprocal scaling factors

$$\alpha = \alpha'_A + w_\alpha t, \tag{30}$$

turning the object A into the $T(\alpha'')$-hull $\langle A\rangle_{T(\alpha'')} = T(\alpha'')$ of A at $t = t_A$. By taking intermediate values of parameter t, various scaled T-hulls are obtained which continuously interpolate between the scaled T-hulls $T(\alpha''_A)$ and $T(\alpha''_B)$, that is, a scaled T-hull of alpha value

$$\alpha = \alpha''_A - \operatorname{sign}\bigl(\alpha''_A - \alpha''_B\bigr) w_\alpha (t - t_A) \tag{31}$$

is generated if $t_A \leqslant t \leqslant t_B$. For large values of the parameter t, $t_B \leqslant t \leqslant 1$, the transformation STTH(A, B, t) turns the scaled T-hull $T(\alpha''_B)$ at $t = t_B$ through a series of $(1/\alpha)$-scaled T-hulls of object B into object B, that is, the T-hulls $B_T(\alpha) = \langle B\rangle_{T(\alpha)}$ of object B with

$$\alpha = \alpha'_B + w_\alpha(1 - t) \tag{32}$$

are obtained if $t_B \leqslant t \leqslant 1$.

Note that this transformation applies in any finite dimension n.

4. Summary

The shape transformation described in this contribution provides tools for the direct comparisons of the relative shapes of molecular electron density contour surfaces (MIDCOs). Various molecular shape constraints, such as those relevant to solvent-solute interactions, are the primary targets for the analysis of electron density in terms of T-hulls.

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