Note

Shape space of achiral simplexes

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We examine the general dimensional relation between the shape space of the *n*-simplexes and the subspace of their achiral sets. It is found that the only simplexes that can be partitioned into "left-handed" and "right-handed" classes are the triangles in Euclidean 2-space.

1. Introduction

Consider the set K of all possible convex polyhedra that can be generated by continuous deformation of a given polyhedron by preserving its polyhedrical structure. K falls into two subsets, achiral K_a and chiral K_c. K_c may be further partitioned into two subsets such that the two mirror images (enantiomorphs) of a given polyhedron must belong to different subsets. The two subsets are therefore of the same order.

In a different context, with reference to models of molecules in which chirality is due to the chiral distribution of achiral ligands on an achiral framework (in which the ligands may be symbolically represented by spheres of different diameter centered at the vertices of this framework), Ruch [1] has pointed out that there are two classes of chiral subsets: those in which the path of continuous deformation that connects two enantiomorphs necessarily requires passage through an achiral form (class a), and those in which this requirement need not be met (class b). In class a, the set of achiral models forms the boundary between the two chiral subsets, and it is therefore meaningful to assign to all models in each subset a common descriptor, indicative of their shared sense of chirality, such as "right-handed" for one subset and "left-handed" for the other. Any two models that belong to a given subset may be termed "homochiral" and any two models that belong to different subsets "heterochiral". In class b, there is no such boundary, and the enantiomorphs in the two chiral subsets are "chirally connected". It is therefore meaningless (or, at best, arbitrary) to attach chirality descriptors to members of the two subsets; by the same token, the "homochiral"–"heterochiral" terminology is inapplicable to members of class b.

We recently asserted [2] that tetrahedra are in general (that is, in the absence of well-defined constraints) chirally connected by continuous deformation. In this note, we show how this condition is a consequence of the difference in shape space dimensions of K_a and K_c, and we generalize this result to higher dimensions.

2. Calculation of shape space dimensions

The size and shape of a tetrahedron is fully defined by a minimum of six geometric parameters (the lengths of the edges, for example). Since our concern is with chirality, and therefore with shape and not with size, only five independent parameters are needed for the complete (and similarity-invariant) definition of a tetrahedron's shape. The set of all shapes may be mapped into a five-dimensional space, the tetrahedron's "shape space" [2]. Consider now the subspace of the shape space that represents the set of all achiral shapes. We would like to know its local dimension. Because an achiral tetrahedron must have at least one plane of symmetry, at most four independent parameters suffice to define the size and shape of any achiral tetrahedron (as proven for the general case below), and three are enough to define its shape. The subspace of achiral tetrahedral shapes is therefore locally parametrized by a three-dimensional subspace. Because a three-dimensional space cannot divide a five-dimensional space into two distinct regions, it follows that a chiral tetrahedron can be continuously deformed into its enantiomorph without passing through an achiral state.

The tetrahedron is the simplex in three-dimensional Euclidean space. In a more general way, we are interested in finding the dimension of the subspace of achiral n-simplexes in the shape space of the n-dimensional simplexes.

Let E^n be the n-dimensional Euclidean space. A simplex is the convex hull of $n + 1$ points that are linearly independent; that is, whenever one of the points is fixed, the n vectors that link it to the other n points form a basis for E^n. An n-dimensional simplex has $n + 1$ vertices and $C_2^{n+1} = n(n + 1)/2$ edges. The dimension of the shape space of n-dimensional simplexes X_n is therefore given by

$$\dim(X_n) = n(n + 1)/2 - 1 = (n^2 + n - 2)/2.$$

It can be shown that among achiral simplexes the type with one hyperplane of symmetry has the most degrees of freedom. Let us call this plane of symmetry H. Only two vertices of the simplex can lie outside H, while the other $n - 1$ must lie in the hyperplane. The reason for this is that if more than two vertices were to lie outside H, there would be at least four points on the same two-dimensional linear subspace, but the choice of one of these four points would yield three linearly dependent vectors, in contradiction to the definition of a simplex. In order to determine the size and shape of this type of achiral simplex, it is therefore sufficient to know the lengths of the edges that lie in H, which number $C_2^{n-1} = (n - 1)(n - 2)/2$, the lengths of the edges that lie on one side of H, which number

$n-1$, and the length of the edge between the two vertices outside H. Thus, Y_n, the subspace of the achiral simplexes in the shape space X_n, will have the following dimension:

$$\begin{aligned}\dim(Y_n) &= (n-1)(n-2)/2 + (n-1) + 1 - 1 \\ &= (n-1)n/2\,.\end{aligned}$$

Our analysis shows that $\dim(X_n) - \dim(Y_n) = n-1$; this difference is equal to unity only when $n = 2$. Therefore, triangles, the simplexes in E^2, are unique in that they alone among all simplexes can be partitioned into heterochiral sets [3].

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References

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