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Landmark Coordinates Aligned by Procrustes Analysis Do Not Lie in Kendall's Shape Space

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The field of geometric morphometrics is concerned with methods for studying shapes of objects. These methods are increasingly used to address a broad range of ecological and evolutionary questions. A few recent examples include the study of ontogenetic

reaction norms (Arnqvist and Johansson, 1998), fluctuating asymmetry (Klingenberg and McIntyre, 1998), and trophic morphology (Caldecutt and Adams, 1998). There has also been recent debate within these pages as to the appropriate place for geometric morphometrics in the context of phylogenetic analysis (Adams and Rosenberg, 1998; Rohlf, 1998a; Swiderski et al., 1998; Zelditch and Fink, 1998; Zeldtich et al., 1998). Much of our theoretical understanding of this powerful and relatively new approach to shape analysis is due to work by Kendall on the geometric and statistical properties of shape spaces defined by the Procrustes metric (Kendall, 1984, 1985). It is important that users of these methods appreciate the relationship between the theoretical aspects of geometric morphometrics and their practical application. This report demonstrates that the geometry of sample variation resulting from the most commonly used geometric method, Procrustes analysis (also known as least squares superimposition), is not the same as the geometry of the shape space described by Kendall. The coordinates of landmarks after the Procrustes superimposition (with unit scaling) of a sample onto a reference lie on the surface of a (hyper)hemisphere of unit radius that, at that reference, approximates the relationships between configurations in Kendall's shape space.

PRELIMINARIES

Most current geometric morphometric methods involve analysis of the Cartesian coordinates of configurations of landmarks (points) that could serve as endpoints for measurements used in more traditional approaches to shape analysis, such as comparisons of ratios of linear distances or of angles between vectors connecting the landmarks. The geometric methods are distinguished from the more traditional morphometric analyses by their strictly enforced retention of all the geometric shape information in the landmark coordinates of each configuration.

Central to geometric morphometrics is the definition of shape as the geometric properties of an object that are invariant to location, orientation, and scale (Slice et al., 1996). The constraints imposed by partitioning total coordinate variation into shape and non-shape (translation, rotation, and size) components can lead to well-defined topological and geometric constraints on the resulting shape variation. Kendall (1984, 1985) showed, for instance, that a specific metric, Procrustes distance, leads to a shape space for planar triangles that is isometric to (has the same distance relationships as) the surface of a two-dimensional sphere of radius 0.5. It is important that users of geometric methods have an understanding of the structure of these spaces and their implications for statistical analyses, because standard linear statistical procedures should not be applied uncritically in such non-Euclidean spaces.

However, as shown below, the most commonly used procedure for removing differences in location, scale, and orientation, Procrustes superimposition, leads not to coordinates in Kendall's shape space, but to coordinates in a space that can be represented as the surface of a (hyper)hemisphere of radius one. In the case of planar triangles, this space has a simple geometric relationship to Kendall's shape space. Furthermore, recent studies (Rohlf, 1999) suggest that when shape variation is linearized by projection into a tangent space for the purpose of statistical analyses, projections from the hemisphere of Procrustes-aligned configurations provide better approximations of intershape distances in Kendall's shape space than do alternative projections from Kendall's space itself.

KENDALL'S SHAPE SPACE AND PROCRUSTES SUPERIMPOSITION

Kendall (1984, 1985) removed location and size differences between sets of point coordinates by centering each configuration on the origin and scaling each configuration to unit "size," where size is defined as the sum of squared, Euclidean distances from each landmark to the configuration centroid. These constraints can be expressed mathematically as

$$\mathbf{X}^t \mathbf{1} = \mathbf{0} \quad \text{and} \quad \text{tr}(\mathbf{X}\mathbf{X}^t) = 1,$$

where $\mathbf{X}$ is a $p \times k$ matrix of the coordinates of p points in k dimensions, $\mathbf{1}$ is a $p \times 1$ vector of 1's, and $\mathbf{0}$ a $k \times 1$ vector of 0's. The square root of the size measure, as defined here, is commonly called Centroid Size (Bookstein, 1991).

Kendall then went on to account for orientation by "quotienting-out" (removing differences due to) special orthogonal rotations (i.e., no reflections) from the centered, scaled configurations to form an equivalence class of shapes. This was done by minimizing the great circle distance, d, between each pair of centered, scaled configurations when considered as $1 \times pk$ vectors:

$$\rho(\sigma_1, \sigma_2) = \inf_{\mathbf{R}} d(\mathbf{RX}_1', \mathbf{X}_2')$$

where $\mathbf{R}$ is a 2×2 special orthogonal rotation matrix, and the primes denote centered and scaled matrices of landmark coordinates. In the above equation, ρ is the Procrustes *angular* (= great circle) distance (see below) between the two shapes, σ_1 and σ_2 and provides a metric for their comparison. ρ has a maximal value of $\pi/2$ and defines Kendall's shape space, Σ_k^p, for configurations of p points in k dimensions, technically, a Reimannian manifold of equivalence classes.

The dimensionality of the sample space of p points in k physical dimensions is, of course, pk. Standardization for location, scale, and orientation reduces the maximal dimensionality of the variation of the data by k, 1 and $k(k - 1)/2$, respectively. This contributes to Kendall's (1984) result that for $k = 2$, shape space is isometric to the complex projective space, CP^{p-2}. In the special case of planar triangles, Σ_2^3 is isometric to the surface of a two-dimensional sphere of radius 0.5.

Figure 1a shows a view of such a sphere onto which has been mapped a sample of 2,000 random triangles (see Appendix). The sphere, in this case, has been oriented so that the north pole represents the shape of an equilateral triangle. The reflection of this triangle maps to the south pole, and those triangles having collinear vertices lie along the equator. Longitude is defined with respect to Bookstein's (1996a) linearized Procrustes estimates of uniform shape differences, u1 and u2. Great circle distances between points equal the Procrustes angular distances between corresponding shapes.
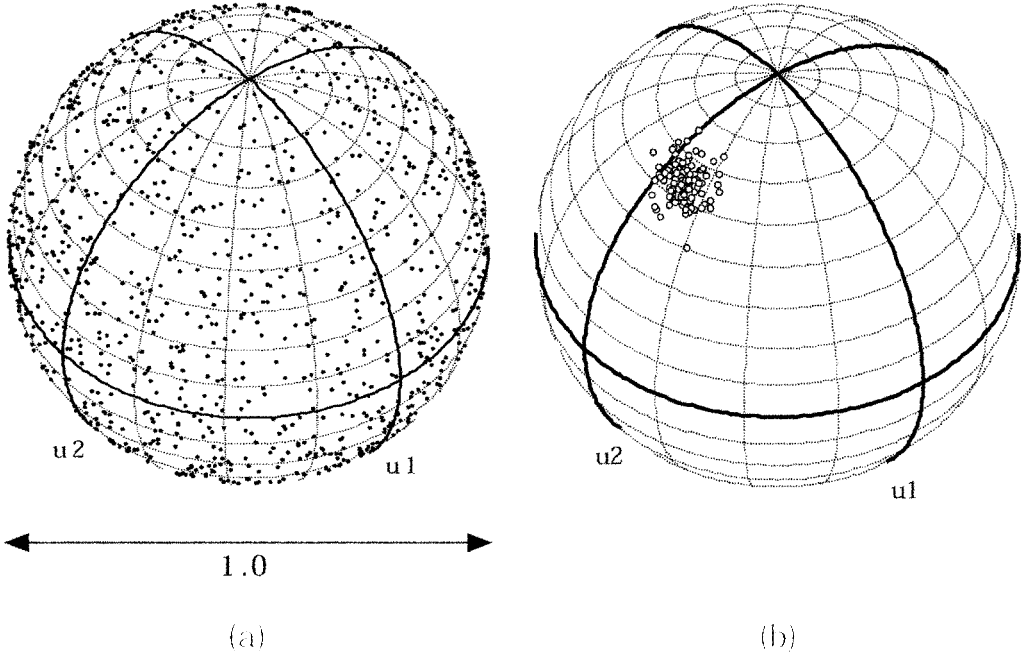

FIGURE 1. A view of Kendall's shape space for triangles showing (a) the mapping of 2,000 random triangles generated by the independent, normal displacement of triplets of points from the origin and (b) the mapping of 110 triangles describing the overall shape of gorilla scapulae. The north pole in both plots corresponds to an equilateral triangle. The south pole corresponds to the reflection of the triangle at the north pole. The equator of each sphere corresponds to triangles with collinear vertices. Longitude is defined with respect to Bookstein's (1996a) linearized Procrustes estimates of uniform shape differences, u1 and u2.

This plot also illustrates Kendall's result that triangles generated by independent, identically distributed, Gaussian displacement of triplets of points from the origin will have a uniform distribution in Σ_2^3 (Kendall, 1985).

Figure 1b shows the same sphere, onto which has been mapped a mixed sample (both sexes from two subspecies) of 110 triangles formed by the extremal angles of gorilla scapulae (Taylor, 1997). This plot is consistent with the important observation that for most biologically derived material, the actual amount of shape variation occupies a relatively small patch of shape space (see also Marcus et al., 2000).

Kendall's development of shape theory is based on the Procrustes metric between pairs of configurations. A convergent approach, and the one used in practical applications of geometric morphometrics, is based on the least-squares superimposition (Ordinary Procrustes Analysis; OPA) of landmark configurations (Boas, 1905; Mosier, 1939; Sneath, 1967; Gower, 1975; Rohlf and Slice, 1990). That is, given the model

$$\mathbf{X}_2 = \alpha(\mathbf{X}_1 + \mathbf{D})\mathbf{H} + \mathbf{1}\tau,$$

where α is a scale factor, $\mathbf{H}$ is a $k \times k$ special orthogonal (no reflection) rotation matrix, $\mathbf{1}$ is a $p \times 1$ vector of 1's, τ is a $1 \times k$ vector of coordinate-wise translations, and $\mathbf{D}$ is a $p \times k$ matrix of shape difference between the two configurations, then the translation and rotation parameters are computed to minimize the sum of squared distances between corresponding landmarks in the two configurations: $\Delta^2 = \mathrm{tr}(\mathbf{D}\mathbf{D}^t)$.

The scale factor, α, can be computed so as to scale each object to a specific, usually unit, centroid size, as in Kendall's work. Such a choice for α does not, however, minimize Δ^2. That is achieved by scaling the specimen to size $\cos(\rho)$, where ρ is the angle between the two centered and aligned configurations written as $1 \times pk$ vectors—the Procrustes angular distance. The difference between these scalings has not always been emphasized in morphometric literature and software, though Goodall (1991) and Kent (1994) make the distinction between partial (unit centroid-size scaling) and full (criterion-minimizing, $\cos(\rho)$ scaling) Procrustes analyses. Scaling to unit centroid size

is the scaling used by Kendall and parallels the approach used in other morphometric analyses with the intent of comparing specimens at a standard size, e.g., dividing measurements by the cube root of body weight or a specified linear dimension (Jungers et al., 1995).

The criterion Δ^2 is a measure of the shape difference between two landmark configurations. The square root of this quantity has also been referred to as Procrustes distance (Bookstein, 1996b). With unit centroid-size scaling, this formulation and the great circle distance used by Kendall are simply related by $\rho = 2\sin^{-1}(\Delta/2)$. These two distances, Δ and ρ, can be distinguished as Procrustes "chord" distance and Procrustes "angular" distance (Dryden and Mardia, 1998), respectively. That convention will be followed here when the distinction is important. Otherwise, both will be synonymized as Procrustes distance.

The OPA superimposition addresses pairwise differences between two configurations. In most practical applications, one is concerned with the analysis of samples of more than two configurations. In such cases, one can fit the individual configurations to a specified reference configuration or, more reasonably (see below), compute a mean configuration and compare samples with it. The latter is referred to as a Generalized Procrustes Analysis (GPA) or a Generalized Least Squares (GLS) superimposition (Gower, 1975; Rohlf and Slice, 1990).

The simultaneous superimposition of configurations to a reference (usually the mean) leads to the geometric properties that are the subject of this report. With either an OPA (fitting one configuration to a reference) or GPA (fitting a sample to an estimated mean configuration) the maximum angular distance between centered, optimally oriented shapes is $\pi/2$ (Kendall, 1984). With unit centroid-size scaling, all shapes superimposed in this manner must lie on the surface of a (hyper)hemisphere of unit radius and of the same dimension as Kendall's shape space. As in the case of Kendall's shape space, this hemisphere can be easily visualized for planar triangles as shown in Figure 2. Figure 2a shows the resulting distribution on the hemisphere of the 2,000 triangles from Figure 1a when Procrustes superimposed onto the equilateral triangle at the north pole
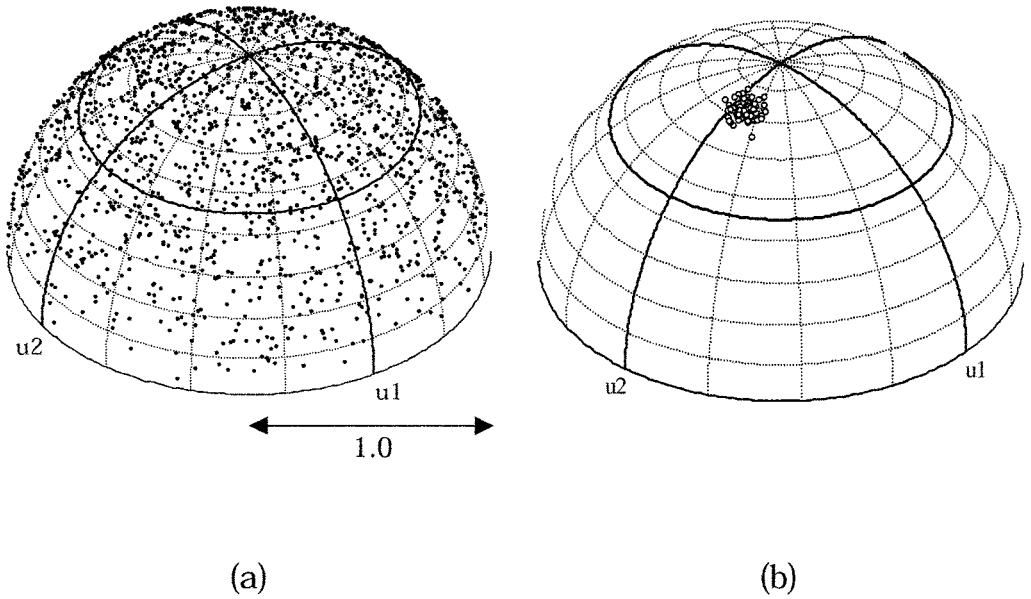
FIGURE 2.   A view of the hemisphere of Procrustes-superimposed triangles showing (a) the mapping of the 2,000 random triangles from Figure 1a and (b) the mapping of the 110 gorilla scapulae from Figure 1b. Both sets of data were fit by using an equilateral triangle (north pole) as the reference configuration. The heavy latitudinal line on each hemisphere corresponds to triangles with collinear vertices that map to the equators of the spheres in Figure 1. The equator of the hemisphere corresponds to the reflection of the equilateral triangle at the north pole. Longitude is defined with respect to Bookstein's (1996a) linearized Procrustes estimates of uniform shape differences, u1 and u2.

in the first figure. Figure 2b shows the distribution of the similarly superimposed gorilla scapulae from Figure 1b.

An important distinction between the mappings of triangles in Figures 1 and 2 is that great circle distances between all pairs of points correspond to Procrustes angular distance *only in Kendall's shape space*. The great circle distance between any shape on the superimposition hemisphere and the reference used for superimposition equals the Procrustes angular distance between the two, but the distance between any two other shapes does not. This is most dramatically illustrated by the fact that on the hemisphere of triangles, the configuration most different in shape from the reference maps to the entire equator of the hemisphere. Points on opposite sides of this equator are separated by a distance of π on the hemisphere but have an actual Procrustes distance of zero. However, the hemisphere of the Procrustes-superimposed triangles can be mapped directly to Σ_2^3 by scaling each point on the hemisphere by $\cos(\rho)$, where ρ is as defined above. The equator of the hemisphere is at the maximal angular distance of $\pi/2$ from

the reference and, thus, is mapped in its entirety to the south pole of Kendall's shape space.

DISCUSSION

Kendall's shape space and the Procrustes (hyper)hemisphere are curved, non-Euclidean spaces. Although researchers have provided some distributional results and statistical procedures that account for the geometry of Kendall's shape space (see Small, 1996; Dryden and Mardia, 1998), applied morphometric analyses usually involve the application of familiar statistical procedures that assume, among other things, distributions in a linear, Euclidean space. This properly requires an additional linearization step whereby data in either of these non-Euclidean spaces are projected onto a linear subspace of the proper dimension. It is through this step that the geometric differences between the two spaces have the greatest potential impact in applied morphometric studies.

Rohlf (1999) considers several choices of linearization suggested for data in both
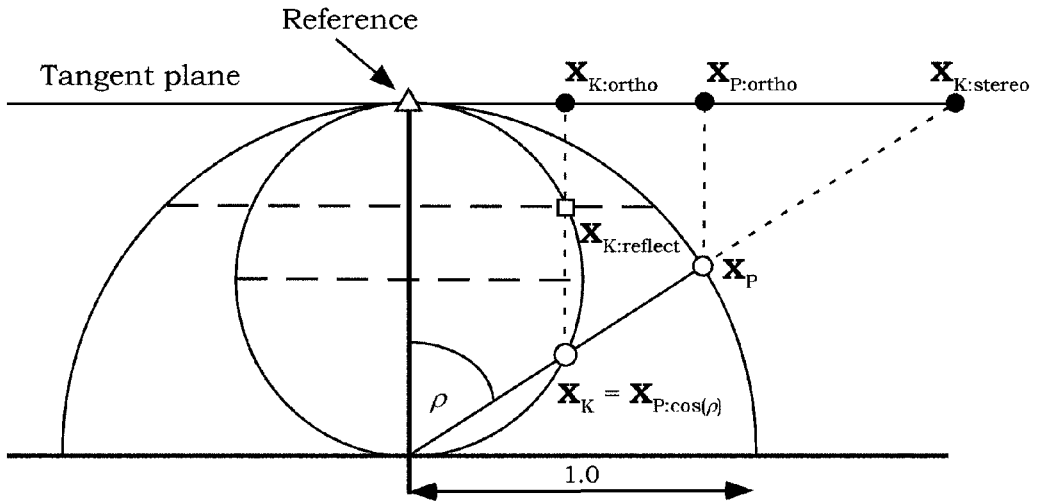
FIGURE 3. The geometric relationship between the Procrustes hemisphere (PH, outer arc, radius = 1.0) and Kendall's shape space (KSS, large inner circle, radius = 0.5) for triangles and alternative tangent-space projections. The open triangle indicates the Procrustes reference triangle and the point used to define the plane tangent to both the PH and KSS. Dotted lines are alternative projections into the linear tangent plane. Open circles indicate a specific, planar triangle either in KSS (K subscripts) or on the PH (P subscripts). Filled circles show orthogonal (ortho subscripts) and stereographic (stereo subscript) projections of the shapes from KSS or from the PH. Note that triangles on the PH map to the KSS when scaled by cos(ρ). Also, the open square symbol denotes the reflection of the triangle X_K across the equator, defined with respect to the reference, of KSS. This reflection represents a reflection of the triangle in physical space if, and only if, the references is an equilateral triangle. If, and only if, the reference is an equilateral triangle, the horizontal dashed lines indicate the position of the triangles with collinear vertices in each space. (This figure was based, in part, on a figure from the help file of an earlier version of tpsRelw [Rohlf, 1998c] showing alternative superimposition scalings.)

spaces (see also Kent, 1994). Some of these choices are illustrated for triangles in Figure 3. For Kendall's shape space, one choice of linearization is an orthogonal projection of the data (X_K) onto a plane (in the case of triangles) tangent to Kendall's shape space ($X_{K:ortho}$). However, this mapping is not single-valued. Points on one side of the equator, defined with respect to the tangent point, are mapped to the same point in the plane as their mirror image across the equator ($X_{K:reflect}$). Note that the two points mapped to the same point in tangent space by this projection are reflections of each other in Kendall's shape space only with respect to the equator as just defined. They are reflections of each other in physical space if, and only if, the tangent point is an equilateral triangle and the equator thus represents triangles with collinear vertices.

A second approach is the stereographic projection of the points from Kendall's shape space onto a tangent plane ($X_{K:stereo}$). Such a projection maps points between the tangent point and the equator, defined with respect to

the tangent point, to the area within a circle of radius 1.0; maps points beyond the equator to the plane outside of this circle; and maps the point antipodal to the tangent point to infinity.

A third choice of linearization is an orthogonal projection of points on the Procrustes hemisphere (X_P) onto the tangent plane at the reference ($X_{P:ortho}$). This provides a unique, one-to-one mapping of points to a disk of unit radius. Note that the cos(ρ)-scaling of Procrustes-superimposed triangles (and only triangles) maps configurations from the Procrustes hemisphere to Kendall's shape space exactly ($X_K = X_{P:cos(\rho)}$) (Fig. 3).

The usefulness of any of these projections depends on how accurately Procrustes distances are preserved in the tangent space. Rohlf (1999) found that for a variety of data the orthogonal projection of points from the Procrustes hemisphere more accurately approximated the true (Procrustes) shape distances than either projection from Kendall's shape space. Those results and the general utility of Procrustes superimpositions

suggest orthogonal projection from the Procrustes hemisphere should be the generally preferred linearization.

Still, for small amounts of shape variation, the methods of linearization described above should produce similar results. For the gorilla data, the uncentered correlation between distances in Kendall's shape space and the interobject distances in the orthogonal and stereographic projections of the points from Kendall's shape space onto a plane tangent at the sample mean is 0.999997 and 1.000000, respectively. The same value for the orthogonal projection from the Procrustes hemisphere onto a similarly defined plane is 1.000000.

Not surprisingly, distortions of the distances between objects are increased for points away from the reference. To minimize such distortions, therefore, one should use the sample mean configuration as the reference for Procrustes superimposition and as the point of tangency for any subsequent projections (Rohlf, 1998a).

The Procrustes hemisphere and the implications of its geometry for the linearization of shape scatter have not been recognized in previous morphometric work—despite the ubiquitous presence of the hemisphere in the analysis of Procrustes-superimposed data sets. The current discussion has focused on shape spaces for planar triangles because accurate and intuitive graphical representations can be provided for the results for such data. For configurations of more landmarks in two dimensions ($p > 3, k = 2$), the geometric structure of the Procrustes (hyper)hemisphere is the same as for triangles except for dimensionality. Similarly, the relationships between various tangent-space projections should be the same for samples with relatively small scatters of shape variation. One noteworthy exception is that the simple relationship between the Procrustes hemisphere and Kendall's shape space for triangles does not hold for more complicated ($p > 3$) planar configurations, because the equator of the Procrustes hemisphere would then correspond to a complex projective space of $p - 3$ dimensions (Kendall, 1984). Thus, multiple maximally different shapes would map to the south pole of a hypersphere after $\cos(\rho)$ scaling; that is, they would not map to Kendall's shape space. For $k \geq 3$, the mathematical consideration of Kendall's shape space is much more complicated (Small, 1996), and a similarly simple relationship between Kendall's shape space and the Procrustes hemisphere to that shown for triangles is unlikely. However, for relatively small amounts of shape scatter, the observations presented here should hold.

As a final point, note that the (hyper)hemispherical scatter of coordinate variation subsequent to Procrustes superimposition is an outcome of the use of Procrustes superimposition and unit scaling. It is a *result* of the superimposition and not a *choice* of representation. Fortunately, linearization by orthogonal projection of the sample onto a plane tangent to the (hyper)hemisphere at the reference configuration provides approximations to shape distances in Kendall's shape space as good as or better than alternative linearizations from Kendall's shape space itself and is more easily obtainable with existing morphometric software. For small shape variation, results using any of these methods should be equivalent.

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APPENDIX

The geometry of the variation of Procrustes-superimposed triangles was first explored with simulated data sets. The procedure is outlined here with specific reference to the Morpheus et al. (Slice, 1999) and NTSYSpc (Rohlf, 1997) programs, but any software capable of superimposing landmarks by using Procrustes methods, carrying out singular value decompositions or computing principal components, and creating three-dimensional plots could be used. Size, scale, and orientation in the simulated data are irrelevant. The steps used were as follows:

1. Compute the coordinates of the vertices of an equilateral triangle, ABC, and of its reflection, for example, (0,0; 0.5,0.866; 1,0) and (0,0; 0.5,–0.866; 1,0).
2. Compute the coordinates of the vertices of six collinear triangles—three with each vertex, A, B, and C, half-way between the other two, respectively, for example, (0,0; 0.5,0; 1,0), (0.5,0; 0,0; 1,0), and (0,0; 1,0; 0.5,0), and three with each pairwise combination of vertices, AB, AC, BC, coincident, for example, (0,0; 0,0; 1,0), (0,0; 1,0; 0,0), and (1,0; 0,0; 0,0).
3. Generate a large data set, say, $n = 2000$, of random triangles by the random, normal (N(0, σ)) displacement of triplets of points from the origin. The magnitude of σ affects only the "size" range of the resulting triangles and, hence, has no effect on the results after superimposition (step 5).
4. Combine the above data, in order, into an NTSYSpc data file.
5. Import the data file into Morpheus et al. and superimpose the data by OPA (= LS) superimposition (finalLSScaling = unity, allowreflections = false) onto the equilateral triangle. This orients the resulting hemisphere so the equilateral triangle is at the north pole. The general geometric results are unchanged for any superimposition of multiple triangles to a single reference, whether to a specific configuration or an iteratively computed mean shape.
6. Export the superimposed configurations to an NTSYSpc file.
7. Use NTSYSpc to carry out a singular value decomposition (SVD) of the data file from step 6 with scaling for the left vectors set to "lambda." Except for rounding error, only the first three dimensions will have nonzero eigenvalues. This can be checked by setting the number of dimensions to the maximal value (for this data set) of six. Finally, set to three the number of dimensions to compute and save the left matrix to a file.
8. Import the left matrix from step 7 into Morpheus et al. as an NTSYSpc data set consisting of numerous objects, each with a single, three-dimensional point. Use

the "group" command to distinguish key triangles from steps 1 and 2 above, for example, group 1 1 3 3, and view "ALL" data to see the hemisphere and the locations of key triangles as described in the text.

Once the hemispherical structure of the Procrustes-superimposed random triangles was determined, the geometric relationships between the Procrustes hemisphere and Kendall's shape space for triangles was worked out and checked by using the key triangles from steps 1 and 2 above. Subsequently, Rohlf developed the program tpsTri (Rohlf, 1998b) specifically for visualizing the Procrustes hemisphere, Kendall's shape space for triangles, the tangent-plane projections, and various other shape spaces (see Rohlf, 2000). tpsTri was used to generate the figures used in this report. The Morpheus et al. and tpsTri programs are available for free download from http://life.bio.sunysb.edu/morph.