A note on statistical analysis of shape through triangulation of landmarks

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In an earlier paper, the author jointly with S. Suryawanshi proposed statistical analysis of shape through triangulation of landmarks on objects. It was observed that the angles of the triangles are invariant to scaling, location, and rotation of objects. No distinction was made between an object and its reflection. The present paper provides the methodology of shape discrimination when reflection is also taken into account and makes suggestions for modifications to be made when some of the landmarks are collinear.

Euclidean distances matrix | logarithm Euclidean distances matrix | triangulation of landmarks | shape analysis

Rao and Suryawanshi, abbreviated as RS in this sequel, developed statistical methodology for analysis of shape of objects in ref. 1 through triangulation of landmarks (TLM) and applied it in a study of sexual dimorphism in hominids. It was observed that the angles of the triangles formed by three landmarks are invariant to scaling, location, and reflection of objects. With k landmarks, there are $k(k-1)(k-2)/6$ triangles and considering two angles of each triangle, the database consists of $k(k-1)(k-2)/3$ measurements (angles) on each object. It was suggested that a subset of $(k-2)$ triangles with $2(k-2)$ angles, which uniquely define the configuration of landmarks of an object, can be used for statistical analysis. But a description of shape differences between objects may need a comparison of all possible triangles, as demonstrated in ref. 1. The present note is intended to clarify some of the issues involved and demonstrate how the study of shape, including reflections through TLM, provides a satisfactory approach to problems of shape comparison, recognition, and discrimination.

What Is Shape Analysis?

We have a set of objects (or their images), each of which is specified by the configuration of some recognizable landmarks on it and identified as a member of a particular class (population) out of a given set of possible alternatives. An object can then be represented by the elements of a matrix of order $k \times p$, where k is the number of landmarks, p is the dimensions (1, 2, or 3 in practice) of the object, and each row gives the coordinates of a landmark when the object is referred to a coordinate system. The coordinates matrix X is not comparable over the objects if they differ in size (S), location (L), and orientation changeable by rotation (R), which will be referred to as SLR. The primary task in shape analysis is to transform X into a vector $y = f(X)$ in such a way that y is invariant to SLR, and the configuration X of landmarks (apart from SLR) can be recovered from y. The elements of y in such a case are called the shape measurements of the object. Two objects are said to be of the same shape if one can be brought into coincidence with the other by suitable SLR.

There will be several choices of y for given x. Some examples are Kendall's and Bookstein's shape coordinates, Euclidean distances matrix (EDM) of Lele (2) and Lele and Richtsmeier (3), logarithm (log) EDM of RS (4), and TLM of RS (1). A description of some of these coordinates and the statistical analyses based on them can be found in books by Dryden and Mardia (5) and Small (6).

For purposes of statistical analysis, any choice of shape measurements will do, provided their probability distribution can be modeled accurately. In such a case, appropriate statistical methods may be used for testing differences between populations and classification of new objects.

In ref. 4, log distances between landmarks and in ref. 1, all possible angles by TLM are suggested as shape measurements. The mean shape of the objects is defined as the set of all arithmetic means (AMs) of different shape measurements. In such a case, the mean shape of a subset of landmarks is simply the set of all AMs associated with these landmarks. In the case of Kendall and Bookstein coordinates, the mean shape of a subset of landmarks depends on all the landmarks, which may not be a desirable feature. The shape measurements used in refs. 1 and 4 in terms of angles and those in ref. 2 in terms of distances between landmarks are direct measurements on landmarks, and differences between individuals and populations in such measurements are easy to interpret. A typical illustration is the explanation of difference in mean shapes of Pan and Pongo skulls in terms of the angles of a triangle formed by three landmarks, as discussed in ref. 1.

In the discussion of the rest of the paper, we keep in view the following aspects of shape analysis.

(*i*) Are the distributions of shape measurements (i.e., SLR invariant) the same in all populations under study?

(*ii*) How do we identify an individual with given shape measurements as belonging to a particular population among several possible alternatives? This is the problem of discrimination.

(*iii*) How do we describe differences in shape between individuals and between populations in terms of easily recognizable measurements, such as angles of triangles formed by triads of landmarks and ratios of distances between landmarks? Such a description may be useful in an in-depth investigation of differences between individuals.

Objects Specified by Three Landmarks

First we consider objects (or images) specified by three landmarks that may be designated as 1, 2, and 3. We adopt the convention of viewing the object with the edge (1, 2) in the west (1)–east (2) direction. In such a case, the third vertex, 3, can be to the north or to the south of the edge (1, 2), as shown in Fig. 1 *A* and *B*. We may call the configuration of landmarks in Fig. 1*A* *L* triangle (where 1, 2, and 3 are in a counterclockwise direction) and that in Fig. 1*B* *R* triangle (where 1, 2, and 3 are in a clockwise direction). Thus we make a distinction between an image and its reflection. Such a distinction may provide a good discriminant in pattern recognition (in diagnosis of diseases, etc.).
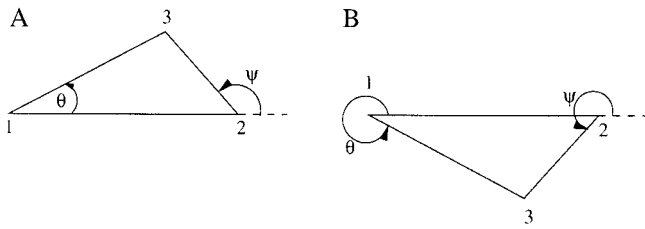

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Fig. 1. (*A*) *L* triangle 1; (*B*) *R* triangle.

We follow the convention of recording the angles at vertices 1 and 2 as shown in Fig. 1 *A* and *B*. In the case of *L* triangles, θ and ψ are in the range of 0 to 180° (or 0 to π radians) with $\psi \geq \theta$, and in the case of *R* triangles, θ and ψ are in the range of 180 to 360° (or π to 2π radians) with $\theta \geq \psi$. Such measurements provide a clear distinction between *L* and *R* triangles.

If the population consists of only one kind of triangle, or if reflection is ignored, we may work with the interior angles at vertices 1 and 2, as shown in Fig. 2, which was the convention followed by RS (1).

The angular measurements, as defined in Figs. 1 *A* and *B* and Fig. 2, are SLR invariant and constitute ideal descriptors of shape. A population of triangles specified by three landmarks may be described as a mixture in a given proportion of the *L* type with a probability distribution of (θ, ψ), where each angle varies in the range (0–180°), and of the *R* type with a probability distribution of (θ, ψ), where each angle varies in the range (180–360°). When comparing two populations for shape differences, it will be more illuminating to test for differences in the proportions of the mixture of *L* and *R* triangles and in the actual distributions of the angles in the *L* and *R* types. In many practical situations, the triangles are likely to be of one type, and the more interesting cases are when both types of triangles exist in a population. However, in any case, because the ranges of (θ, ψ) are different for the *L* and *R* triangles, the joint distribution of (θ, ψ) is uniquely defined.

It has been pointed out by Dryden and Mardia (4) that when three landmarks are collinear, two of the angles are zero whatever the positions of the landmarks on a line, and the angular approach fails to discriminate between shapes in terms of the positions of the landmarks.

Collinearity of landmarks in an observed specimen raises a number of questions. It may be an isolated pathological case, in which case it needs careful investigation. It may be a natural characteristic of the objects of a populations that three landmarks are collinear (absolutely or nearly because of minor perturbations). In such a case, the problem becomes one dimensional, and we need only consider a single measurement such as the distance of landmark 3 from 1 in the positive or negative direction, after scaling the length of the edge (1, 2) to unity. Or it may be that collinearity of landmarks is one of the possible configurations in a population of triangles. If such objects have a finite probability, then we may have to consider the population as a mixture of three types of objects, *L* and *R* triangles and straight lines. If necessary, collinearity of three landmarks may be viewed as a limiting case of a triangle with angles $\varepsilon, \lambda\varepsilon$ and
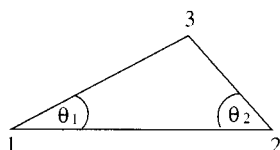

Fig. 2. Triangle specified by two interior angles.

$180\text{-}\varepsilon\text{-}\lambda\varepsilon$, where ε is small and λ determines the position of one of the landmarks with respect to the others on a line.

Statistical Analysis of Triangles

Let us consider populations with only one type of triangle. In such a case, the shape measurements may be chosen as the interior angles of a triangle, and the mean shape can be defined as the triangle whose vertex angles are the mean values of the corresponding angles of individual triangles. No anomaly arises so long as we are working with one type of triangle. Variation in shape can be defined by the variance–covariance matrix of any two interior angles. Differences in shape distributions between populations may be explained in terms of differences in mean shapes of triangles and possibly in their variance–covariance matrices. Such a simple interpretation of differences in shape of three landmarks, which will be of some practical value, may not be available when Kendall or Bookstein coordinates are used.

How do we test for difference in mean shape on the basis of samples of angular data from each of the populations under comparison? We can derive appropriate tests if the stochastic model for the distribution of angles is known. In ref. 1, Hotelling's T^2 and Mahalanobis distance were used to test and explain differences between populations of one type of triangle considering two interior angles θ_1, θ_2 as samples from a bivariate normal distribution. This was justified because a prior test showed no significant departure from bivariate normality. If the distribution is found to be nonnormal, there are several alternatives. If the sample sizes are large, Hotelling's T^2 can be used approximately as a χ^2. Adjustments can also be made in the T^2 statistic if the variance–covariance matrix of θ_1, θ_2 is different in different populations. Another possibility in large samples is the use of bootstrap methodology as suggested by Lele and Cole (7). If exact tests under nonnormality are required, one could use permutation and other nonparametric tests. Other possibilities are transforming the angles to induce normality, such as taking logs as mentioned in ref. 1.

Suppose that each of the populations to be compared is a mixture of two types of triangles. Then we may compare the distributions of *L* triangles and *R* triangles separately by using the method developed for comparing one type of triangle in ref. 1 and further elaborated in this paper. We also have the opportunity to test for differences in the proportion of the mixture of *L* and *R* triangles in different populations. When a population consists of a mixture of *L* and *R* triangles, the concept of a mean triangle may not be meaningful.

A single test of difference in the overall distribution of two angles (*L* and *R* triangles put together), if necessary, can also be carried out on standard lines by using Kolmogorov- and Smirnov-type tests.

For a graphical representation of the objects, the interior angles of triangles of the *L* type can be plotted as aerial coordinates in the upper equilateral triangle and of the *R* type in the lower equilateral triangle. If s is the side of the equilateral triangle, then the triangle with angles $\theta_1, \theta_2, \theta_3$ ($\theta_1 + \theta_2 + \theta_3 = 180°$) can be represented by the point (x, y), where x, the distance from 1 along the side 1, 2, and y, the distance perpendicular to 1, 2 are given by

$$x = s\,\frac{\theta_1}{180} + (s \cos 60)\,\frac{\theta_3}{180},$$

$$y = (s \sin 60)\,\frac{\theta_3}{180},$$

The shapes of the triangles at different points are shown in Fig. 3. The degenerate cases when the vertices are collinear can be represented on the dotted line depending on the position of vertex 3 in relation to vertices 1 and 2, as shown in Fig. 3.
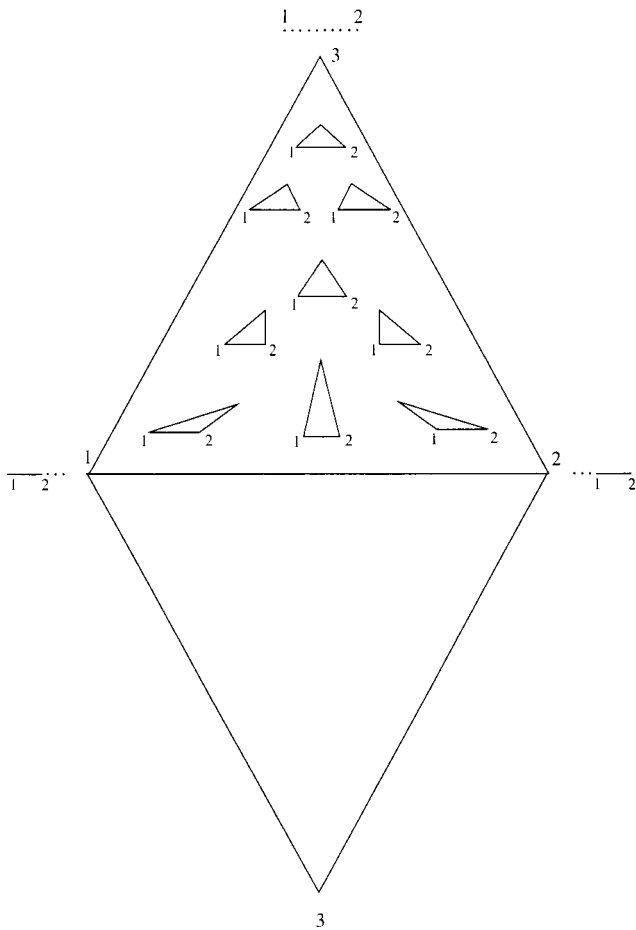
Fig. 3. Different shapes of triangles at different points of aerial coordinates are indicated.

More Than Three Landmarks

When there are more than three landmarks, say k, the possible number of triangles is $k(k-1)(k-3)/6$, but the configuration of landmarks can be fixed by choosing $(k-2)$ triangles. Considering two angles of each triangle, we have a total of $2(k-2)$ angles as shape measurements. The choice of $(k-2)$ triangles can be made in a number of ways. We have addressed the problem of the choice of triangulation in ref. 1. It was suggested that, for purposes of testing differences in shape and for discrimination between populations, any particular triangulation will do, provided we can find an appropriate stochastic model for the distribution of $2(k-2)$ angles. This may not be known, and in practice nonparametric or large sample methods may have to be used. It is recommended that a few possible triangulations may be chosen and statistical analysis done on each to test for consistency. It is suggested that Delaunay triangulation may have
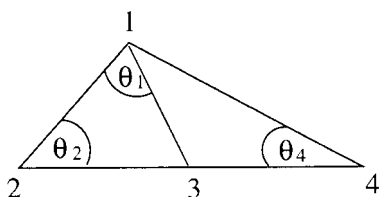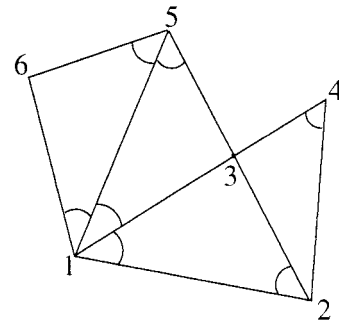

Fig. 5. TLM of which three (1, 3, 4) are collinear.

some advantages, because they provide triangles that are close to the equilateral.

If the problem is one of classification of individuals by shape, neural networks or other nonparametric procedures may be used to choose a set of angles, with appropriate transformations if necessary, which minimize the percentage of errors in classification.

If differences in shape between populations are established by appropriate tests, it may be necessary to explain the nature of differences by considering each possible triangle, as demonstrated in ref. 1. Some precautions are needed in triangulation in view of the possibilities that some landmarks may be collinear and some triangles may not be of the same type (L or R) for all sample objects.

The collinearity problem can be handled easily provided not all landmarks are collinear. Fig. 4 shows the case of four landmarks of which three landmarks, 2, 3, and 4, are collinear or nearly collinear.

We can choose two triangles and angles θ_1, θ_2 and θ_4, as shown in Fig. 4. We thus have one angle less to deal with in our analysis. Fig. 5 shows the case of 6 landmarks of which 2, 3, and 4 are collinear. In such a case, the choice of $4 = (6-2)$ triangles and 7 angles (one less because of collinearity), as marked in Fig. 5, may be chosen.

Although it is important to distinguish between L and R triangles, when the configuration of any set of three landmarks is considered, it would be simpler for purposes of global statistical analysis, when there are more than three landmarks, to choose a TLM where each triangle is of only one type in all the samples, which is usually possible in practical situations. In the extreme case, it may be possible to choose two landmarks such that all the other landmarks are on one side of the (base) line joining the two landmarks. Then the triangles chosen as indicated in Fig. 6 are all of one type.

The statistical analysis with such choice of triangles can be carried out as indicated in ref. 1.

Conclusions

The angles of triangles are natural SLR invariant measurements that can be made directly on an object. Differences in angular

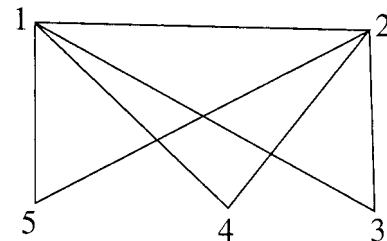**Fig. 4.** Four landmarks, three of them (2, 3, 4) nearly collinear.

Fig. 6. All triangles have the same base line (1, 2).

measurements between objects provide simple descriptors of shape differences and may be of value in practical applications. The problem of distinguishing between objects that are reflections of each other can be handled easily through the study of angles as described in *Objects Specified by Three Landmarks* (above). The distribution of the SLR invariant coordinates of Kendall and Bookstein, and the distances between landmarks of Lele can be examined through the distribution of angles, because the former are functions of the latter. The EDM is invariant to reflection also. We donote such a situation by SLRr invariant, where r stands for reflection.

The choice of a stochastic model for any set of SLR invariant measurements poses a difficult problem. Consider for instance the choice of a particular stochastic model for Bookstein's coordinates by using the line joining two chosen landmarks as the base line for registering each sample objects. The same model cannot hold if a different base line is chosen. So there is no way of making an *a priori* recommendation for the choice of the stochastic model without reference to the chosen base line. This problem does not arise if one considers all distances in EDM or all possible angles and finds a suitable stochastic model. Of course, if a subset of these measurements is used, the same difficulty arises. The same stochastic model may not hold for all subsets. This is why a preliminary examination of data for model selection is recommended for any chosen set of SLR invariant measurements before deciding on appropriate statistical methodology for analysis.

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