CHAPTER ONE

Modern Morphometrics

Dennis E. Slice

INTRODUCTION

The quantification of human proportions has a long history. As far back as the Middle Kingdom (*c*. 1986–1633 BC), Egyptian artisans used square grids and standard proportions to produce consistent depictions of human (and other) figures, even establishing different formulae for males and females (Robins, 1994) (Figure 1). The German anatomist Johann Sigismund Elsholtz formalized the scientific measurement of living individuals, "anthropometry," in his 1654 Doctoral dissertation (Kolar and Salter, 1996), and his particular interest in symmetry would appeal to many present-day anthropologists and general biologists. From the 19th century to the present day, the measurement and analysis of human beings and their skeletal remains have been a central theme in anthropology, though not always with beneficent motivation (e.g., Gould, 1981). During this time, anthropologists have often taken advantage of the state-of-the-art in statistical methodology, but they have not been just passive consumers of technological innovation. Indeed, pervasive interest in our own species, its artifacts, and our closest relatives has motivated and contributed much to the development of statistical methods that are now taken for granted in areas far afield from anthropology. The early work of the biometric laboratory established by Galton and Pearson bears witness to the vital

Dennis E. Slice • Institute for Anthropology, University of Vienna, Vienna, Austria.
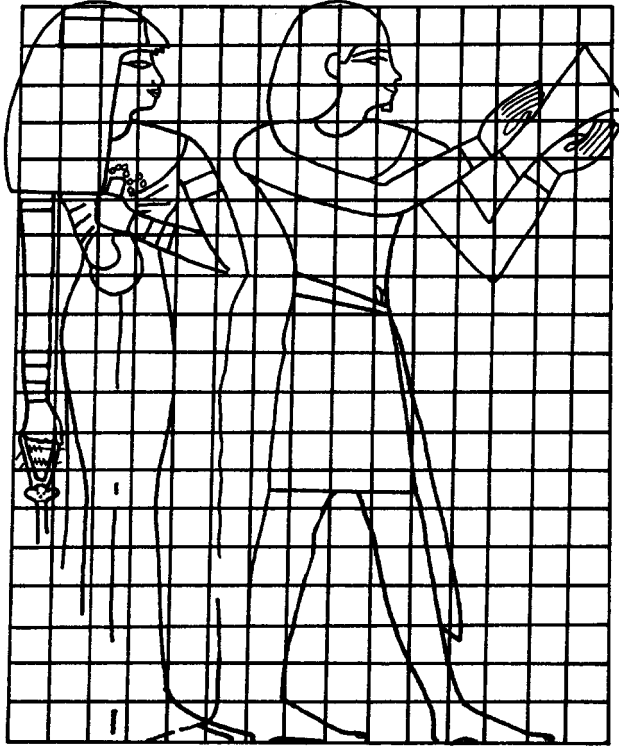
Figure 1. Nakht and wife (New Kingdom: *c*. 1570–1070 BC). Note same number of gridlines (18) from soles of feet to hairline and different waist heights for male and female figures. Grid completed from surviving traces. Drawing by Ann S. Fowler in Robins (1994). Reproduced by permission of the author.

interplay between the development of statistical methodology and anthropological research (e.g., Mahalanobis, 1928, 1930; Morant, 1928, 1939; Pearson, 1903, 1933).

This dynamic interaction between physical anthropology and statistical development continues today as new methods of shape analysis are inspired by anthropological problems. In turn, the availability of new morphometric tools opens new avenues of research or offers more powerful alternatives to traditional methods. The current volume provides a snapshot of this state of affairs in the early 21st century. Contributions include speculations on new directions in morphometrics, the development and extension of tools for shape analysis, and illustrations of how the latest morphometric methods have provided better and more powerful means to address basic research questions.

In this introductory chapter, I have tried to provide an overview of the basic terminology, concepts, and methods relating to the vast field that is modern morphometrics. My intention is to both relieve individual authors of having to reiterate methodological summaries and to provide an accessible introduction to students and researchers new to the field. Additional information to any level of technical detail can be found through the cited literature. Adams et al. (2004) provide a similar summary from a slightly different perspective. The reviews by Bookstein (1993, 1996) and Reyment (1996) include interesting and valuable historic components in addition to useful technical information.

We begin with some definitions.

DEFINITIONS

The field of morphometrics brings with it a plethora of terms and concepts that are seldom part of a biological, or even mathematical, curriculum. Slice et al. (1996) and the updated online version available at the Stony Brook website (see below) provide definitions of many of these. Here we present only the most fundamental terms necessary for an appreciation of modern morphometric methods.

Shape—the geometric properties of an object that are invariant to location, scale, and orientation.

Shape is the property about which we are most concerned here, and the definition contains two important points. The first is that we are interested in the geometric properties of an object. By focusing on geometry, we exclude properties, such as color and texture, that would otherwise meet the invariance requirements set out above (but see the Chapter 2 by Bookstein and Chapter 7 by Prossinger, this volume).

The second point is the invariance to location, scale, and orientation. By this we confine ourselves to geometric properties that do not change if the position or orientation of the specimen changes and, furthermore, would not change with the magnification or reduction of the object. This can be achieved either by the use of invariant measures, such as distance ratios or angles, or through methods that register all data into a common coordinate system, for example, the Procrustes superimpositions. In the latter case, the parameters for location, orientation, and scale built into the superimposition models are referred to as *nuisance* parameters. This is, in fact, only a technical designation as the relationship

between shape and these other sources of variation, especially and usually size, may be of scientific interest and not just sources of annoyance. Morphometricians use the term *form* to refer to data containing only size and shape.

Size measure—any positive, real-valued measure of an object that scales as a positive power of the geometric scale of the form.

For the most part, we are concerned here with linear measures of size, say $g(\mathbf{X})$, that can be characterized by:

$$g(a\mathbf{X}) = ag(\mathbf{X})$$

$\mathbf{X}$ is our data, $g(\mathbf{X})$ is our size measure, and a is some magnification factor. This equation means that if we compute our size measure for our original data and for the same data scaled by some factor, a, the size measure for the scaled data will be a times that of the original data. In more concrete terms, if we multiply our data by a factor of two, a proper, linear size measure will be doubled.

Size has long been recognized as an important component of the comparison of structures (e.g., Burnaby, 1966; Huxley, 1932; Mosimann, 1970). It tends to dominate the variability between sexes, populations, species, and even individuals, and the researcher is interested in methods for separating size variation from that due to other factors. Even though the above provides a precise definition for what is a proper size variable, there are any number of measures that are consistent with that definition, but each may behave differently in the presence of shape variation. For instance, the distance between two well-defined points on an object is a proper size measure, but for the same data set, different distances could indicate no changes, increases, or decreases in size when individuals or groups differ in shape. The question of which size measure to use is only partially answerable in that under certain circumstances some size measures have optimal properties that can be used to argue for their use, for example, centroid size described below. In other situations, or depending upon the ultimate research focus, a case can be made for other measures, for example, the cube root of body weight in allometry studies.

Shape variable—any geometric measure of an object that is invariant to the location, scale, and orientation of the object.

Shape variables are the grist for the analytical mill that will be used to answer research questions. Coordinates of well-defined points, sufficient sets of distances between such points, the coordinates of points used to sample an outline,

and angular differences used to encode the arc of a curve are all proper shape variables so long as they possess, or have been processed to achieve, the requisite invariances and capture geometric information about the structures for which they have been defined.

Geometric morphometrics—the suite of methods for the acquisition, processing, and analysis of shape variables that retain *all* of the geometric information contained within the data.

Geometric morphometrics brings together all of the acquisition, processing, analysis, and display methods for the study of shape that is characteristic of modern morphometric methods. Generally attributed to Les Marcus, to whom this volume is dedicated, and first used in print, perhaps, by Rohlf and Marcus (1993), this term is specifically meant to represent those methods that rigorously adhere to the exhaustive acquisition and analysis of shape information as defined above. This distinguishes these methods from what have been referred to as "traditional" morphometric methods that do not necessarily capture or retain sufficient information to reconstruct the spatial relationships among structures by which the measurements are defined. A key benefit to the use of geometric morphometric methods is that since all geometric information is retained throughout a study, results of high-dimensional multivariate analyses can be mapped back into physical space to achieve appealing and informative visualizations that are frequently not possible with alternative methods. The current volume is filled with examples.

MORPHOMETRIC DATA

The specific variables used in a morphometric analysis are chosen based on the question being investigated, the material under study, the equipment available for data acquisition, and to a greater or lesser extent the biases or experience of the researcher. However, there are several general classes of variables that are most frequently used for shape analysis. These classes each have their own benefits and/or limitations and admit different types of processing, analysis, and interpretation. Many of these are illustrated in Figure 2 and discussed below.

One thing that these different types of variables have in common is the assumption of the identity of data recorded for each individual, for example, the width of my head is the "same" variable as the width of your head. This implicit sameness of measurements may apply to individual variables, like head width,
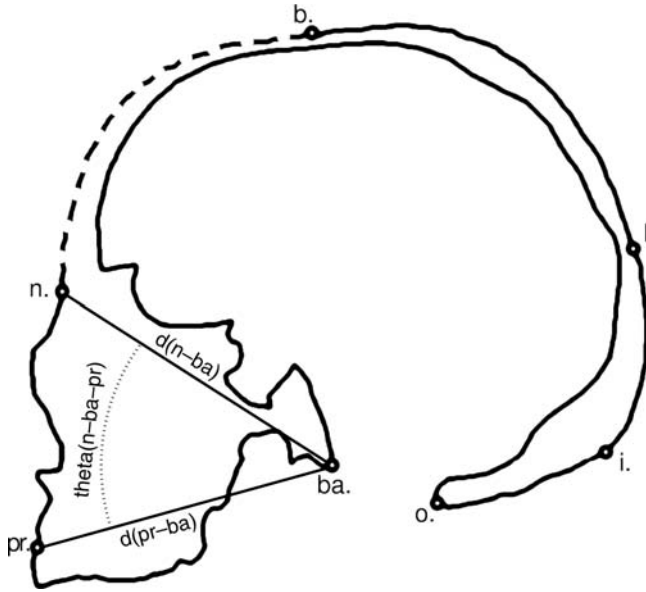
Figure 2. Morphometric data. Distances, angles, outlines, and landmarks: b.—
bregma, n.—nasion, pr.—prosthion, ba.— basion, o.—opisthion, i.—inion, l.—lambda.
See text for details.

but must sometimes be extended to suites of variables, such as an ordered series
of points recorded along a curve where several variables (the coordinates of the
points) are used to characterize a single structure of interest. This distinction
has implications in the processing of data and the interpretation of results. This
issue is discussed in greater detail as it arises in subsequent sections.

Distances, Ratios, and Angles

Distances are perhaps the oldest and most familiar variables used for morpho-
metric analysis. They are measured by ruler, caliper, or other specialized device
either between well-defined points, such as nasion, basion, and prosthion illus-
trated in Figure 2, or according to some rule, such as maximum cranial breadth
(Howells, 1973). They may be linear, straight-line distances, or they may be
curvilinear as, for example, the arclength of the frontal bone indicated by the
dashed line in the figure.

  Distances have the advantage of being inherently independent of orientation
and position. Size is the only information that must be removed from a set

of distances to achieve an analysis of shape. One way to meet this invariance is through the use of ratios or indices that encode the *relative* magnitudes of two distances. In Figure 2, one could use as a variable for shape analysis the ratio of the distance between nasion and basion, "d(n-ba)," to the distance between prosthion and basion, "d(pr-ba)," (×100). This is called the gnathic, or alveolar, index (e.g., Howells, 1989; Hanihara, 2000) and encodes some information about the shape of the face. However, it also introduces the statistical shortcomings associated with ratios (Atchley and Anderson, 1978; Atchley et al., 1976; Pearson, 1897).

A significant problem with distances is that unless they are carefully selected, one may not be able to determine the relative locations of all the endpoints of the measurements, and thus, they can omit information about the shape of the structure. In the current example, the distances between nasion and basion and between prosthion and basion (and their ratio) lack information about the positions of nasion and prosthion relative to each other. In fact, there are any number of face shapes that could have same nasion–basion and prosthion–basion distances. A way to address this deficiency is to add to our variables the angle formed by nasion–basion–prosthion, as shown in the figure as "theta(n-ba-pr)." Angles have the quite desirable property of being invariant not only to location and orientation as are distances, but also are invariant to size. The combination of the two distances and the angle fixes the relative positions of the three points up to a reflection, but mixing variables of different units may cause problems in multivariate analyses (like principal components analysis discussed below) that utilize information about the variances and covariances of variables. In such cases, one must resort to the standardization of the data and the analysis of correlations (not covariances). This introduces another level of abstraction between the analysis and the original specimens.

A better solution would be the addition of another distance variable—the distance between nasion and prosthion. This new set of three distances completely fixes the relative positions of the three points up to a reflection, is invariant to position and orientation, but still contains size information.

A shortcoming of both these solutions is that the selection of a sufficient set of variables to fix the shape of a structure becomes more difficult and tedious as the number of anatomical points or distance definitions increases. There is also the additional, unfortunate situation that such data (even if carefully selected to fix geometry) might yield multivariate summaries (sets of distances) of anatomy

that are impossible to realize in space of the original data, that is, in two or three dimensions (Lele and Richtsmeier, 2001; Rao and Suryawanshi, 1996).

Landmark Coordinates

Cartesian coordinates are another type of data that can address many of the problems of distances and angles, but they introduce new ones of their own. They are, in fact, a special set of distances—signed distances of specified points from a set of mutually perpendicular axes. When these points are anatomical structures on a specimen, they are often called landmarks and are frequently the same points used to define traditional distances or angles.

The collection of landmark coordinates can proceed either by the direct recording of point locations on the specimen using specialized digitizing hardware or by the use of software operating on representations of the specimen like digital images (two dimensional) or medical imaging data (three dimensional).

Figure 2 shows a number of landmarks familiar to physical anthropologists, but as presented their coordinates are undefined. We must first establish a coordinate system with respect to which we can record the positions of the landmarks. Once recorded, the advantages and efficiency of coordinates become apparent as every possible distance and every possible angle that could be defined using these landmarks can be computed using classical geometry and elementary trigonometry.

The analysis of landmark coordinates has its own problems, however. These arise because it is difficult, if not impossible, to define a biologically meaningful set of axes with which to record them. Attempting to define such axes with respect to anatomy, such as in the use of the Frankfurt orientation, nonlinearly transfers variability in the anatomical structures used to define the axes to the landmark coordinates. Instead, coordinate data are usually collected with respect to some convenient, but arbitrary, axes, and these axes are unique with respect to individual specimens. Coordinates so obtained thus have encoded in them orientation and location both with respect to the different axes used in their collection, and, equivalently, the different positioning of the specimens during data collection. The estimation and extraction of these nuisance parameters are important steps in modern, coordinate-based morphometrics, and various approaches to this problem are discussed below.

Besides the fundamental problem of coordinate comparability, landmark coordinates also differ in the quality of the information they encode. This has

been codified to a degree by Bookstein's (1991) classification of landmarks as Type I, II, or III. Type I landmarks are those defined with respect to discrete juxtapositions of tissues, such as triple points of suture intersections, Type II landmarks are curvature maxima associated with local structures usually with biomechanical implications, and Type III landmarks are extremal points, like the endpoints of maximum length, breadth, etc., defined with respect to some distant structure. Of these, the two- or three-dimensional locations of Types I and II are most often fully defined with respect to local morphology, and all dimensions are more-or-less biologically informative. Type III landmarks, however, are "deficient" in that they contain meaningful information only in line with the remote defining structure. Variation orthogonal to this direction has a substantial arbitrary component. A similar situation arises in the analysis of outlines discussed later.

Landmark coordinates afford us the opportunity to examine two topics that are more difficult to consider when dealing with other types of morphometric data. The first is the importance of triangles. Triangles, triplets of points, are the simplest geometric structure to have shape. A single point has only location, and a line segment defined by the two endpoints is completely described by its location, orientation, and length (size). Triangles have all of these attributes plus an additional component that is shape.

The second topic made more accessible by landmark coordinates is the consideration of the dimensionality of shape variation, that is, the number of dimensions (degrees of freedom) necessary to represent shapes. The triangle's simplicity makes it a good starting point. Any triangle in a plane requires only six numbers (the coordinates) for its complete geometric description. One degree of freedom is attributable to translation along each axis, one to scaling, and another to orientation. This results in $6 - 2 - 1 - 1 = 2$ degrees of freedom for variation in shape. Note that with only two dimensions left to encode shape we have a chance to graphically explore the structure of this space. This is one reason triangles are such an important part of research into shape theory.

Since the number of nuisance parameters are fixed for planar configurations, the general formula for the dimensionality of shape variation for p points in two dimensions is $2p - 2 - 1 - 1 = 2p - 4$. For three dimensional data the formula is $3p - 3 - 3 - 1 = 3p - 7$, where we have three dimensions in which to translate, three angles of rotation, but still one scale parameter to estimate. To be completely general, the dimensionality of shape variation for an arbitrary

number of points, p, in any number of dimensions, k, is $pk - k - k(k-1)/2 - 1$. We return to this topic in our discussion of shape spaces.

Outlines

Some anatomical structures, like brow ridges, orbital rims, or the foramen magnum, do not lend themselves to characterization by well-defined, discrete landmarks. They are, instead, partial or complete boundaries of another structure or traces of local maximum surface curvature that are continuous, one-dimensional features.

Such curve or outline data are usually represented by ordered sets of discrete point coordinates. These can be superficially similar to landmark data, but they are conceptually quite different. It is the entire underlying continuous structure that is to be compared across specimens and not the individual points used to characterize the outline. This deceptive similarity is even more reinforced when equal numbers of points are used to sample individual outlines. In fact, the coordinates of outline points only contain one piece of useful information— the position of the outline in the region around the sample point relative to its position at similar surrounding points.

This distinction usually requires special methods of analysis, and different methods are available for different types of outlines. In general, outlines can be classified as simple or complex, where simple outlines can be expressed as a single-valued function of some other variable, say $y = f(x)$, and complex outlines cannot. Outlines can also be closed or open, where closed outlines have no beginning or end and can be traced repeatedly without lifting the pencil or reversing direction on the outline, while open outlines have distinct starting and ending points. Rohlf (1990) provides a good survey of outline data and earlier methods for their analysis.

Two types of outlines are shown in Figure 2. The arc between bregma and nasion is the mid-sagittal profile of the frontal bone and could be treated as an open, simple curve. The mid-sagittal outline of the entire cranium in the figure would be a complex, closed outline.

Surfaces

Surfaces, two-dimensional regions within some defined boundaries, are not simple extensions of outlines. An immediate problem introduced in the

transition from the analysis of outlines to that of surfaces is that the concept of the one-dimensional ordering of sample points is lost. Thus, the analysis of surfaces requires unique morphometric methods that are few. Niewoehner (Chapter 13, this volume) uses projected grids to construct sets of points with which to sample surfaces, and the chapter by Gunz et al. in this volume (Chapter 3) provides some new possibilities for analyzing surfaces within the superimposition framework established for landmarks.

TRADITIONAL METHODS

The bulk of biological literature dealing with shape analysis has used methods that are today called "traditional" morphometrics (Marcus, 1990). These methods are characterized by the application of multivariate statistical procedures to collections of distances, distance ratios, and/or angles gathered to sample the shape of an object. Thus, such approaches are also known by the appellation "multivariate morphometrics" (Blackith and Reyment, 1971).

As described earlier, the distances, ratios, and angles used in traditional, or multivariate, morphometrics more often than not fail to encode all of the geometric information about the biological structures by which they are defined. Without recording and maintaining this geometry, morphometric analyses cannot provide an exhaustive assessment of shape variability or differences and may unnecessarily neglect important, but unanticipated, geometric relationships among the structures under investigation. Furthermore, such incomplete analyses make it difficult to produce graphical depictions of results that can be related to the actual physical specimens.

Bookstein et al. (1985) attempted to remedy these limitations with the development of the truss—a systematic series of measurements designed to fix the geometry (up to a reflection) of the anatomical landmarks. Another method for dealing with the same problem is to simply analyze all possible distances between the landmarks of interest. This is the basis for the Euclidean Distance Matrix Analysis (EDMA) methods described in the section on coordinate-free methods.

SUPERIMPOSITION-BASED MORPHOMETRICS

The deficiencies of distance- and angle-based morphometrics can be addressed by the direct analysis of the coordinates of the landmarks by which traditional

measurements are, or could be, defined. Raw coordinates, however, also contain information about the location, orientation, and size of the configuration of landmarks that must be factored out or subtracted off to achieve an analysis of shape. Proper geometric morphometric methods do not simply discard the information in these nuisance parameters, but, rather, sequester it (a phrase due to Bookstein) into a separate suite of non-shape variables available for later consideration.

One way of partitioning the total variation of raw coordinate data into shape and non-shape components is by superimposing all of the configurations within a common reference system and scaling them to a common size. Various ways to do this are described in the following sections.

The data used to illustrate some of the methods are presented in Figure 3 (left) that shows a set of five landmarks on a gorilla scapula whose two-dimensional coordinates were recorded from scanned photographs (provided by Andrea Taylor) using tpsDig (Rohlf, 2001). The complete data set consists of coordinates for 52 male and 42 female adult, west African lowland gorillas, and we seek to compare sexes with respect to scapular shape. Taylor and Slice (Chapter 14, this volume) use similar data (though not exactly the same landmarks) to investigate biomechanical predictions of scapular shape in *Pan* and *Gorilla*.

Two-Point Registration

There are any number of ways one could define measures of size, location, and orientation for a particular set of landmark coordinate data. For two-dimensional data one could simply specify the coordinates of one landmark to define location and the length and direction of a line segment, or baseline, between that point and another to define orientation and scale. This is the "two-point registration" extensively developed by Bookstein (1986, 1991). It is also often called base-line registration or edge-matching.

The operations involved in the two-point registration of planar configurations can be expressed quite concisely in complex notation (Bookstein, 1991), but here and throughout this chapter I use the more general matrix notation that is readily extended to three- and higher-dimensional data. Let

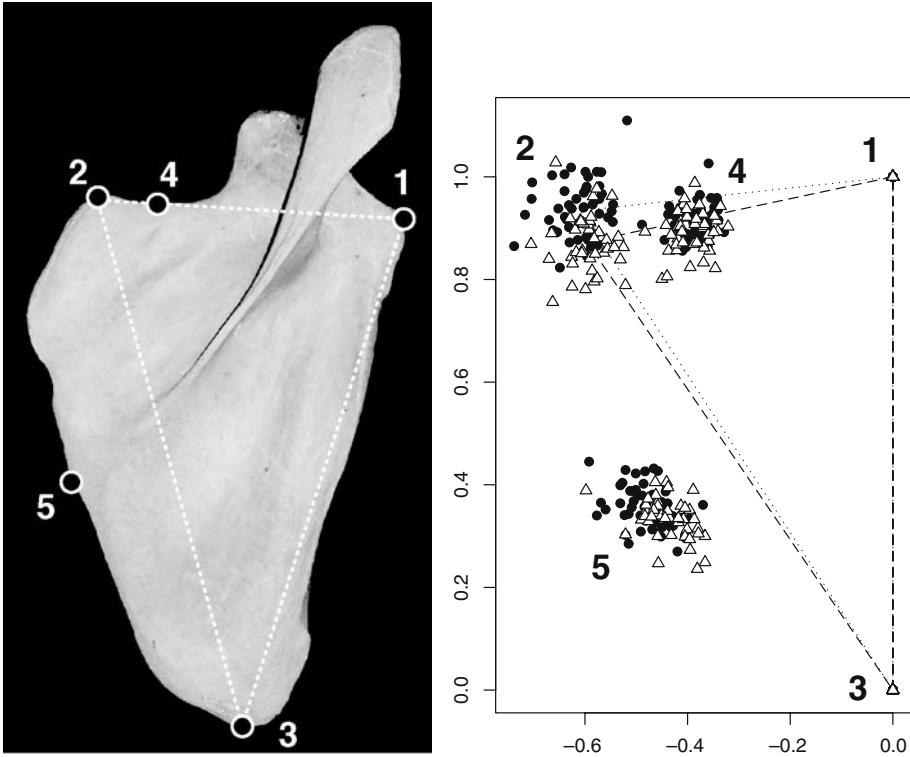$$\mathbf{X} = \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix}$$

Figure 3. Data used to illustrate various morphometric methods. Left, gorilla scapula and landmarks. Right, boths males (circles, $n = 52$) and females (triangles, $n = 42$) superimposed using two-point registration with landmarks 1 and 3 as the baseline. Mean triangles between extremal angles shown for males (dotted) and females (dashed). Superimposition done with Morpheus et al. (Slice, 1998). Plot generated with R (http://www.r-project.org).

be the x and y coordinates of the three labeled vertices of a triangle, and let us specify that we will use points in the first and second position for our registration. Subtracting off location as encoded in the coordinates of the first point we get

$$\mathbf{X}' = \mathbf{X} - \mathbf{1t}$$

$$= \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \begin{bmatrix} x_1 & y_1 \end{bmatrix}$$

$$= \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix} - \begin{bmatrix} x_1 & y_1 \\ x_1 & y_1 \\ x_1 & y_1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 \\ x_2 - x_1 = x_2' & y_2 - y_1 = y_2' \\ x_3 - x_1 = x_3' & y_3 - y_1 = y_3' \end{bmatrix}$$

Next, we rotate the baseline so that it is in some standard alignment that is usually taken to be coincident with the positive x-axis:

$$\mathbf{X}'' = \mathbf{X}'\mathbf{H}^t = \begin{bmatrix} 0 & 0 \\ x_2'' & 0 \\ x_3'' & y_3'' \end{bmatrix}$$

$$\mathbf{H} = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

$$\theta = \cos^{-1}\left((\mathbf{x}_2' \cdot \mathbf{e}_1) \big/ \left(\sqrt{\mathbf{x}_2' \cdot \mathbf{x}_2'} \sqrt{\mathbf{e}_1 \cdot \mathbf{e}_1} \right) \right)$$

$$\mathbf{x}_2' = \begin{bmatrix} x_2' & y_2' \end{bmatrix}^t$$

$$\mathbf{e}_1 = \begin{bmatrix} 1 & 0 \end{bmatrix}^t$$

Finally, we divide by the length of the baseline, which because of the standardizations so far, is simply x_2'':

$$\mathbf{X}''' = \frac{1}{x_2''}\mathbf{X}'' = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ x_3''/x_2'' = x_3''' & y_3''/y_2'' = y_3''' \end{bmatrix}$$

These operations are applied separately to all triangles in a sample. Notice that after these transformations, the coordinates of the first two landmarks are fixed at $(0, 0)$ and $(0, 1)$ for any triangle in the sample. Thus, all information about the shape of a triangle is encoded in the coordinates of the third landmark (x_3''', y_3'''). These are known as Bookstein coordinates or Bookstein shape coordinates for triangles. However, this same method was used by Galton (1907) to characterize facial profiles.

For more than three landmarks, one simply extends the rows of the $\mathbf{X}$ and $\mathbf{1}$ matrix and applies the same transformations to any additional landmarks. For

each additional landmark, the dimensionality of the shape variation is increased by two, since the number of dimensions lost due to the standardizations is fixed.

One might ask, how does the choice of baseline effect the resulting shape coordinates and can such effects impact the findings of the analysis? As Bookstein (1991) points out, for small shape variation the use of different baselines effects mainly translations, rotations, and rescalings of the scatter of shape coordinates that will not effect multivariate statistical analysis. The magnitude of the rescaling effect is a function of the relative lengths of alternative baselines, and problems do occur for baselines approaching zero length. Rohlf (2000) showed, for instance, that the power of statistical tests for group differences is severely reduced when the landmarks defining the baseline are nearly coincident. This is not a serious problem in practice, since investigators are likely to make more reasonable choices of baseline that span the object under consideration.

It is somewhat difficult to extend the Bookstein coordinates to three-dimensional data. One possibility was implemented by Slice (1994) and described by Dryden and Mardia (1998). This involves the specification of a third point to establish a baseplane. The data are then transformed, as before, so that the first point is situated on the origin and the vector between first and second points is coincident with the positive x axis. Finally, the configurations are rotated such that the plane defined by the three base points is coincident with the x, y plane with the third point on the positive side of the y axis. The algebra is a bit more complicated than in the two-dimensional case, but the principles remain the same. These operations result in the variation at the third landmark not being completely removed, yet it is not fully three dimensional, either. There can be up to two dimensions of variation at this point, and the interpretation of such results becomes much more difficult. As a result, this method of three-dimensional shape variable construction has been little used.

An example of using two-point registration to construct Bookstein shape coordinates is illustrated in Figure 3 (right), that shows the registration of the sample of male and female gorilla scapula data mentioned above. The triangle between the extreme angles is highlighted, but the entire five-landmark suite of data can be analyzed through the coordinates of the three non-baseline points. Apparent differences between male and female lowland gorillas can be seen in the differences in the locations of sex-specific scatter at the various landmarks.

Procrustes Superimposition

Instead of using just one or two landmarks to estimate the requisite parameters, one might consider methods to incorporate information from all of the landmarks in a configuration. This is the basis for the most widely used method in geometric morphometrics today—the Procrustes superimposition. Major theoretical investigations into Procrustes-based methods are due to David Kendall (1984, 1985, 1989), who was motivated, in part, by questions in archeology (Kendall and Kendall, 1980). Specifically, it was proposed that megalithic sites in England were linearly situated. The statistical question, then, is how can one tell if sets of points are more linearly arranged than one would expect from random placement, and Kendall's approach was to develop the theoretical constructs to test if triangles formed by triplets of these points (sites) were flatter than expected by chance. Since there is no obvious correspondence between sites like there is in anatomical landmarks, Kendall's investigations included a component allowing for the permutation of vertices.

Kendall's work resulted in the deep and elegant mathematical results that form the basis of much of modern shape theory. Kendall's and Bookstein's research intersected in Bookstein's (1986) *Statistical Science* paper for which Kendall was a discussant. Goodall (1991) provides an extensive treatment of the practical and theoretical aspects of the Procrustes methods, and Small (1996) and Dryden and Mardia (1998) are recent statistical texts.

Much theoretical work on Procrustes methods is due to Kendall, but much applied work preceded his endeavors. The earliest known matrix formulation of the two object Procrustes method is due to Mosier (1939) for psychometric application. The matrix formulation of Generalized Procrustes Analysis (see below) for superimposing samples was set forth by Gower (1975), who was concerned with comparing the multivariate scoring of carcasses by meat inspectors. Similar algebraic and geometric comparisons of landmark configurations for anthropological purposes were used by Sneath (1967), and Cole (1996) points out that the earliest use of this technique was, in fact, suggested by the eminent anthropologist Franz Boas (1905) to address shortcomings of the Frankfurt orientation.

Procrustes superimposition is a least-squares method that estimates the parameters for location and orientation that minimize the sum of squared distances between corresponding points on two configurations. A least-squares estimate for scale is also available, but its use does not lead to symmetric results between configurations of different sizes, so all specimens are most often scaled to a

standard size. When the least-squares estimate of scale is used, the analysis is called a full Procrustes analysis. It is termed a partial Procrustes analysis in the usual case when configurations are scaled to a common size. The square root of the sum of squared coordinate differences after superimposition is a measure of the shape difference between configurations.

For a particular configuration of p landmarks in k dimensions written as a $p \times k$ matrix, $\mathbf{X}_1$, we model difference in coordinate values relative to a mean-centered reference configuration of corresponding landmarks, $\mathbf{X}_0$, by

$$\mathbf{X}_1 = \frac{1}{r_1}(\mathbf{X}_0 + \mathbf{E}_1)\mathbf{H}_1^t + \mathbf{1}\mathbf{t}_1,$$

indicating that numerical values in $\mathbf{X}_1$ differ from those in $\mathbf{X}_0$ by scaling, $1/r_1$, rotation, $\mathbf{H}_1^t$, translation, $\mathbf{t}_1$, and actual shape differences, $\mathbf{E}_1$, which would include measurement error. $\mathbf{1}$ is a $p \times 1$ matrix of ones. Some rearrangement leads to

$$r_1(\mathbf{X}_1 - \mathbf{1}\mathbf{t}_1)\mathbf{H}_1 = \mathbf{X}_0 + \mathbf{E}_1$$

that exposes the shape differences in $\mathbf{E}_1$. The estimates of the requisite parameters are

$$\mathbf{t}_1^t = \frac{1}{p}\mathbf{X}_1^t\mathbf{1} = (\bar{x}_1, \bar{y}_1)^t,$$

$$\mathbf{H}_1 = \mathbf{V}_1\mathbf{\Sigma}_1\mathbf{U}_1^t, \quad \text{where } \mathbf{X}_1^t\mathbf{X}_0 = \mathbf{U}_1\mathbf{D}_1\mathbf{V}_1^t,$$

and

$$r_1 = \frac{1}{\sqrt{\mathrm{tr}\left((\mathbf{X}_1 - \mathbf{1}\mathbf{t}_1)^1(\mathbf{X}_1 - \mathbf{1}\mathbf{t}_1)\right)}} = \frac{1}{\mathrm{CS}_1}$$

It can be shown fairly easily (Boas, 1905; Sneath, 1967) that to superimpose two configurations to minimize the sum of squared distances between landmarks one need only translate the configurations so that the average coordinate in each dimension is the same for both specimens. The exact coordinates of the average location are irrelevant, so both configurations are centered on the origin as indicated in the $\mathbf{t}_1$ vector above.

$\mathbf{H}_1$ is an orthogonal matrix that rigidly rotates the $\mathbf{X}_1$ configuration about the origin to minimize the sum of squared distances between its landmarks and the corresponding landmarks of $\mathbf{X}_0$. It is computed as the product of three matrices, of which $\mathbf{U}$ and $\mathbf{V}$ are derived from the singular value decomposition

of the product of the transpose of X_1 and X_0. The matrix Σ is a diagonal matrix with positive and negative ones along the diagonal, each having the same sign as the corresponding element of D_1, which is also diagonal. This substitution is to prevent any stretching of X_1 to achieve a better (in a least-squares sense) fit to X_0—the non-unity elements of D_1 correspond to stretching or compression. As expressed, the rotation could also effect a reflection to improve fit. If such is not desired, H_1 must be tested to see if it is reflecting (has a negative determinant) and adjusted accordingly (change the sign of the diagonal element of Σ in the same position as that of the smallest value of D_1).

The scalar, r_1, is the scale factor and is most frequently computed as the inverse of the configuration's centroid size (CS). Each configuration involved in an analysis is similarly scaled so that all configurations have a standard size—unit CS. CS is used because small, circular, random variation at individual landmarks does not generate a correlation between shape and this measure of size (Bookstein, 1991). It is also the length of the vector containing all of a centered specimen's landmark coordinates written out as a *pk* row or column.

The above formulae can all be derived using matrix notation, and they apply to two-, three-, or higher-dimensional configurations of landmarks. One simply appends columns to the various X_i and other matrices to allow for the additional coordinates.

So far, the discussion has focused on the superimposition of one configuration of landmarks onto another, specified configuration. Such fitting of two specimens has been called ordinary Procrustes analysis, OPA (Goodall, 1991). Researchers, though, are usually interested in the analysis of samples of more than two specimens. In such cases, it is usual to relate members of a sample to their mean. The problem is that meaningful mean coordinates cannot be computed prior to superimposition and superimposition requires knowledge of the mean configuration. The solution to this is an iterative process in which any specimen is initially selected to stand for the mean. All of the configurations in the sample are fit to that reference, then a new mean is computed as the arithmetic average location of the individual landmarks in the sample and scaled to unit CS. The process is repeated, fitting the sample to the new estimate, and it is guaranteed to produce monotonically decreasing sum-of-squared deviations of the sample configurations around the estimated mean (Gower, 1975). The procedure is terminated when this sum-of-squares no longer decreases by some critical value or, equivalently, when the change in mean estimate from one iteration to the next is deemed negligible. The term used for the fitting of a sample

onto an iteratively computed mean is generalized Procrustes analysis (GPA) (Gower, 1975), and it is the superimposition method used for most geometric morphometric studies.

Figure 4 shows the effects of the separate translation, scaling, and rotation steps of a GPA on the gorilla data. The triangles between the extreme angles of the scapulae are highlighted in the last panel for later reference, but the superimposition was based on all five landmarks. In general, one can see a "condensation" of the original variability into nearly circular, apparently unstructured variation around the mean landmark locations as the superimposition translates, scales, then rotates the configurations to minimize their sum of squared differences to the iteratively computed mean. Also, one can see subtle differences between the males and females in average landmark location that suggests sexual dimorphism in scapula shape (tested and visualized below). Both sexes were fit to the grand mean by generalized Procrustes superimposition, and the sex-specific means computed separately afterwards.

In this volume (Chapter 9), McKeown and Jantz compare the results of coordinate-based, generalized Procrustes analysis with those of traditional, distance-based data in the investigation of spatio-temporal affinities in samples of Native American crania.

Resistant Fit

One criticism of the Procrustes superimposition is of its use of a least-squares criterion in estimating the translation and rotation parameters (Seigel and Bensen, 1982). If one or a few landmarks are greatly displaced relative to the others in one specimen or in one sample, these localized differences would inflate the squared distance between configurations. The least-squares Procrustes methods, therefore, spread such large local differences across all of the landmarks to produce a number of smaller differences. This is called the Pinocchio effect referring to the shape of the puppet's head before and after lying. The only real difference would be in the length of the nose, but a Procrustes superimposition would suggest differences over the entire head.

An approach developed to help identify local differences is resistant fitting (Rohlf and Slice, 1990; Seigel and Bensen, 1982; Slice, 1993a, 1996). These are methods based on the use of medians or medians of medians (repeated medians) to estimate the translation, scale, and rotation parameters for superimposition. Seigel and Benson (1982) describe the method for pairs of two
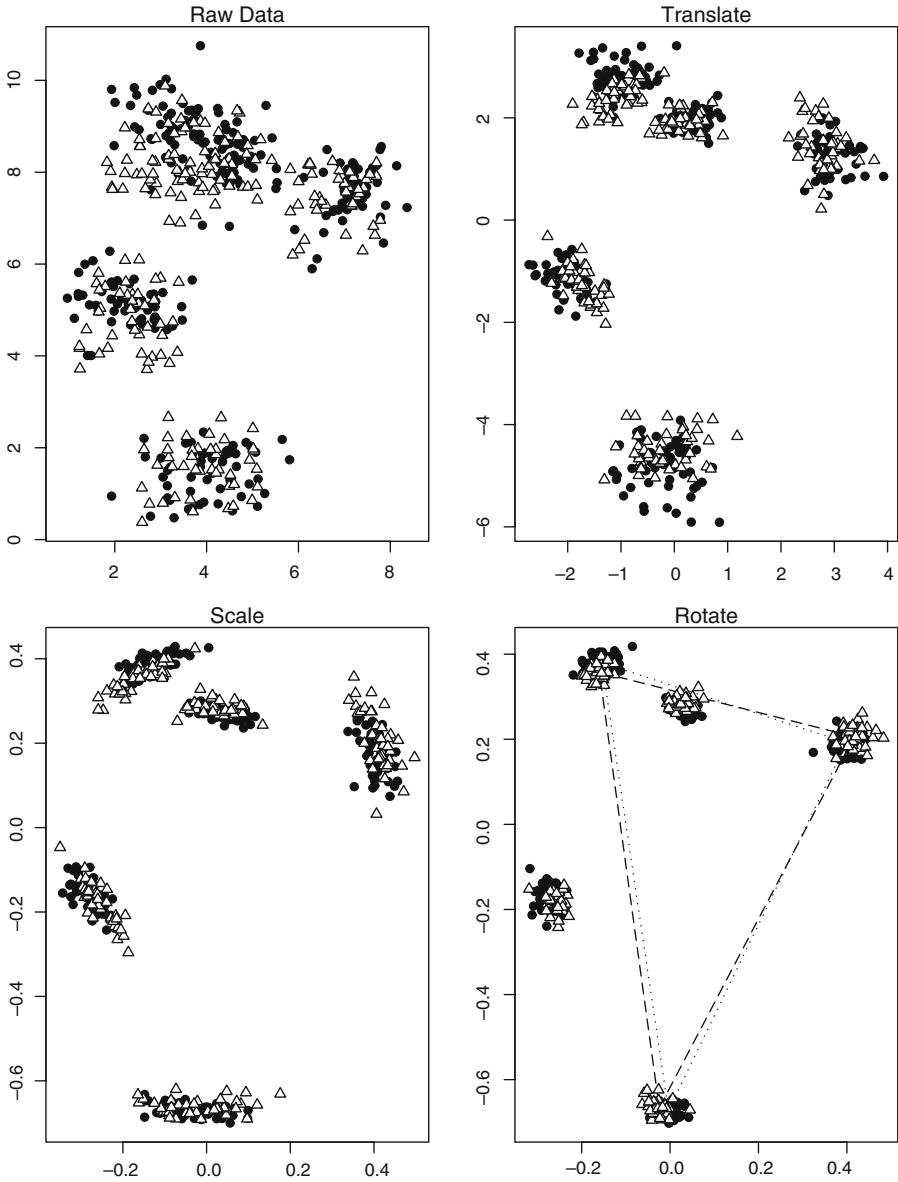
Figure 4. Generalized Procrustes superimposition of the scapula data. Upper left, raw data as digitized. Upper right, data after translation to the origin. Lower left, translated data after scaling to unit CS. Lower right, translated and scaled data after least-squares rotation of individual specimens to their iteratively-computed sample mean. Mean triangles between extremal landmarks shown for males (dotted) and females (dashed). Superimposition done with Morpheus et al. (Slice, 1998). Plots generated with R (http://www.r-project.org).

dimensional configurations, Rohlf and Slice (1990) extend the method to allow for the generalized resistant fitting of two-dimensional data, and Slice (1993a, 1996) develops methods for the generalized resistant fitting of three and higher dimensional samples based on similar work for two configurations by Siegel and Pinkerton (1982). Dryden and Mardia (1998) discuss other alternatives.

Despite its intuitive appeal, the median-based results do no allow nearly as sophisticated a theoretical development as the Procrustes methods (e.g., Dryden Mardia, 1998; Kendall, 1984, 1985; Small, 1996). The current consensus is that the Procrustes methods are to be preferred for use in statistical analysis. The resistant methods, though, can still be useful, especially through the comparison of the results of Procrustes and resistant superimpositions (e.g., Slice, 1996) and, like two-point registration, can be used for suggestive visualizations after statistical analyses based on Procrustes methods have been performed.

SHAPE SPACES

The square root of the sum of squared differences of corresponding landmark coordinates in two (partial) Procrustes-superimposed figures is equivalent to the distance between the tips of the two vectors containing all of the landmark coordinates for each of the two configurations. Given this "Procrustes distance," it is possible to ask about the geometry of a space in which the distance between all points representing shapes is that same distance. Such an inquiry was a major component of the theoretical work of Kendall (1984, 1985) who was able to fully describe the geometry of what is generally referred to as "Kendall's shape space."

Some of Kendall's key results are that the shape space of planar triangles is two-dimensional, but that it is non-Euclidean (curved) and isometric to the surface of a sphere of radius $\frac{1}{2}$. This is consistent with our earlier conclusion about the dimensionality of the shape space for triangles obtained by counting degrees of freedom. Because of the spherical geometry of shape space, Kendall and other mathematicians often prefer to work with great-circle, or Riemannian, distance, ρ, instead of the straight-line, or chord, partial Procrustes distance, d, but there is a simple relationship between the two, $\rho = 2\sin^{-1}(d/2)$ for two-dimensional configurations (Kendall, 1984).

An important corollary of Kendall's results for planar triangles is that it is possible to visualize shape space for such data. Figure 5 shows Kendall's shape
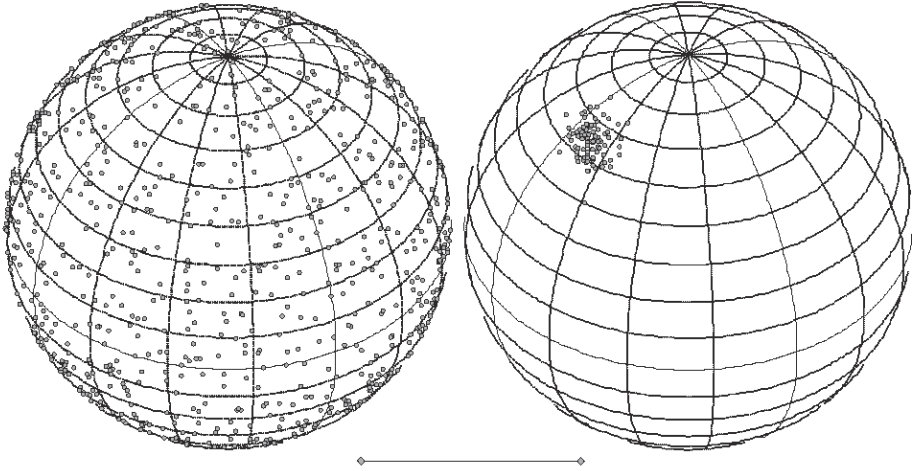
Figure 5.   Representation of Kendall's shape space for triangles. Left, 2,000 random triangles generated by normal displacement of vertices from the origin. Right, 94 gorilla scapulae. Males and females not distinguished. Scale bar is 0.5 units. Plots created with tpsTri (Rohlf, 2002).

space for triangles. The plot on the left illustrates one of his other results—that triangles generated by the independent, normal displacement of points from the origin are uniformly distributed in shape space (Kendall, 1984). The positions of 2,000 such points are shown. The right plot illustrates another important point—that the biological variability of interest to researchers is usually concentrated in a relatively small area of shape space. The right panel shows the positions of the triangles formed by the extreme angles of the 94 gorilla scapulae. This is an important feature of biological material for the statistical analysis of shape data. It is also interesting to note that Bookstein shape coordinates are a special, stereographic projection of points in Kendall's shape space (Small, 1996).

   Kendall's results are based on the shape distance between two configurations of landmarks. The situation is somewhat different for the generalized Procrustes analysis, where multiple configurations in a sample are fit to in iteratively-computed mean (Slice, 2001). In that case, the geometry of superimposed planar triangles is that of a hemisphere of unit radius. The key difference in the two geometries arises from the fact that in Kendall's shape space the distances between all points are Procrustes distances. With GPA, the specimens are individually superimposed onto the consensus. Only distances between individual specimens and the consensus equal the Procrustes distance on the GPA
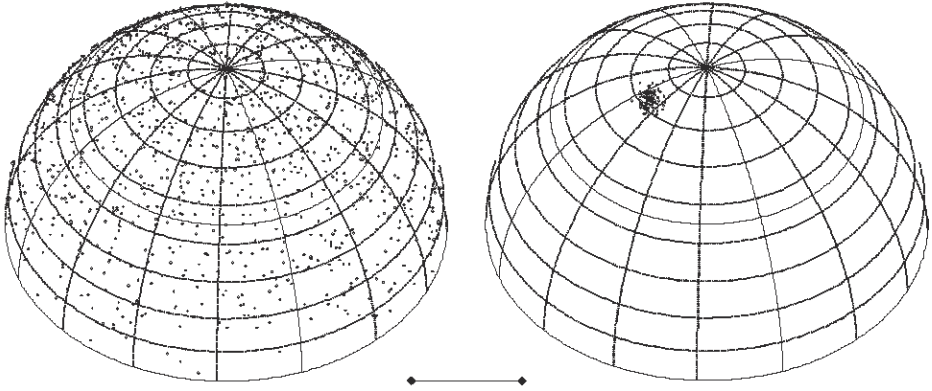
Figure 6. The generalized Procrustes hemisphere for triangles. Data are the same as in the previous figure. Scale bar is 0.5 units. Plots created with tpsTri (Rohlf, 2002).

hemisphere. Distances between specimens do not. For more than three landmarks in two dimensions, the geometry of GPA space is still the surface of a hyper-hemisphere. Like Kendall's shape space, though, the geometry for configurations in three or more dimensions is likely to be much more complicated (Dryden and Mardia, 1993; Small, 1996).

The GPA spaces for the random triangles and gorilla scapulae are illustrated in Figure 6. Rohlf (1999a) and Slice (2001) discuss the simple relationship between the Kendall's shape space, the GPA hemisphere, and various projections into linear tangent spaces (see section on Multivariate analysis). These relationships, however, hold only for planar triangles (Slice, 2001).

MULTIVARIATE ANALYSIS

The purpose of the superimposition methods is to register landmark configurations in a common coordinate system in which the coordinates of the landmarks can be used as shape variables. This is not an end in itself, but provides the researcher with suitable data to explore the structure of shape variation, assess the significance of differences in mean shapes, relate the observed variation to extrinsic factors, and the like. For this, the whole suite of multivariate methods familiar to traditional morphometrics is available for the analysis of differences and variation in superimposed landmark coordinates. For these methods, the student of morphometrics is free to consult standard texts on multivariate statistics, such as Johnson and Wichern (1982) or Krzanowski (1988). One

especially useful text is Carroll and Green (1997) that focuses on the geometric interpretation of multivariate analyses. This nicely compliments the geometric theme at the core of modern morphometric analysis.

There is one caveat in the application of parametric multivariate methods to Procrustes-processed data. The theory underlying many multivariate methods assumes a linear, Euclidean space. We have seen, though, that the geometry of Kendall's shape space and that of generalized Procrustes analysis is non-linear, thereby violating this key assumption. One way around this problem is to analyze not the Procrustes coordinates, but their projection into a linear space tangent either to Kendall's shape space or the Procrustes hemisphere. Rohlf (1999a) and Slice (2001) describe and assess various projections (see also Dryden and Mardia, 1998 and Small, 1996). In general, an orthogonal projection from the GPA hemisphere to a linear space tangent at the sample mean seems to best preserve the distances between specimens, though for the relatively small variation found in most biological samples any of the reasonable alternative projections does a fairly decent job and, conversely, using no projection does not violate the assumptions of a linear space too badly.

Singleton in this volume (Chapter 15) uses principal components analysis and regression of Procrustes-superimposed landmarks to investigate allometric, functional, and phylogentic aspects of the shape of masticatory structures in cercopithicines.

An alternative to parametric methods with their restrictive assumptions is the use of nonparametric, randomization tests to effect similar tests (Bookstein, 1997). See, for instance, Manly (1997) for a discussion of randomization and related non-parametric tests. In the case of the gorilla data used so far, differences in mean shape between male and female gorillas are significant for both Bookstein's shape coordinates ($p = 0.001$) and GPA coordinates ($p = 0.001$) when judged by a simple randomization test that compares the observed between-group sum-of-squares to the same value for 999 random shufflings of group membership. Sex accounted for about 12% of total sample variation in Bookstein shape coordinates (Figure 3) and about 11% in GPA coordinates (Figure 4, lower right).

Similar permutation tests are used here by Wescott and Jantz (Chapter 10) to document recent, secular change in the craniofacial shape of Black and White Americans, and Bastir et al. (Chapter 12) use randomized version of partial least-squares analysis (Bookstein, 1991) to examine the integration of the cranium and mandible in hominoids.

VISUALIZATION

Once one has superimposed the configurations, computed means, quantified variation, and/or assessed significant differences or associations, one can take advantage of a geometric approach to morphometrics to generate visualizations of differences, associations, variability, etc. in the space of the original specimens. There are several ways to do this.

Vector Plots

Perhaps the simplest method for visualizing the results of a geometric morphometric analysis is with vector plots. This is done by taking the coordinates of the landmarks of a key configuration, say, a grand mean or the mean of one group in a two-group comparison, and drawing vectors from the landmark locations on that configuration to points specified by the results of your statistical analysis. For instance, say you are comparing two mean shapes, $\bar{\mathbf{X}}_1$ and $\bar{\mathbf{X}}_2$, which have been computed after fitting the members of both samples to their joint grand mean. The relevant vectors for display might then be the difference vectors between the two groups, $\Delta\bar{\mathbf{X}}_{1,2} = \bar{\mathbf{X}}_2 - \bar{\mathbf{X}}_1$. One would then plot the landmarks of $\bar{\mathbf{X}}_1$ and draw vectors from them to the points $\bar{\mathbf{X}}_1 + \Delta\bar{\mathbf{X}}_{1,2}$. Note that these will be just the locations of the points of $\bar{\mathbf{X}}_2$. One can also exaggerate (or diminish) differences by multiplying the displacement matrix by some appropriate factor, for example, $2\Delta\bar{\mathbf{X}}_{1,2}$ would double the difference between the two groups, but preserve the direction of the differences. For more than two groups one could plot all pairwise differences as vector differences or plot the differences between group means and the grand mean.

This type of plot is shown in Figure 7 where the shape difference between average male and female gorilla scapula from a five-landmark GPA are shown. The reference configuration is that of the average male, and the vectors (their length multiplied by a factor of two) point in the direction of the shape of the average female.

The machinery of geometric morphometrics and linear statistical analysis make it equally easy to plot results from analyses more complicated than mean comparisons. The results of familiar multivariate analyses like principal components analysis, canonical variates analysis, etc. are expressed as linear combinations of the original variables—the superimposed landmark
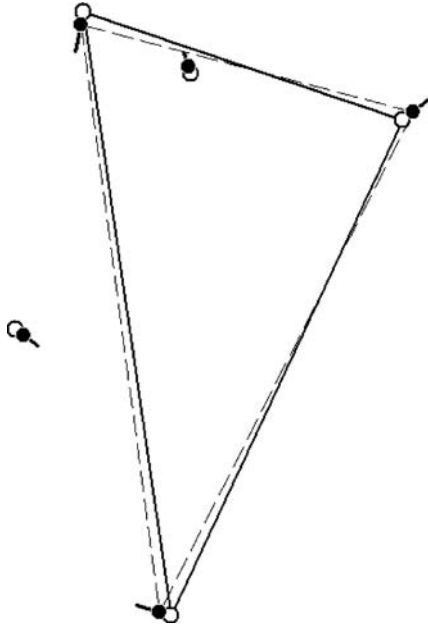
Figure 7. Difference between male and female gorilla scapulae shown as vectors (magnified ×2). Open circles are mean male landmark coordinates. Solid circles are mean female coordinates. Plot created with Morpheus et al. (Slice, 1998).

coordinates. Furthermore, these results are usually in the form of vectors scaled to unit length. To visualize, say, the shape variability captured by the principal component axis associated with the largest amount of variation (usually called the 1st principal component, the one with the largest eigenvalue), one takes the grand mean configuration and adds to it the coefficients of the first PC to generate the positions of the vector tips as described previously. The position of the tips of these vectors corresponds to the shape of a configuration displaced one unit in the positive direction along the first principal component (It is often not appreciated, but the positive/negative directions of individual components are perfectly interchangeable. They are defined only up to reflection). Likewise, the coefficients from a multiple regression of shape onto some other variables can be used to generate the predicted shape for any value of the independent variables, and this can be used as to define the tips in a morphometric vector plot.

One problem with vector plots is that it becomes irresistibly tempting to discuss them in terms of individual points moving or being displaced. Such statements are not justifiable simply on the basis of the plots, and this kind of

information is generally unknowable given landmark coordinate data. Consider two triangles of different shapes. Which landmarks in one are in different relative locations compared to the other? One cannot say. The procedures used for shape analysis examine shape differences in their totality, not one landmark position at a time. So, is there a graphical device that can take into account the relative positions of all the landmarks? Yes, the thin-plate spline.

Thin-Plate Splines

The thin-plate spline was adapted for use in morphometrics by Bookstein (1989, 1991). It addresses both the problem of integrating information about the relative locations of all landmarks and the classic problem posed by D'Arcy Thompson (1942) of expressing shape differences between two specimens as a global mapping of the Cartesian space of one specimen into that of another. This latter goal, in fact, has a much longer history with Renaissance artists like Albrecht Dürer using deformed grids to express normal variation and methods of pictorial caricature (Bookstein, 1996b).

The theoretical justification for the method is rather complicated, but the algebra is relatively straightforward. First, one configuration, usually a group or grand mean, is used as a reference and the differences between the landmark locations and those of another specimen, the target, along each coordinate axis are processed separately. That is, one computes the required parameters for the differences in x coordinates between the two specimens, then the y coordinates, and so on. For each coordinate dimension, the differences between the two configurations are treated as displacements at right angles out of the plane of the reference configuration (for the two-dimensional case). The equations so derived are then recombined to express the totality of differences between the two configurations (Figure 8).

To achieve this, we need the coefficients for the equation:

$$f(x, y) = a_1 + a_x x + a_y y + \sum_{i=1}^{p} w_i\, U\left((x_i, y_i) - (x, y)\right) \qquad (1)$$

This function maps a pair of coordinates, (x, y), to a scalar incorporating inform- ation about the possesive proximity to each of the p reference landmarks. What we seek are the coefficients such that that scalar at the positions of the landmarks in the reference configuration equals the heights above or below the plane that, in turn, correspond to the coordinate differences between the reference and the
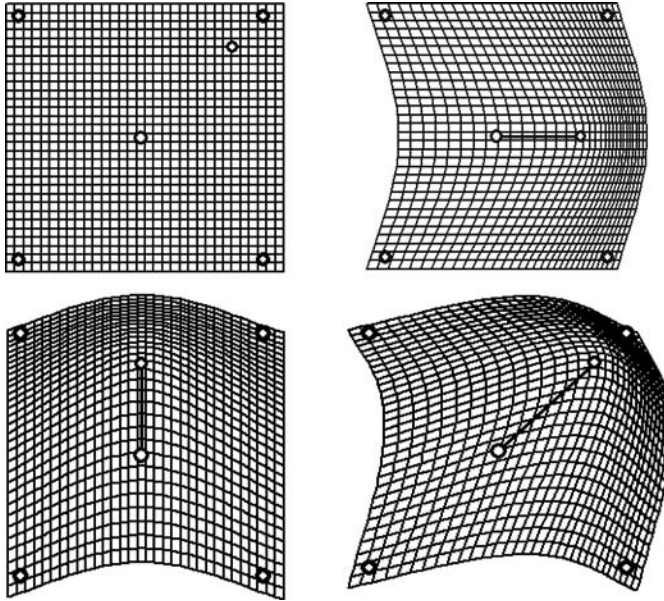
Figure 8. Construction of the thin-plate spline deformation grid. Shown in the upper, left are two five-landmark configurations differing only in the right and upward displacement of the central landmark on the target configuration. To produce a deformation grid for the difference, interpolation formulae are computed separately for the x displacement (upper, right) and the y displacement (lower, left), then combined (lower, right). Note, this construction works even though the configurations are not in Procrustes alignment. Plots created with Morpheus et al. (Slice, 1998).

target. Note that although we set this as a condition for the above equation, the resulting formula can still be applied to any position in the plane of the reference to interpolate heights at points not coincident with reference landmarks. With the addition of one more condition—that the resultant surface be the least bent of any surface passing through the specified heights at the locations of the reference landmarks—the derived surface will be the thin-plate spline. This specification comes from engineering where the equation is used to model the deformation of an infinite, infinitely-thin metal plate, hence the name.

To compute the coefficients for a configuration of p points in $k = 2$ dimensions meeting our requirements, we begin with the construction of a partitioned matrix:

$$\mathbf{L} = \left[\begin{array}{c|c} \mathbf{P}_{p \times p} & \mathbf{Q}_{p \times 3} \\ \hline \mathbf{Q}^{t}_{p \times 3} & \mathbf{0}_{3 \times 3} \end{array} \right]$$

where $\mathbf{P}$ is symmetric with zeros on the diagonal and off-diagonal elements $p_{i,j} = p_{j,i} = U(r_{i,j}) = r_{i,j}^2 \ln(r_{i,j}^2)$, where $r_{i,j}$ is the Euclidean distance between points i and j of the reference specimen. $\mathbf{Q}$ is a matrix of the landmark coordinates of the reference specimen augmented by an initial column of ones, and $\mathbf{0}$ is a matrix of zeros.

The required coefficients are obtained from the equation:

$$\mathbf{L}^{-1}\mathbf{Y}_{p+3,1} = (\mathbf{w}|a_1, a_x, a_y)^t \tag{2}$$

where $\mathbf{Y}$ is the vector of differences between the reference and the target specimen along the axis currently being considered (the constraints placed on the equation mentioned earlier) augmented by three zeros at the end. The individual elements of $\mathbf{w}$ are the w_i in the earlier equation. Each is associated with one (the ith) landmark on the reference configuration.

We are now free to use Equation (1) and the new coefficients to compute the height of the surface at any point in the plane of the reference. As required, heights at reference landmarks will equal differences between the reference and the target configuration along the coordinate axis under consideration, and heights at other positions will be interpolated so that the resulting surface has minimal bending. For application in morphometric visualization, we then assemble the heights, separately computed with different coefficients for each coordinate axis, into displacement vectors for a given point in the plane of the reference.

To use this information to achieve the thin-plate spline plots seen throughout this book, one constructs a grid of square cells over the reference configuration and computes the interpolated displacement vectors for points on the gridlines. Redrawing the connections between the displaced points results in the thin-plate spline plot (Figure 8). It is important that the initial grid cells be square so that deviations from "squareness" can be interpreted as oriented stretching within the cells of the resulting spline plot. This is not a mathematical requirement. It is just harder to assess how a cell has changed in a plot if you are unsure of its initial shape and distinguishing between initial rectangles and resultant quadrilaterals is more difficult than spotting deviations from squareness.

Note that this construction has no prerequisites about the superimposition of the reference and the target configurations. The construction is also very robust and can represent extreme shape differences beyond any to be encountered in anthropological research. The only exception is that the formulae "blow up" if two points are coincident on the reference, but distinct on the target. This

is perceived as a "tearing" of the thin-plate spline model. In biological terms such a situation would represent the genesis of a new biological feature through either evolution or development. Bookstein and Smith (2000) proposes the use of "creases" to model such occurrences.

The w_i used in the thin-plate spline provide the coordinates of an individual specimen with respect to the eigenvectors of the bending energy matrix (see the section on "Warps" below)—the upper, left $p \times p$ submatrix of $\mathbf{L}^{-1}$ (Bookstein, 1991). These eigenvectors are a set of orthonormal axes for local, or non-affine, components of shape differences with respect to the reference configuration. The remainder of the total shape difference between an individual specimen and the reference is the global, affine, or uniform shape difference. These are those differences that can be characterized as stretching or compressing the space in orthogonal directions. Such transformations have the properties that they leave parallel lines parallel and affect the local space precisely the same way everywhere, hence the term global (Figure 9, upper right and lower left). In contrast, the local shape differences represented by the eigenvectors of the bending energy matrix encode different compressions, expansions, displacements, or reorientations of local regions of the space (Figure 9, lower right). The w_i encode the local difference between shapes, but use of such scores in the analysis of total shape difference requires the quantification of the affine component, as well.

Bookstein (1996a) presented a method to compute the affine terms for two-dimensional data based on the Procrustes metric, but this method does not extend easily to higher-dimensional configurations. Recently, Rohlf and Bookstein (2003) have presented more general, complimentary approaches to quantifying affine variation. One is based on the Burnaby-like projection of data (Burnaby, 1966) into a space orthogonal to that of local variation. The other is based on the linear regression of a specimen onto the consensus or reference that is similar to the affine least-squares fitting described in Rohlf and Slice (1990). Regardless of the form of computation, the concatenation of the variables for purely affine shape differences with those for local variation provides a linear space suitable for the application of standard, parametric multivariate statistical tests.

The discussion so far has been modeled differences in two-dimensional configurations as deviations out of the plane of the reference. The situation is a little different, but not by much, for generating thin-plate splines for three-dimensional configurations. Here the model is less-intuitive, with
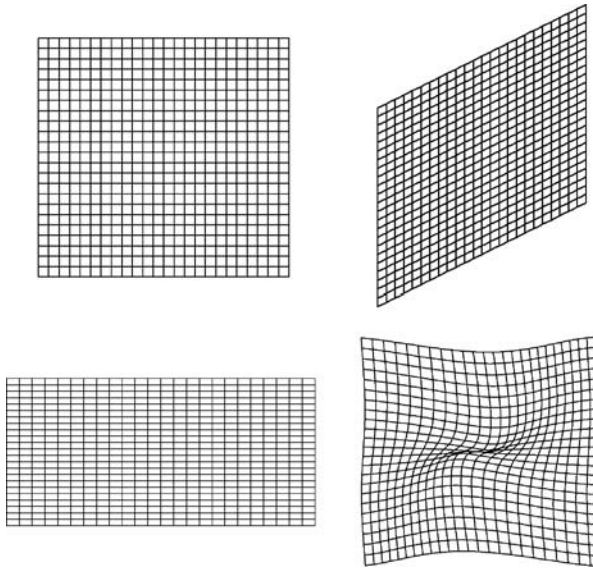
Figure 9. Affine transformations (upper, right and lower, left) are global in the sense that they involve only a simple stretching/compression in orthogonal directions and are the same everywhere in the space. Non-affine, or local, deformations involve twisting, stretching, and shifting of small regions as shown in the lower, right. An exact position must be specified to discuss the effects of such deformations. Plots created with Morpheus et al. (Slice, 1998).

coordinate-wise differences being considered as orthogonal displacements out of the volume of the reference specimen, but it is identical in spirit to the two-dimensional case. Some adjustment is also needed in the U function, which becomes $|r_{i,j}|$ to achieve the requisite minimization (Bookstein, 1991, appendix 1).

Figure 10 shows a thin-plate spline mapping the shape of the average male gorilla scapula landmarks onto those of the average female gorilla. This figure was generated using the average male gorilla landmark locations as the reference in the thin-plate spline equations and the average male–average female difference vectors ($\times 2$) in the **Y** matrix in Equation 2. One can now appreciate the regional expansions, rotations, etc. taking into account the relative positions of all landmarks simultaneously. As with vector plots, any reasonable source of displacements can be used to generate the splines. For instance, one can spline an average configuration using the coefficients of a principal component or the coordinates of a predicted configuration based on a regression analysis.
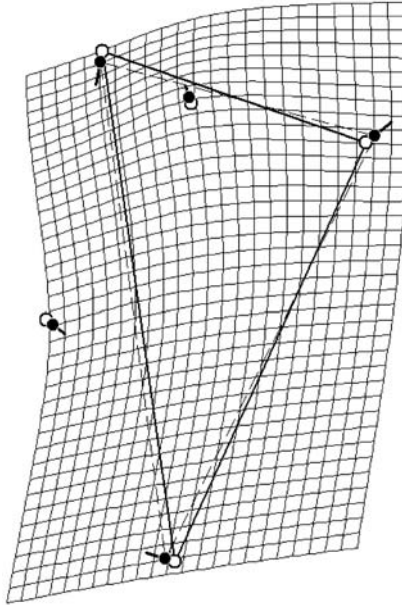
Figure 10. Thin-plate spline deformation grid showing the difference between mean male and female gorilla scapulae (magnified ×2) as a transformation of the male scapula. Vectors are also shown. Compare with Figure 7. Plot created with Morpheus et al. (Slice, 1998).

The thin-plate spline mapping can also be used in other ways. For instance, it can be used to associate other information, such as pixel intensity, in the space around the landmarks of the target configuration with specific locations in the space of the reference. In this way, images associated with individual specimens can be used to construct an average image associated with the reference. This method of image "unwarping" is used by Gharaibeh (Chapter 5, this volume) in his study of the geometric effects of head orientation in the anthropometric analysis of archival photographs.

WARPS, WARPS, AND MORE WARPS

Researchers new to the world of geometric morphometrics are often confused by unfamiliar terminology. One especially noteworthy case is that of the various "warps" that are often referred to in the literature and derive from the thin-plate spline formulation just discussed. There are principal warps, partial warps, relative warps, and singular warps.

Principal warps are the eigenvectors of the *bending energy matrix*, which is the upper, left $p \times p$ submatrix of the $\mathbf{L}^{-1}$ matrix used to compute the coefficients for the thin-plate spline. This matrix encodes the local aspects of shape differences, and its eigenvectors are linear combinations of orthogonal displacements of the landmarks of the reference configuration ordered by the energy required to fit the hypothetical metal sheet to those displacements. That is, the first principal warp associated with the largest eigenvalue (bending energy) is the most local deformation of the reference configuration. The second requires the most energy of deformations geometrically orthogonal to the first, and so on. A key feature of the principal warps is that they are functions of the reference configuration alone. They are computed without using any other data configurations, and therefore, carry no information about the sample other than vaguely through the contributions of sample configurations to the mean (if the reference used is the sample mean).

Partial warps are pairs or triplets of principal warps used to encode differences between individual specimens and the reference. The scores on these warps or axes come in multiples since real coordinate axes (x, y, and z) are modeled separately in the thin-plate spline computations. The partial warp scores are the scores for each individual for each coordinate for each principal warp axis, and taken together, the partial warps provide an orthogonal basis for the space of non-affine shape variation. The scores, themselves, are shape variables.

Relative warps are linear combinations of the partial warps and affine components computed to decompose total shape variability into uncorrelated, variance-maximizing variables. In more familiar terms, the relative warps are the principal components of sample variability in shape space with respect to the partial warp and affine scores. Rohlf (1993) describes how this principal component analysis can be tuned to emphasize larger- or smaller-scaled shape variation if the researcher has a reason for doing so.

Recent additions to the morphometric jargon are the *singular warps*. There are pairs of covariance-maximizing linear combinations of two sets of variables observed on individuals. One or both sets can be shape variables, and in the case of the former, the second set can be environmental or other variables the researcher wishes to relate to shape (Bookstein et al., 2003).

EXTENSIONS TO PROCRUSTES ANALYSIS

The combination of multivariate Procrustes analysis, multivariate statistics, and thin-plate spline visualizations is what Bookstein (1993, 1996b) called

the "Morphometric synthesis." It also represents the foundation of most coordinate-based analyses to be found in the literature to date. Still, there are a number of current or potential elaborations that are likely to take the approach beyond the now-familiar comparison of mean shapes or the regression of shape on size or extrinsic factors like temperature or epoch. These are mentioned only briefly here, but this economy should not be taken to represent any limitation on the potential of these methods in morphometrics.

One intriguing area of research is that of asymmetry (Palmer, 1996; Palmer and Strobeck, 1986) in which the differences in the relative size of two sides of a bilaterally symmetric structure or bilateral structures of an individual organism are examined across populations. The idea is that in the absence of developmental instability, environmental perturbations, or within-organism substrate competition, organisms should manifest perfect symmetry. Deviations from perfect symmetry, therefore, can give insight into developmental programs, environmental stress, and/or other putative factors. Such variation can be divided into various classes such as: directional asymmetry—where one side always differs in the same way, antisymmetry—where one side differs by some degree, but which side is more-or-less random, and fluctuating asymmetry—where variations are random with respect to the average shape or form. The latter is often interpreted as an indicator of environmental perturbation, but to get to that component, other types of asymmetry must either be partitioned out or discounted.

An early investigation of asymmetry using geometric morphometrics is that of Smith et al. (Bookstein, 1991; Smith et al., 1997), who partition shape variation in right and left honey bee wings into fluctuating and directional components. Klingenberg and McIntyre (1998) and Klingenberg and Zaklan (2000) analyze asymmetry in fly wings using standard MANOVA methods applied to Procrustes coordinates. Mardia et al. (2000) and Kent and Mardia (2001) present a comprehensive methodology for the analysis of asymmetry entirely within the Procrustes geometry, though this has yet to find its way into general morphometric use.

Kimmerle and Jantz (Chapter 11, this volume) use MANOVA methods and regression to examine trends in asymmetry in the crania of both sexes of whites and blacks in the United States. An alternative to the Procrustes framework for the analysis of asymmetry is the use of Euclidean Distance Matrix Analysis (see the section on Coordinate-free methods) presented in the current volume by Richtsmeier et al. (Chapter 8).

The Procrustes methods are restricted by their requirement of named (in most cases) landmarks and the assumption of equipotent information in all coordinate directions. As indicated by Bookstein's landmark classification, this is not always the case. To address this restriction, Bookstein (1991, 1997) proposed sliding such two-dimensional semi-landmarks in the uninformative direction(s) to enhance the relative contribution of informative variability. Bookstein et al. (1999) uncover some rather surprising results using this approach. They find that the inner, midsagittal profile of the frontal bone is invariant with respect to shape between modern and archaic humans. Furthermore, it is nearly indistinguishable in these groups from that of Australopithicines or Pan! In the current volume, Gunz et al. (Chapter 3) extend the method of sliding landmarks both to two-dimensional curves embedded in three-dimensions (space curves) and to the analysis of surfaces. Relevant formulae for these and Bookstein's original two-dimensional case are found there as well.

Quantitative genetics is another area in which the integration of modern morphometric techniques could have a significant impact. Procrustes-derived shape variables have been used by Klingenberg et al. (2001) and Klingenberg and Leary (2001) to explore quantitative trait loci and the relationship between genetic and phenotypic covariance using similar data. Monteiro et al. (2002) investigate the heritability of shape using Procrustes shape variables.

COORDINATE-FREE METHODS

It has been suggested that the Procrustes and other registration-based methods are undesirable since they involve a distinct and unnecessary superimposition step after which analyses involve an inestimable coordinate covariance structure (e.g., Lele and Richtsmeier, 2001). To avoid this, several "coordinate-free" approaches have been suggested that utilize variables that are invariant to orientation and location within a specific coordinate system (size may be factored out separately). Rao and Suryawanshi (1996, 1998) suggested the use of sufficient sets of interior angles between landmarks and combinations of interlandmark distances as variables to quantify and analyze shape. The early truss methods of Bookstein et al. (1985) would also be included in this category.

The most widely used method of this school, however, is based on Euclidean Distance Matrix Analysis, or EDMA (Lele and Cole, 1995, 1996; Lele and Richtsmeier, 1991, 2001). The Euclidean Distance Matrix (EDM), or Form Matrix (FM) is simply a symmetric, $p \times p$ matrix in which the off-diagonal

elements, $e_{i,j} = e_{j,i}$, are the Euclidean distances between landmarks i and j. Diagonal elements are zero, and in practice, only one set of off-diagonals is used for statistical testing. These measurements are a highly redundant set of variables that completely fix the geometry of the landmarks up to a reflection and are invariant to any choice of orthogonal basis vectors with respect to which the original coordinates might have been collected. Note that, while invariant to location and orientation, such an assemblage still contains size information that must be partialled out if a pure shape analysis is desired.

Analysis proceeds via the pairwise comparison of EDMs, which might be two configurations or mean EDMs for two groups. Mean form matrices can be computed using the method of moments (Stoyan, 1990; Lele, 1993), but there is a problem in that the resulting average interpoint distances might not represent a physically realizable structure. Lele (1993) suggests one "flattens" the estimates back into image/physical space by using only the first two/three eigenvectors of the mean form matrix scaled by their associated eigenvalues.

The developers have proposed several methods for the statistical assessment of pairs of EDMs. In its first incarnation, EDMA I (Lele and Richtsmeier, 1991), ratios of corresponding distances in the two EDMs are used to construct a relative form difference matrix (rFDM). If the two configurations are precisely the same, these values will be all unity, and if the two differ only by size, the elements will be some constant value. It is seldom the case that configurations will be identical, so the authors proposed a non-parametric test for shape differences. The test statistic, T, is the ratio of the largest ratio in the rFDM to the smallest. The significance of T is assessed relative to confidence limits obtained from bootstrap resampling of the two populations (Richtsmeier and Lele, 1993). Lele and Cole (1995, 1996) proposed another approach for heteroscedastic samples, EDMA II, that uses the test statistic, Z, the maximum absolute value of the arithmetic difference of elements in two EDMs. The significance of Z is tested by a parametric bootstrap procedure in which on generates normally distributed samples with the same mean shape and covariance structure as the original samples and determines if the resulting confidence limits on Z contain zero. To achieve a shape, instead of form, analysis, EDMs in EDMA II may be scaled by some user-specified measure of size, for example, baseline length or CS (Lele and Cole, 1995, 1996).

The relative merit of EDMA vs. the Procrustes approaches has been one of the more contentious issues of modern morphometrics. The proponents of EDMA (Lele, 1993; Lele and McCulloch, 2002; Lele and Richtsmeier, 2001)

argue that the use of inestimable landmark covariance matrices and inconsistent mean and covariance estimates are serious problems with Procrustes-based methods ("consistency" is a statistical term meaning that as the sample size goes to infinity, the estimated value converges in probability on the true value). Rohlf (1999b, 2000, 2003) compared a number of morphometric methods including EDMA and GPA using simulations of random triangles generated with independent, isotropic error. He found the EDMA methods introduced artifactual covariance structure into randomly generated samples (Rohlf, 1999b), had a more complicated and structured power surface (Rohlf, 2000), and for realistic sample sizes, produced more biased mean estimates (Rohlf, 2003). EDMA supporters counter that the simplistic models of isotropic error are not representative of real-world data sets (Lele and Richtsmeier, 1990) and reject the power comparisons as being artifactual and lacking valid, analytical support (Richtsmeier, personal communication).

Lele and Richtsmeier (2001) is a comprehensive outline of the case for EDMA and with contributions from Cole, provides extensions of the EDMA approach to the study of growth, classification, clustering, asymmetry, molecular structures and phylogenetics. In this volume, Richtsmeier et al. present an EDMA-based method for the study of asymmetry using a mouse model for Trisomy 21, Down syndrome.

OUTLINE METHODS

The differences between outline data and landmark coordinates usually require special consideration, and different methods are available for different types of outlines (see Rohlf, 1990). One method of particular importance in morphometrics is elliptic Fourier analysis (EFA) (Kuhl and Giardina, 1982) for two-dimensional, closed contours. This method does not require evenly spaced sample points or equal numbers of points across specimens, can handle arbitrarily complex outlines, provides parameterization of the entire outline, and includes optional standardizations for size, location, orientation, and digitizing starting point to support the analysis of shape. In general, though, one would like to seamlessly combine outline and landmark data in a single analysis. An outline might pass through bona fide landmarks, or it could have structurally associated landmarks nearby. In Chapter 6, this volume, Baylac and Frieß combine EFA and GPA to study the effects of cranial deformation using partial and complete cranial outlines and landmarks.

Another possibility is to develop a common framework for the joint analysis of landmarks and outlines. McNulty (Chapter 16, this volume) uses equally spaced sample points between anatomical landmarks on brow ridges superimposed using only the anatomical landmarks to quantify supraorbital morphology in extant and fossil hominoids. The sliding landmarks method developed by Bookstein (e.g., 1997) allows sample points to slide along tangents to the outline in a Procrustes analysis in order to reduce uninformative variation in that direction. Their use in analyzing curves in three-dimension is discussed by Gunz et al. in Chapter 3, this volume. Reddy et al. (Chapter 4) present a modification of the sliding landmark method to take advantage of the usually high density of initial sample points collected when quantifying such curves, and apply the method to the study the Neanderthal "bun."

FRACTALS

The concept of a fractal is an interesting one with many potential applications in biology (Slice, 1993b), including physical anthropology. In general, a fractal is "a set for which the Hausdorff-Besicovitch dimension strictly exceeds the topological dimension" (Mandelbrot, 1983). Such sets can be point sets or outlines or surfaces or volumes, and all possess a distinguishing property call self-similarity (see Feder, 1988; Peitgen and Saupe, 1988). This means that some geometric aspect of the set is repeated at different scales. The similarity may be exact, with larger-scale features being composed of smaller-scale copies of a fundamental structure, or statistical, where scale-adjusted variability at all scales is similar. The implication of such self-similarity for morphometrics is great. One finds, for instance, that genuinely fractal closed outlines have an infinite perimeter since no matter how small a measurement scale is used the perimeter never "smoothes out" into a two-dimensional Euclidean curve (Slice, 1993b). The characterization of a biological structure in the form of the fractal dimensions, d, can be used to quantify the complexity of a shape over some finite range of measurement scales.

Structures amenable to such analysis include complex sutures like those in ammonite shells and cervid skulls examined by Long (1985). The comparison of the fractal dimensions of sutures from a more accurate tracing was used by Palmqvist (1997) to challenge the previous hominid affinities of the Orce skull fragment supported by Gilbert and Palmqvist (1995). In this volume,

Prossinger (Chapter 7) argues for the fractal nature of frontal sinuses and presents a plausible model for the development and modeling of such structures.

FINAL COMMENTS

This chapter has been a rather fast-paced and necessarily superficial overview of the large and growing field of modern shape analysis with a slight bias toward applications in physical anthropology. It is hoped that this will provide readers having relatively little exposure to morphometric methods with sufficient information to follow and appreciate subsequent chapters. Newcomers are not expected to master, or necessarily fully grasp, all of the subtleties and mathematical details summarized here, but at least they will have been exposed to the material. If, as is likely, these same readers want to learn more about the methods and begin to use them in their own research, the references cited herein will provide a good place to start. In addition, a number of user-friendly resources are available to enhance their education. One is the morphometrics website at the State University of New York at Stony Brook (http://life.bio.sunysb.edu/morph) developed and maintained by F. James Rohlf. The site contains free, downloadable software for data acquisition and morphometric analysis, downloadable data sets, and a morphometrics bulletin board, bibliographies, book reviews, and links to other sites. A second valuable resource is the morphometric mailing list, morphmet, started by Les Marcus. Over four hundred people from around the world are subscribers and are inevitably willing to assist others. Subscription information can be found at the Stony Brook morphometrics site, http://life.bio.sunysb.edu/morph/morphmet.html.

ACKNOWLEDGMENTS

REFERENCES

Adams, D. C., Rohlf, F. J., and Slice, D. E., 2004, Geometric morphometrics: Ten years of progress after the "revolution," *Italian Journal of Zoology.* 71(1):5–16.

Atchley, W. R. and Anderson, D., 1978, Ratios and the Statistical Analysis of Biological Data, *Syst. Zool.* 27(1):71–78.

Atchley, W. R., Gaskins, C. T., and Anderson, D., 1976, Statistical properties of ratios. I. Empirical results. *Syst. Zool.* 25(2):137–148.

Blackith R. and Reyment R. A., 1971, *Multivariate Morphometrics*, Academic Press, New York.

Boas, F., 1905, The horizontal plane of the skull and the general problem of the comparison of variable forms, *Sci.* 21(544):862–863.

Bookstein, F. L., 1986, Size and shape spaces for landmark data in two dimensions (with discussion), *Stat. Sci.* 1:181–242.

Bookstein, F. L., 1989, Principal warps: thin-plate splines and the decomposition of deformations, *IEEE Trans. on Pattern Anal. and Machine Intell.* 11:567–585.

Bookstein F. L., 1991, *Morphometric Tools for Landmark Data: Geometry and Biology*, Cambridge University Press, Cambridge.

Bookstein, F. L., 1993, A brief history of the morphometric synthesis, in: *Contributions to Morphometrics*, L. F. Marcus, E. Bello, and Garciá-Valdecasas, eds., Monografias del Museo Nacional de Ciencias Naturales 8, Madrid, pp. 15–40.

Bookstein, F. L., 1996a, A standard formula for the uniform shape component in landmark data, in: *Advances in Morphometrics*, L. F. Marcus, M. Corti, A. Loy, G. J. P. Naylor, and D. E. Slice, eds., Plenum Press, New York, pp. 153–168.

Bookstein, F. L., 1996b, Biometrics, biomathematics and the morphometric synthesis, *Bull. of Math. Biol.* 58:313–365.

Bookstein, F. L., 1997, Landmark methods for forms without landmarks: Localizing group differences in outline shape, *Med. Image. Anal.* 1:225–243.

Bookstein F. L. and Smith, B. R., 2000, Inverting development: geometric singularity theory in embryology, in: *Mathematical Modeling, Estimation, and Imaging*, D. Wilson, H. Tagare, F. Bookstein, F. Préteaux, and E. Dougherty, eds., Proc. SPIE, vol. 4121, pp. 139–174.

Bookstein, F. L., Chernoff, B., Elder R. L., Humphries, J. M. Jr., Smith, G. R., and Strauss, R. E., 1985, *Morphometrics in Evolutionary Biology*, Special Publication 15, Academy of Natural Sciences Press, Philadelphia.

Bookstein, F. L., Gunz, P., Mitteröcker, P., Prossinger, H., Schäfer, K., and Seidler, H., 2003, Cranial integration in *Homo*: Singular warps analysis of the midsagittal plane in ontogeny and evolution, *J. Hum. Evol.* 44(2):167–187.

Bookstein, F. L., Schäfer, K., Prossinger, H., Seidler, H., Fieder, M., Stringer, C. et al., 1999, Comparing frontal cranial profiles in archaic and modern Homo by morphometric analysis, *Anatomi. Rec. (New Anatomist)* 257:217–224.

Burnaby, T. P., 1966, Growth-invariant discriminant functions and generalized distances, *Biometrics* 22:96–110.

Carroll, J. D. and Green, P. E., 1997, *Mathematical Tools for Applied Multivariate Analysis*, Academic Press, San Diego.

Cole, T. M. III., 1996, Historical note: early anthropological contributions to "geometric morphometrics," *Am. J. Phys. Anthropol.* 101(2):291.

Dryden, I. L. and Mardia, K. V., 1993, Multivariate shape analysis, *Sankhya* 55:460–480.

Dryden, I. L. and Mardia K. V., 1998, *Statistical Shape Analysis*, John Wiley & Sons, New York.

Feder, J., 1988, *Fractals*, Plenum Press, New York.

Galton, F., 1907, Classification of portraits, *Nature* 76:617–619.

Gilbert, J. and Palmqvist, P., 1995, Fractal analysis of the Orce skull sutures, *J. Hum. Evol.* 28:561–575.

Goodall, C. R., 1991, Procrustes methods in the statistical analysis of shape, *J. Roy. Statistical Society, Series B*, 53:285–339.

Gould, S. J., 1981, *The Mismeasure of Man*, W.W. Norton & Company, New York.

Gower, J. C., 1975, Generalized Procrustes analysis, *Psychometrika*, 40:33–51.

Hanihara, T., 2000, Frontal and facial flatness of major human populations, *Am. J. Phy. Anthropol.* 111(1):105–134.

Howells, W. W., 1973, *Cranial Variation in Man: A Study by Multivariate Analysis of Difference Among Recent Human Populations*, Papers of the Peabody Museum of Archaeology and Ethnology, No. 67. Harvard University, Cambridge, MA.

Howells, W. W., 1989, Skull shapes and the map: craniometric analyses in the dispersion of modern *Homo*, Papers of the Peabody Museum of Archaeology and Ethnology, No. 79. Harvard University, Cambridge, MA.

Huxley, J. S., 1932, *Problems of Relative Growth*, Methuen, London. Reprinted 1972, Dover Publications, New York.

Johnson, R. A. and Wichern, D. W., 1982, *Applied Multivariate Statistical Analysis*, Prentice-Hall Inc., Inglewood Cliffs, New Jersey.

Kendall, D. G., 1984, Shape-manifolds, Procrustean metrics and complex projective spaces, *Bulletin of the London Mathematical Society* 16:81–121.

Kendall, D. G., 1985, Exact distributions for shapes of random triangles in convex sets, *Advan. Appl. Prob.* 17:308–329.

Kendall, D. G., 1989, A survey of the statistical theory of shape, *Stat. Sci.* 4:87–120.

Kendall, D. G. and Kendall, W. S., 1980, Alignments in two dimensional random sets of points, *Advan. Appl. Prob.* 12:380–424.

Kent, J. T. and Mardia, K. V., 2001, Shape, Procrustes tangent projections and bilateral symmetry, *Biometrika* 88:469–485.

Klingenberg C. P. and Leamy, L. J., 2001, Quantitative genetics of geometric shape in the mouse mandible, *Evolution* 55:2342–2352.

Klingenberg, C. P. and McIntyre, G. S., 1998, Geometric morphometrics of developmental instability: Analyzing patterns of fluctuating asymmetry with Procrustes methods, *Evolution* 52:1363–1375.

Klingenberg, C. P. and Zaklan, S. D., 2000, Morphological integration between developmental compartments in the *Drosophila* wing, *Evolution* 54(4):1273–1285.

Klingenberg C. P., Leamy L. J., Routman E. J., and Cheverud J. M., 2001, Genetic architecture of mandible shape in mice: Effects of quantitative trait loci analyzed by geometric morphometrics, *Genetics* 157:785–802.

Kolar, J. C. and Salter, E. M., 1996, *Craniofacial Anthropometry*, Charles C. Thomas Publishers Ltd., Springfield.

Krzanowski, W. J., 1988, *Principles of Multivariate Analysis*, Claredon Press, Oxford.

Kuhl, F. P. and Giardina, C. R., 1982, Elliptic Fourier features of a closed contour, *Comp. Graph. Imag. Process.* 18:236–258.

Lele, S. R., 1993, Euclidean distance matrix analysis: estimation of mean form and form difference, *Math. Geol.* 25:573–602.

Lele, S. R. and Cole T. M. III, 1995, Euclidean distance matrix analysis: a statistical review, in: *Current Issues in Statistical Shape Analysis, Volume 3*, University of Leeds, Leeds, pp. 49–53.

Lele, S. R. and Cole, T. M. III, 1996, A new test for shape differences when variance-covariance matrices are unequal, *J. Hum. Evol.* 31:193–212.

Lele, S. R. and McCulloch, C., 2002, Invariance and morphometrics, *J. Am. Stat. Assoc.* 97(459):796–806.

Lele, S. R. and Richtsmeier, J. T., 1990, Statistical models in morphometrics: Are they realistic? *Syst. Zool.* 39(1):60–69.

Lele S. R. and Richtsmeier, J. T., 1991, Euclidean distance matrix analysis: A coordinate free approach for comparing biological shapes using landmark data, *Am. J. Phy. Anthropol.* 86:415–427.

Lele, S. R. and Richtsmeier, J. T., 2001, *An Invariant Approach to Statistical Analysis of Shapes*, Chapman & Hall/CRC, New York.

Long, C. A., 1985, Intricate sutures as fractal curves, *J. Morph.* 185:285–295.

Mahalanobis, P. C., 1928, On the need for standardization in measurements on the living, *Biometrika* 20A(1/2):1–31.

Mahalanobis, P. C., 1930, A statistical study of certain anthropometric measurements from Sweden, *Biometrika* 22(1/2):94–108.

Mandelbrot, B. B., 1983, *The Fractal Geometry of Nature, 2nd Edition*, W. H. Freeman and Company, New York.

Manly, B. F. J., 1997, *Randomization, Bootstrap and Monte Carlo Methods in Biology, 2nd Edition*, Chapman & Hall/CRC, New York.

Marcus, L. F., 1990, Traditional morphometrics, in: *Proceedings of the Michigan Morphometrics Workshop*, F. J. Rohlf and F. L. Bookstein, eds., Special Publication Number 2, University of Michigan Museum of Zoology, Ann Arbor, MI, pp. 77–122.

Mardia, K. V., Bookstein, F. L., and I. J. Moreton, I. J., 2000, Statistical assessment of bilateral symmetry of shapes, *Biometrika* 87:285–300.

Monteiro, L. R., Diniz-Filho, J. A. F., dos Reis, S. F., and Araújo, E. D., 2002, Geometric estimates of heritability in biological shape, *Evolution* 56:563–572.

Morant, G. M., 1928, A preliminary classification of European races based on cranial measurements, *Biometrika* 20B(3/4):301–375.

Morant, G. M., 1939, The use of statistical methods in the investigation of problems of classification in anthropology: Part I. The general nature of the material and the form of intraracial distributions of metrical characters, *Biometricka* 31(1/2): 72–98.

Mosier, C. I., 1939, Determining a simple structure when loadings for certain tests are known, *Psychometrika* 4:149–162.

Mosimann, J. E., 1970, Size allometry: size and shape variables with characterization of the log-normal and generalized gamma distributions, *Jour. Amer. Stat. Assoc.* 65:930–945.

Palmer, A. R., 1996, Waltzing with asymmetry, *BioScience* 46:518–532.

Palmer, A. R. and Strobeck, C., 1986, Fluctuating asymmetry: measurement, analysis, patterns, *Annu. Rev. Ecol. Syst.* 17:391–421.

Palmqvist, P., 1997, A critical re-evaluation of the evidence for the presence of hominids in Lower Pleistocene times at Venta Micena, Southern Spain, *J. Hum. Evol.* 33: 83–89.

Pearson, K., 1897, Mathematical contributions to the theory of evolution—on a form of spurious correlation which may arise when indices are used in the measurement of organs, *Proceedings of the Royal Society of London* 60:489–498.

Pearson, K., 1903, Craniological notes: Professor Aurel von Torok's attack on the arithmetical mean, *Biometrika* 2(3):339–345.

Pearson, K., 1933, The cranial coordinatograph, the standard planes of the skull, and the value of Cartesian geometry to the craniologist, with some illustrations of the uses of the new methods, *Biometrika* 25(3/4):217–253.

Peitgen, H. and Saupe, D., 1988, *The Science of Fractal Images*, Springer-Verlag, New York.

Rao, C. R. and Suryawanshi, S., 1996, Statistical analysis of shape of objects based on landmark data, *Proceedings of the National Academy of Sciences, U.S.A.* 93:12132–12136.

Rao, C. R. and Suryawanshi, S., 1998, Statistical analysis of shape through triangulation of landmarks: A study of sexual dimorphism in hominids, *Proceedings of the National Academy of Sciences, U.S.A.* 95:4121–4125.

Reyment, R. A., 1996, An idiosyncratic history of early morphometrics, in: L. F. Marcus, M. Corti, A. Loy, G. J. P. Naylor and D. E. Slice, eds., *Advances in Morphometrics*, Plenum Press, New York, pp. 15–22.

Richtsmeier, J. T. and Lele, S. R., 1993, A coordinate-free approach to the analysis of growth-patterns: Models and theoretical considerations, *Biol. Rev.* 68:381–411.

Robins, G., 1994, *Proportion and Style in Ancient Egyptian Art*, University of Texas Press, Austin.

Rohlf, F. J., 1990, Fitting curves to outlines. Proceedings of the Michigan morphometrics workshop, in: *Proceedings of the Michigan Morphometrics Workshop*, F. J. Rohlf and F. L. Bookstein, eds., Special Publication Number 2, University of Michigan Museum of Zoology, Ann Arbor, MI, pp. 167–177.

Rohlf, F. J., 1993, Relative warp analysis and an example of its application to mosquito wings, in: *Contributions to Morphometrics*, L. F. Marcus, E. Bello and Garciá-Valdecasas, eds., Monografias del Museo Nacional de Ciencias Naturales 8, Madrid, pp. 131–159.

Rohlf, F. J., 1999a, Shape statistics: Procrustes superimpositions and tangent spaces, *Journal of Classification* 16:197–223.

Rohlf, F. J., 1999b, On the use of shape spaces to compare morphometric methods, *Hystrix* 11:9–25.

Rohlf, F. J., 2000, Statistical power comparisons among alternative morphometric methods, *Am. J. Phys. Anthropol.* 111:463–478.

Rohlf, F. J., 2001, tpsDig, Version 1.31. Department of Ecology and Evolution, State University of New York at Stony Brook, Stony Brook, New York.

Rohlf, F. J., 2002, tpsTri. Version 1.17. Department of Ecology and Evolution, State University of New York at Stony Brook, New York.

Rohlf, F. J., 2003, Bias and error in estimates of mean shape in morphometrics, *J. Hum. Evol.* 44:665–683.

Rohlf, F. J. and Bookstein, F. L., 2003, Computing the uniform component of shape variation, *Syst. Biol.* 52:66–69.

Rohlf, F. J. and Marcus, L. F., 1993, A revolution in morphometrics, *Trends in Ecology and Evolution* 8:129–132.

Rohlf, F. J. and Slice, D. E., 1990, Extensions of the Procrustes method for the optimal superimposition of landmarks, *Syst. Zool.* 39:40–59.

Siegel, A. F. and Benson, R. H., 1982, A robust comparison of biological shapes, *Biometrics* 38:341–350.

Siegel, A. F. and Pinkerton, J. R., 1982, Robust comparison of three-dimensional shapes with an application to protein molecule configurations, Technical Report No. 217. Series 2, Department of Statistics, Princeton University.

Slice, D. E., 1993a, Extensions, comparisons, and applications of superimposition methods for morphometric analysis, Ph.D. dissertation. Department of Ecology and Evolution, State University of New York, Stony Brook, New York.

Slice, D. E., 1993b, The fractal analysis of shape, in: *Contributions to Morphometrics*, L. F. Marcus, E. Bello, and Garciá-Valdecasas, eds., Monografias del Museo Nacional de Ciencias Naturales 8, Madrid, pp. 161–190.

Slice, D. E., 1994, GRF-ND: Generalized rotational fitting of N-dimensional data, Department of Ecology and Evolution, State University of New York at Stony Brook, New York.

Slice, D. E., 1996, Three-dimensional, generalized resistant fitting and the comparison of least-squares and resistant-fit residuals, in: *Advances in Morphometrics*, L. F. Marcus, M. Corti, A. Loy, G. J. P. Naylor and D. E. Slice, eds., Plenum Press, New York, pp. 179–199.

Slice, D. E., 1998, Morpheus et al.: Software for morphometric research. Revision 01-31-00, Department of Ecology and Evolution, State University of New York at Stony Brook, New York.

Slice, D. E., 2001, Landmark coordinates aligned by Procrustes analysis do not lie in Kendall's shape space, *Syst. Biol.* 50:141–149.

Slice, D. E., Bookstein, F. L., Marcus, L. F., and Rohlf, F. J., 1996, A glossary for morphometrics, in: *Advances in Morphometrics*, L. F. Marcus, M. Corti, A. Loy, G. J. P. Naylor and D. E. Slice, eds., Plenum Press, New York, pp. 531–551.

Small, C. G., 1996, *The Statistical Theory of Shape*, Springer-Verlag, New York.

Smith, D., Crespi, B., and Bookstein, F. L., 1997, Asymmetry and morphological abnormality in the honey bee, *Apis mellifer*: Effects of ploidy and hybridization, *Evolutionary Biology* 10:551–574.

Sneath, P. H. A., 1967, Trend surface analysis of transformation grids, *J. Zool., London* 151:65–122.

Stoyan, D., 1990, Estimation of Distances and Variances in Booksteins landmark model, *Biometrical J.* 32:843–849.

Thompson, D'A. W., 1942, *On Growth and Form*, Cambridge University Press, Cambridge.