in the linear $\mathbf{x}_i - \bar{\mathbf{x}}$ term relating A to $\mathbf{y}_i - \bar{\mathbf{y}}$ (1). With this model the δ should be compared directly, with triangle dimension entering only in estimating the precision.

2. For large strains $d\mathbf{Q}$ is not invariant (to within a rotation) to choice of base edge (10).

3. One difficulty with the approach via triangles is that measurement error is propagated through the choice of a common baseline (in a quadrilateral say) whereas variance considerations suggest averaging. Only for each triangle of landmarks is the translation of a single landmark always equal to the translation of the landmark centroid, $\mathbf{y}_i - A\bar{\mathbf{x}}_1 = \bar{\mathbf{y}} - A\bar{\mathbf{x}}$.

The modelling inconsistencies in using triangles have already been considered. However, this approach does define a basis direction comparable across individuals and does extend the homology between individuals from landmarks to the whole form (using pseudo-landmarks). As mentioned previously, modelling of interindividual variation requires at least the definition of a basis direction, and some tacit notion of extended homology also. These are the principal conceptual impediments to development of a theory of morphometrics along the lines of this discussion. They are no novelty to morphometrics, and it is substantially to Bookstein's credit that he has dealt with them.

As a final remark, the next generalization is to longitudinal data, for which the positions of a set of landmarks, possibly evolving in time, are recorded at several time points. The deformation tensor field is varying in space and time. Technically, many of the issues are the same, as in fact approaches for the analysis of finite deformation have been borrowed from the analysis of longitudinal data itself.

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Rejoinder

Fred L. Bookstein

Five able discussants have persuaded me that my essay, however long already, spent too little space reviewing themes other than its own. Each discussion points out connections between morphometrics and diverse topics both within biometrics and without.

Kendall's shape space $\sum_2^3$. David Kendall surmises, correctly, that I had not previously encountered his work. Indeed we have approached nearly the same problem from two very different directions. Although permutations and reflections of landmark configurations are prohibited on biological grounds, the algebra of my shape space is still that of a tangent space at the point of his $\sum_2^3$ corresponding to the mean shape. In the large, the plane of shape coordinates Q represents all of his shape space, except for one point $Z_1 = Z_2$, six times over.

The tensors supply a canonical geometric description of directions in any tangent plane of this space. Also, they lead to a metric geometry throughout the space, with infinitesimal element of distance equal to $|dQ|/\mathrm{Im}\, Q$, the difference of the log principal strains. The geodesic arcs of this geometry are curves corresponding to triangular shapes whose transformations from a fixed starting triangle have the same principal axes—the shapes that can be reached by fractional powers of the same affine transformation. The geodesics, then, must be the circles involved in the construction of the principal axes (Figure 11), the circles orthogonal to the real axis. In this metric construction for shape space we recognize one of the classic models of hyperbolic geometry, the Poincaré half-plane (cf. Coxeter, 1965, Section 14.8).

Such a space has negative Riemannian curvature, whereas Kendall's shape space, under the metric inherited from Euclidean distance, has positive curvature. This and other interesting differences between Kendall's geometry and mine derive from the differences between their fields of principal application. My morphometric shape space has a line of metric singularities all down the real axis. Points (triangles) not on this axis may not be transformed into points upon it or across it by any proper affine transformation. That axis, representing triangles of zero area, is the Absolute of the hyperbolic geometry, the locus infinitely far away. Its exclusion expresses the restriction of the deformation model to transformations of positive Jacobian, so that straight angles are not rendered oblique or the sign of small triangular areas changed. In the vicinity of the real axis, the shape coordinates Q in tangent space work perfectly well, but the tensor-based metric breaks down: reports of mean differences around straight angles cannot take the form of tensors. In summary, the tangent spaces of Kendall's space Σ_2^3 are equivalent to the space of shape algebra, whereas the hyperbolic half-plane is the space of shape change interpretation.

Goodall's two-stage procedure. Colin Goodall suggests an alternative set-up for morphometrics in which the deformation itself is taken as the primary object of observation and its natural parameters p, q, θ, ψ modeled by some joint distribution. This is feasible for strictly longitudinal analyses—growth, follow-up after surgery, and the like—but longitudinal series make up only one morphometric study design. The other designs, not suited to this framework, include the comparison of sample means, the analysis of clinical deformity by matching to normative forms, studies of allometry and other influences on shapes observed singly, and the computation of deformations from serial data in order to study processes other than individual change, such as the canonical deformation visualizing shape stability in Figure 18.

Goodall's own analysis of plant growth exploit points at rather close spacing. Although such data permit increased precision in the observation of true deformations across time, specimen by specimen, the multiplicity of points tends not to correspond across specimens, making problematic the comparison of deformations or their averaging in population samples. The principal strains p and q are tensor invariants, but their gradients, and the angles θ and ψ, are not. For comparisons of p, q, θ, and ψ to be biologically interpretable across forms, one needs bridges among the multiple coordinate systems involved. In the system of morphometrics put forward in this essay, such bridges are supplied by landmarks, whereupon θ is no longer a particularly natural parameter—rather, one needs the full size-shape machinery. In other systems of measurement the bridges between coordinate systems may be supplied instead by gravity, by an axis of coiling or translation, or by fixed metallic implants. For a single triangle of landmarks observed at two times over a sample of organisms, I believe that Goodall's analysis is equivalent to the matched allometric analysis of shape coordinates demonstrated in Section 6. For more extensive collections of landmarks, there is indeed a choice to be made between interpolation and smoothing; I will return to this matter at the end of this comment.

Shape as fixed vector. Gregory Campbell rejects the stated purpose of my essay, the fusion of the geometric and multivariate approaches to morphometrics. He claims, for instance, that because my shape coordinates are homeomorphic to ratios of edge lengths (whenever the assumption of small shape variance applies), it follows that "the geometry is effectively removed from the problem, to be replaced by functions only of distances," with which one might work "just as easily." Such a statement misconstrues the role of morphometrics in biological and biomedical research. Morphometrics serves as the empirical link between geometry and biology, the matching of geometric measurements to the comparative biological context. The morphometrician's task is only secondarily statistical testing of hypotheses; it is primarily the construction of a sensible set of descriptor variables by which the biological phenomenon under study may be captured.

In the presence of K landmarks, one has access to $K(K-1)/2$ interlandmark distances. To avoid singularities of the joint distribution, one must restrict one's attention to a basis of no more than $2K-3$ of these distances, or $2K-4$ of their ratios. The appropriate basis for reporting an analysis is not, in general, a subset of the larger, redundant basis, but instead is a collection of linear combinations computable only after statistical analysis is complete. Changes in a network of interlandmark distances, whether measured in millimeters or in fractions of change, are best reported as a pattern of loadings (conjoint changes) along other directions entirely, directions whose specification depends crucially upon the mean form as well as upon the pattern of distance changes. This dependence of report on mean form is nonlinear even when linear statistics suffice for the study of shape variations about that mean.

From a biological point of view, the existence of discrete, recognizable landmarks is accidental. They lie arbitrarily upon the form with respect to the biological processes taking place inside. The morphometrician's description must be as independent of the landmarks as possible, even when they are the only data available. Our job is the extraction of the most useful variables, not merely the statistical processing of those edges of convenience or any other arbitrary data archive. In summary, geometry is not "effectively removed" from morphometric analysis by recourse to any predetermined size or shape basis. It is only sequestered; it must be restored at the end of an analysis by a change of basis if the findings are to be of any biometric use.

Robustification. Paul Sampson shows by example how one supersedes multivariate normal assumptions by a bootstrapped computation of realistic sampling distributions. It would be captious to disagree with a suggestion so reasonable. Noel Cressie, also concerned with robustness, may find Sampson's idea a satisfactory resolution. There is already robustness in the method by virtue of its recourse to factor loadings rather than multiple regression coefficients for the depiction of systematic effects upon shape, especially in dealing with size allometry or shape stability (Figures 17 and 18). As another instance, an elliptical distribution of the shape coordinates Q for a triangle may be tentatively modeled as the superposition of a circular distribution, of radius equal to the minor diameter, over a distribution constrained to the major axis and having variance equal to the difference between the squared axis lengths of the ellipse. This rank one component of shape is now available for attribution to an external factor, such as mean sample size in the example of Figure 7. On the model put forward here, only that part of shape variation need be circular which cannot be attributed to the influence of exogenous shape determinants in this fashion. Goodall's stricture that factor analysis is "a technique to be viewed with caution" applies mainly to factor rotation in its various psychometric incarnations, not to the straightforward summary of directional derivatives which is the role of the morphometric factor.

In contrast to Sampson's and Cressie's concerns about robustness, Gregory Campbell develops the algebra of covariance terms which are $O(\sigma^2)$, attends to the difference between zero correlation and independence, and, generally, deals with matters I would label as "antirobustification." In the face of the great redundant span of biologically interpretable variables with which morphometrics must cope in the applied literatures, I think it is sufficient to explore mainly their algebraically simplest aspects; one is not thereby misled about real data. The lesser stringency of the normal model—the replacement of probability by linear geometry—is inseparable from the simplicity of the diagrammatic descriptions of morphometric phenomena to which that model leads. Perhaps Campbell could show us a landmark data set for which the difference between the linearized normal model and the generalized gamma model is sufficient to affect one's scientific inferences; I have never encountered such an example.

Some clarifications. (1) Colin Goodall points out that one cannot expect a nonaffine deformation to corroborate the behavior of distance ratios among all the constructed landmarks. This is not as great a problem as it seems. In practice, the pairs of landmarks involved in the productions of Theorem 2 tend to belong to the convex hull of the form—the optimal distance measure tends to be an expression of growth gradients that can be modeled as monotone. The interpolation used in Figures 1 and 15 and elsewhere is driven by just such a strictly linear correspondence of computed landmarks around the boundary, so that it meets the needs of Goodall's requirement in practice. It happens that this particular interpolator, like the thin plate spline mentioned by Sampson, is based on harmonic functions, so that it cannot lead to extrema of any directional derivative except at landmarks. This suits it well to the visualization of the results of Theorem 2. (2) Gregory Campbell observes that the null model appears not to apply to several of the examples. Naturally it does not; it was rejected. Both the data of Figure 7 and the data of Figures 13 through 17 show allometry: in one case, a correlation of size with shape; in the other, a correlation of size changes with shape changes. This is not the negation of the null model, but its refinement, credible whenever the scatter of shape coordinate residuals from the allometric model appears suitably circular. (3) The point of my Theorem 1 is not that criticized by Campbell in his first paragraph ("Such approximations encourage zero covariances"). Theorem 1 is not about the covariances of size S with ratios for which it serves as denominator. Its subject is the covariance of S with any ratio of distances between constructed landmarks, whatever the denominator. That the covariances Campbell discusses are zero for any size variable has nothing to do with the covariances involved in Theorem 1, which are all zero, to first order, only for variables equivalent to S. Incidentally, the shape vector H of Campbell's first paragraph is not satisfactory for morphometric studies, as it is not invariant under rotation or translation of the coordinate system in which the landmarks Z_i are located. (4) Sampson and Campbell both note that I omitted a crucial clause in my restatement of Mosimann's main theorem. The variables V_i of the first paragraph in Section 4 are, of course, to be taken as multivariate normal. (5) Noel Cressie describes the possible role of the symmetric axis in one's thinking about landmarks. There is a discussion along similar lines in Section 4.1 of Bookstein et al. (1985); we share his optimism.

Inhomogeneity and smoothing. I shall use the remainder of my space to speculate along a line suggested by Sampson and Goodall. Together they have raised complementary horns of a morphometric dilemma. To detect deviations from homogeneity of transformation in the individual case, one needs many landmarks, so as to test for and localize significant failure of fit in Goodall's regression (1); but to detect any signal at all in sample to sample comparisons, as Sampson points out, one loses power as the number of landmarks rises.

I suggest resolving this tension by considering *components* of transformation loosely analogous to Sneath's (1967) polynomial regressions but tied tightly to the algebra of landmark mean locations. Consider first a quadrilateral of landmarks, taken, for simplicity, in the form of an exact square. Choosing either diagonal of the square, one can divide this square into two triangles sharing that diagonal as baseline. The net shape change of the quadrilateral from the square form to another can be described by a four-variable shape basis made up of the pair of pseudovectors describing the shape changes of either pair of opposing triangles. Denote these two pseudovectors as dQ_1 and dQ_2. In Figure 13 the scatters of such a pair of dQ's for the diagonal Sella-Menton are shown in frames (*a*) and (*b*). The matching of scattered points dQ_1, dQ_2 between the frames is not shown, but is crucial to the analysis to follow.

There are two summary quantities for the shape change of a quadrilateral that, when properly corrected for baseline change, are independent of the triangulation chosen. Details of this invariance are presented in Bookstein (1985). For a starting form which is square, they take a particularly simple algebraic form.

The *homogeneous component* of the transformation is the vector *difference* $dQ_1 - dQ_2$, representing the average of the transformations on either side of the diagonal, changes in lengths or angle of the diagonals without change in their point of intersection; and the *purely inhomogeneous component* of the shape change is the vector *sum* $dQ_1 + dQ_2$. This component measures the amount of translation of either diagonal with respect to the other without change in length or angle. Clearly the two components together are as informative as their sum and difference, the pseudovectors dQ_1 and dQ_2 with which we started.

The purely inhomogeneous transformations (reviewed in Bookstein, 1985) seem to be unfamiliar to many applied geometers. A typical transformation of this class is that taking the unit square with corners at (±1, ±1) to the kite with corners at (−1.5, −1.5), (1, −1), (0.5, 0.5), and (−1, 1). If this transformation is to be modeled as linear upon the edges of the starting square, then a reasonable interpolated distortion is the *bilinear* map $(x, y) \to (x, y) - \frac{1}{4}(1 + xy, 1 + xy)$, as shown in Figure 23a. This map bends one diagonal and transforms the other diagonal nonlinearly along itself. From its affine derivative, the matrix

$$\begin{bmatrix} 1 - \dfrac{y}{4} & -\dfrac{x}{4} \\ -\dfrac{y}{4} & 1 - \dfrac{x}{4} \end{bmatrix},$$

we see that the map has a singularity of principal directions at the center (0, 0) of the square, where this matrix is the identity. The biorthogonal grid for this

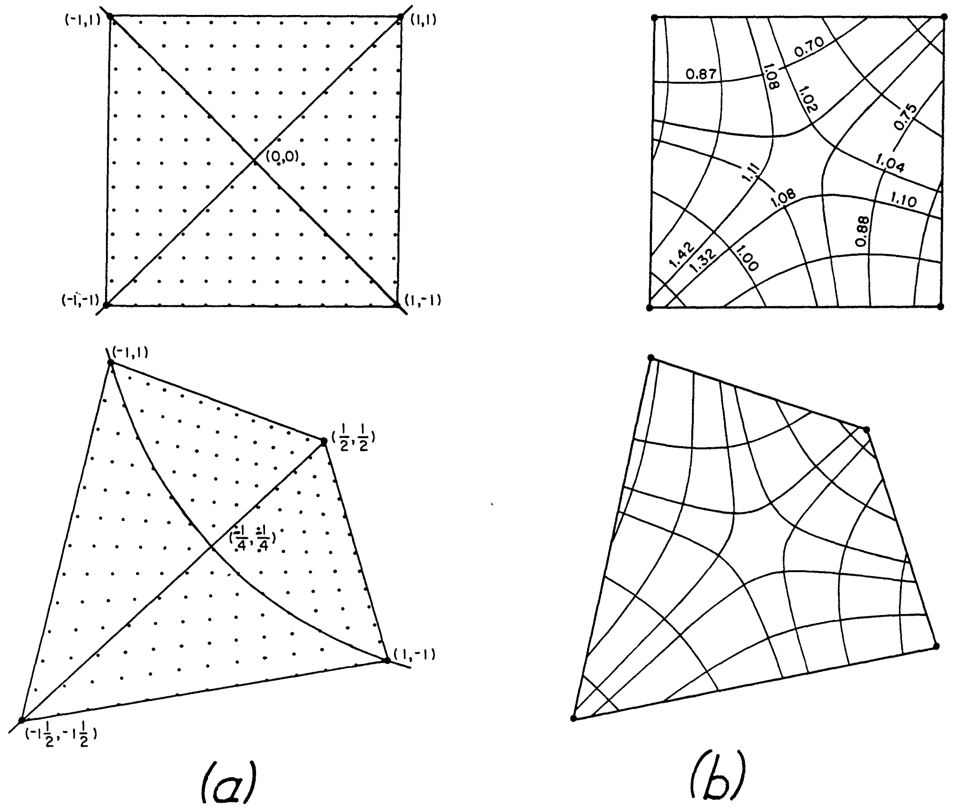

FIG. 23. *Every shape change of a quadrilateral of landmarks has a purely inhomogeneous component, the extent to which its diagonals are translated with respect to each other without change of length or angle. This component can be visualized as a transformation of the interior of the quadrilateral.* (a) *The interpolated bilinear map, linear on all four edges of the quadrilateral but not on the interior diagonals.* (b) *The biorthogonal grids for the map in* (a). *There is a singularity around which the integral curves and principal strains show unexpected threefold or sixfold symmetry* (*cf.* Bookstein, 1985).

map (shown in Figure 23b) has exactly hexagonal symmetry of the grid lines and triple symmetry of the principal strains near that singularity. (This pattern was already hinted at in Figure 18.)

Another candidate for interpolating the distortion from square to kite is the ordinary projection leaving all straight lines straight, the diagonals as well as the edges. The projection is not linear around the edges of the starting square, and has a different singularity inside, analogous to that at the origin of a parabolic coordinate system. Other distinctions between these two interpolants are reviewed in Bookstein (1985).

The simple shape variables suggested by the purely inhomogeneous mapping are not ratios of perpendicular distances through a single point but either (i) ratios of lengths of parallel edges on opposite sides of the singularity, or (ii) ratios of collinear lengths measured away from the singularity in opposite directions. Figure 23 suggests two ratios of the first kind, that of the vertical edges and that of the horizontal edges. Their composite is the sum of the north and east edge lengths divided by the sum of the south and west edge lengths. On the null model for variation around the kite shape, this ratio is statistically equivalent to the ratio of the heights of the two triangles upon the diagonal from $(1, -1)$ to $(-1, 1)$, a ratio of the second sort. Compare the less symmetrical analysis of Figure 18, which afforded only one simple shape ratio.

In a sample of forms represented by four landmarks, the net T^2 for shape may be partitioned into one component testing the homogeneous part and another testing the inhomogeneous part. Applied to the data of Figure 13, for instance, we find that both these components of change are statistically significant. A biometric description of the growth of this splanchnocranial quadrilateral must refer to both the net affine transformation and its regional variation. For a quadrilateral, the regional variation cannot be localized; like an interaction term in the analysis of variance, it is instead the assertion of a gradient (in this context, a growth-gradient) across the form in one or two directions.

This simple algebraic decomposition should be extendable to components of higher order for landmark configurations more complex than quadrilaterals. Such a scheme would replace the smoothing that Goodall suggests by a noise-suppressing decomposition of the exactly interpolated transformation, a decomposition which applies both to the individually observed deformations (whenever the data support such a notion) and to deformations representing differences of sample means, allometry, or other designs. These components will be somewhat analogous to orthogonal polynomials, which are at once expressions of the geometry of a domain and also planned comparisons suited to linear modeling. Just as the purely inhomogeneous transformation can be recognized by the characteristic hexagonal singularity of its grid, as in Figure 23, a reasonable set of higher order components might be expected to bear characteristic grid "fingerprints." I agree with Sampson that the influence of exogenous factors upon these or other components of deformation could be construed as a factor regression and studied very effectively under a version of Wold's soft modeling.

I thank the discussants for their conscientious scrutiny of an unusually long manuscript and for their aid in establishing morphometrics as an arena for serious biometrical thought. As did David Kendall, I would also thank the Editor for boldly offering considerable space to this new topic. If our development of this field will further combine geometrical, biological, and statistical themes so diverse, it will continue to be worth the attention of the general statistical community.

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