Committee II
Theoretical Empiricism: A General Rationale for Scientific Model-Building

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SOFT MODELING AND THE MEASUREMENT OF BIOLOGICAL SHAPE

by

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I. The Comparison of Biological Forms as a Latent Variable

In his classic *On Growth and Form* of 1917, the great British natural philosopher D'Arcy W. Thompson introduces the study of form-comparisons thus:

> ...The morphologist, when comparing one organism with another, describes the differences between them point by point, and 'character' by 'character'. If he is from time to time constrained to admit the existence of 'correlation' between characters ..., yet all the while he recognizes this factor of correlation somewhat vaguely, as a phenomenon due to causes which, except in rare instances, he can hardly hope to trace; and he falls readily into the habit of thinking and talking of evolution as though it had proceeded on the lines of his own descriptions, point by point, and character by character.
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> ... But when the morphologist compares one animal with another, point by point or character by character, these are too often the mere outcome of artificial dissection and analysis. Rather is the living body one integral and indivisible whole, in which we cannot find, when we come to look for it, any strict dividing line even between the head and the body, the muscle and the tendon, the sinew and the bone. Characters which we have differentiated insist on integrating themselves again; and aspects of the organism are seen to be conjoined which only our mental analysis had put asunder. The coordinate diagram throws into relief the integral solidarity of the organism, and enables us to see how simple a certain kind of correlation is which had been apt to seem a subtle and a complex thing.
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> But if, on the other hand, diverse and dissimilar fishes can be referred as a whole to identical functions of very different co-ordinate systems, this fact will of itself constitute a proof that variation has proceeded on definite and orderly lines, that a comprehensive 'law of growth' has pervaded the whole structure in its integrity, and that some more or less simple and recognisable system of forces has been in control. (Thompson 1961[1917]:274-275)

In this manner Thompson explicitly identifies the object under discussion, namely the relationship between biological forms, with a **latent variable** (LV): an abstraction for the efficient explanation of diverse, covarying comparisons distributed over the organism. His identification of this LV with a "system of forces" reflects the biomechanical understanding typical of his era, obsolete now; what remains, the idea of a "simple and recognisable" geometrical pattern of explanation (Figure 1), has fascinated mathematical biologists and morphologists from Thompson's day to the present.

The endurance of Thompson's insight owes to its felicitous blending of two previously unrelated descriptive traditions. The latent variable of which he speaks had hitherto been studied in biology and in mathematics separately, where it went by two different names. The biologist knew it as **homology**, the rules by which parts of different organisms were understood to correspond, whereas the mathematician knew it as the pointwise **deformation**, "Cartesian transformation," acting to distort a picture plane or other specifically geometric representation of form. The identification of these two formal models in the study of a single empirical problem lies at the foundation of modern morphometrics (Bookstein, 1982a; Bookstein et al., 1985).

Landmarks. To reliably quantify the forms of organisms varying in shape, the biologist needs to pass from a homology of parts to one of (mathematical) points. The observed form is thereby abstracted into a configuration of **landmarks** having both a geometric location and a biological identification: for instance, "the bridge of the nose, there on the x-ray." The two attributes correspond to the two sources of information combined in the LV model. Each landmark, located in all the forms of a series, is a systematic one-point sample of the homology function. For instance, the bridge of this nose is homologous to the bridge of that nose, by definition, and so the point-deformation which is the homology of these two x-rays must map this point to that one.

Such a representation of deformation, the mention of one point at a time along with its image, is mathematically clumsy. From configurations of landmarks the researcher usually passes directly to an explicit homology function by an **interpolation** (Bookstein, 1978) that is smooth in-between the landmarks at which it is observed. For empirical comparative studies of biological form, a LV may thus be operationalized as a geometrically smooth effect on shape: a systematic shape difference spatially distributed over the interior of a configuration of N homologous landmarks. Because a LV is an explicit deformation, we will be able to diagram it directly as an effect upon the typical form. In place of dry parameter vectors of inner and outer weights, we will be able to visualize the actual geometrical quantities explained by the LV, the spatial pattern of correlated changes in form.

Morphometric variables. In practice, a LV is inseparable from its manifest indicators. What sort of indicators might be appropriate in the study of deformation? One might guess that the natural space of indicators is spanned by the $2N$ Cartesian coordinates of the N landmarks under study. However, it is not biological forms separately that we seek to measure, but relations between forms; these are not measured by vectors (two coordinates per point) but by symmetric tensors (three parameters per point), as will be explained in Part II. Although landmark coordinates make up the raw archive of our data, their comparison requires a different, richer set of constructs: the **shape** and **size measures** that can be derived from the coordinate records by manipulations of greater or lesser complexity.

A **size measure** is a function of the landmark coordinates which is linear in geometric scale and which is computed homologously from form to form. Examples include the distances between landmarks in pairs, the distance from one landmark to a point 30% of the way from a second to a third, etc. By a **shape measure** we mean, in essence, the ratio of a pair of size measures. Such ratios will be of dimension zero in geometric scale. The more familiar shape measures are functional transformations of such ratios; for instance, an angle is the arc-tangent of the ratio of distances which is the tangent function. Particular comparisons of form can always be described by a systematic pattern of size measures representing geometrically parallel or perpendicular extents upon the organism—the **biorthogonal grid** to be sketched in Part III. These patterns encapsulate the LV under study with optimal descriptive efficiency.

II. Analysis of a Single Triangle of Landmarks

In landmark-based morphometrics, the universe of indicators of form has only a finite number of degrees of freedom. The coefficients of any LV are capable of carrying all the information needed to reconfigure the landmarks appropriately. It is convenient to introduce the study of these LVs and their indicators, the shape and size variables, using a measurement space of the simplest possible structure. When landmarks are taken three at a time, in triangles, there are only three degrees of freedom for form-description: two for shape and one for size. We therefore begin the study of deformation with shape changes of triangles. The LVs which result from conventional soft modeling in this context can be made manifest as new indicators, and remain manifest even when we restore size information (the third degree of freedom) to an analysis. The later examples of Part III deal with more extensive configurations of landmarks. In these models for LVs, the indicators corresponding to one triangle will make up one first-order LV; the set of these will make up a block of their own, each contributing to the representation of a deformation as a second-order LV.

Shape coordinates for a triangle. Shape measures, by definition, are ratios of size measures. In the study of triangles, the most convenient size measures are the lengths of edges. Let us select one edge of the triangle ΔABC—say, the edge AB—and scale the triangle so that the length of that edge is constant at 1.

After scaling so, we may register landmark A at the Cartesian point (0,0) and landmark B at the point (1,0) (Figure 2). If landmark A were originally at (x_A,y_A), B at (x_B,y_B), and C at (x_C,y_C), then the normalization on edge AB assigns landmark C the Cartesian coordinates (ν_1,ν_2) where

$$\nu_1 = \frac{(x_B-x_A)(x_C-x_A) + (y_B-y_A)(y_C-y_A)}{(x_B-x_A)^2 + (y_B-y_A)^2},$$

[1]

$$\nu_2 = \frac{(x_B-x_A)(y_C-y_A) - (y_B-y_A)(x_C-x_A)}{(x_B-x_A)^2 + (y_B-y_A)^2}.$$

Because all triangles of the same Euclidean shape will yield the same point (ν_1, ν_2), all information about the shape of the triangle ΔABC must be coded in this coordinate pair.

One degree of freedom for shape variables. Consider any shape variable that can be computed from a triangle of landmarks. Figure 3a, for instance, illustrates the variable $\angle ACB$. Any shape variable is constant on some curve through C; the angle $\angle ACB$ happens to be constant along the circle through A, C, and B. Neighboring curves, in this case other circles through A and B, correspond to neighboring, nearly equally spaced values of the shape measure.

In a small region of this plot, this set of curves can be approximated by a family of parallel, equally spaced straight lines, Figure 3b. The shape variable varies fastest perpendicular to these curves, in the direction of the axis *G*, the *gradient* of the shape variable. The smaller the variation in a population of triangles, the better a shape variable is characterized by the direction of its gradient.

There is thus one family of linearly equivalent shape variables for every direction through the point C. For instance, the direction G in Figure 3c is the gradient of the angle $\angle AQC$, where Q is the point at 1.5 on the x-axis (in the coordinate system with A at 0 and B at 1). Another measure with the same gradient is the ratio to AB of the distance to the midpoint of AB. These two unfamiliar shape measures are linearly equivalent at C, as are all others bearing the same gradient there.

Every useful shape variable has a gradient in some direction. Since there is a semicircle's worth of directions around any point C, there is only a semicircle's worth of linearly different shape variables in the vicinity of a typical shape ΔABC. For any two distinct shape gradients G_1, G_2 at C, every other shape variable G is linearly equivalent to (i.e., has the same gradient near C as) some linear combination $aG_1 + bG_2$ of G_1 and G_2.

The effect of changing the choice of baseline—for instance, from $\overline{AB}$ to $\overline{BC}$—is to rotate all three edges $\overline{AB}$, $\overline{BC}$, $\overline{CA}$ of the mean triangle by the same angle, and rescale them all inversely to the change in baseline length. For any triangle, the constructed (ν_1,ν_2) following upon this change will differ from the former (ν_1,ν_2) by that additional rotation together with the same rescaling. Therefore, under change of the choice of baseline, the entire (ν_1,ν_2) scatter corresponding to a sample of triangles mainly rotates and changes its scale. To this order of approximation, any statistical analysis in the (ν_1,ν_2) plane which is invariant to rotations, translations, and rescaling will yield the same findings whatever baseline was chosen for the construction. Our soft models will all have this property, and hence will represent analysis of shape independent of the (arbitrary) choice of a size measure.

From gradient to shape variable: making a latent variable manifest. The obverse of this reduction of shape variables to gradients is the realization of particular gradients by particularly useful shape variables. For triangles, the deformation modeling any statistical summary of change in the configuration may be taken as geometrically uniform. Such a deformation may be represented everywhere inside the triangle by the **principal axes** of its **strain tensor**: the directions which bear the greatest and least ratios of change of length between the poles of the comparison. These directions must remain at 90° over the course of the contrast or trend they describe, just as the axes of an ellipse, longest and shortest diameters, lie at 90°. Figure 4 summarizes this representation and indicates how the principal strains may be observed directly by reference to two measurable distances upon the form. The shape aspect of this change is best summarized by change in the proportion between these two measured distances; incorporation of information about size change further specifies the ratios of change for the distances separately.

The particular proportion optimally reporting an observed mean shape difference in the (ν_1,ν_2) plane is constructed as in Figure 5. A small displacement $\Delta\nu$ of the mean form (r,s) in this plane corresponds to a principal cross of length-change ratios differing by $|\Delta\nu|/|s|$ and oriented at ±45° to the angle bisectors between $\Delta\nu$ and the baseline (Bookstein, 1984a). Form by form, each of these lengths is measured as a transect from one vertex through a computed aliquot of the opposite edge; as these endpoints correspond according to the model of uniform deformation, the segments are homologous over a sample, and so their lengths are proper size variables. The shape variable which is the ratio of these measured lengths has gradient precisely along $\Delta\nu$. Whatever the net size change, distances along one of these axes have the algebraically largest mean ratio between poles of the contrast, and those along the other have the algebraically smallest mean ratio, of all distances homologously measured over the set of triangular forms.

In matrix notation, this is the **polar decomposition** for an affine transformation (Bookstein, 1978, Chapter 8), its representation as a product $\mathbf{O}(\theta')\mathbf{D}\mathbf{O}^{-1}(\theta)$ of three simple transformations. Each **O** is a rotation ("O" for "orthogonal") taking principal axes from horizontal and vertical to their orientations as observed in the starting form (θ) or the ending form (θ'), while **D** is a diagonal matrix of the differential extension ratios along the two perpendicular principal directions. If the analysis is to be drawn upon a single form, as when the second configuration is free to rotate, then the leftmost factor $\mathbf{O}(\theta')$ may be omitted.

Indicators for a single triangle. A sample $\Delta A_iB_iC_i$ of triangular forms may be normalized upon their edges A_iB_i, form by form. Information about the size of $\Delta A_iB_iC_i$ is thereby lost; but the shape of each triangle, unaltered by this maneuver, must be embodied explicitly in the position of the movable vertex C_i. Shape variation of the population of triangles can therefore be studied in the scatter of the points C_i after this construction, Figure 6a, and shape change may be studied in the scatter of pairs (C_i, C_i') at two times, Figure 6b.

To adumbrate a true LV (the mean transformation) having the matrix $\mathbf{DO}(\theta)$, a 2x2 matrix, we use as indicators the two vector components $(1,0)L_3\mathbf{O}'\mathbf{DO}$, $(0,1)L_3\mathbf{O}'\mathbf{DO}$, where L_3 is the column vector encoding the position of the third landmark using the other two landmarks as baseline that the (arbitrary) rotation $\mathbf{O}'$ has sent to horizontal. From the observation of these two components we can reconstruct $\mathbf{D}$ and θ up to the change of scale of the baseline.

In all the soft models to follow, triangle by triangle the shape indicators will be such pairs of coordinates (ν_1, ν_2). Linear combinations of these will always be sums of simple regressions, Wold's "Mode A," because the gradient directions represented by the shape coordinates ν_1, ν_2 are always geometrically orthogonal vector components whatever their covariance in a sample. The first-order LVs corresponding to these little blocks of two will always be linear predictors of some other variable in the model, whether manifest (size, or age group, or sex) or latent (future shape or shape change). To the formula for the LV on such a block, the weighted combination of ν_1 and ν_2, corresponds a gradient in the shape space of its triangle. That gradient, playing the role of $\Delta\nu$ in the preceding discussion, yields up a particular shape measure, ratio of two distances at 90°, which measures it perfectly. Therefore, *to each first-order LV corresponds a new manifest indicator identical with it as estimated case by case.*

Under a suitable null model (Bookstein, 1985), change in perimeter is nearly uncorrelated with the shape coordinates for a variety of triangular configurations. (It is exactly uncorrelated in the case of circular landmark location error for an equilateral triangle.) When size is measured in this way, change in mean size and change in mean shape may be interpreted as separate aspects of the net change observed in a triangle of landmarks, with all coefficients of the soft model to be estimated Mode A. Such an interpretive decomposition is valid even if this size measure is correlated with shape in the sample under study. Alternatively, size may be regressed on shape by using any pair of the (ν_1, ν_2) coordinates. The result is a canonical description of **allometry**, the covariance of shape with size, which may be used to predict size from shape or shape from size.

III. The Computation of Deformations by Soft Modeling

The geometric and algebraic machinery is now entirely in place for describing systematic effects on shape and size in terms of latent variables of deformation. The present Part of this essay presents examples of the soft modeling of deformation for research designs at various levels of geometric or temporal complexity. These examples hint at a wider role for the generation of indicators after estimation, hints expanded in Part

IV.

Arrow diagrams including triangles. In the models to follow, each first-order LV stands for one triangle and represents a tensor, such as that of Figure 4, acting on that triangle. The position of these LVs in the model, together with the role of second-order LVs if any, will vary from example to example. The first-order LVs will be indicated by circles, after the usual semiotics of arrow diagrams; but inside each circle is sketched the triangle the LV represents. Inside that triangle there will appear, after the model is estimated, a diagram of the manifest shape variable (ratio of a pair of distances at 90°) equivalent to the first-order LV identified.

A cephalometric data base. In craniofacial biology it is customary to produce x-rays of the bony cranium and jaws in a standardized fashion. The patient's head is placed some six feet from the x-ray tube and a few inches from a film cassette; the central beam of rays passes along the line joining his ear holes and intersects the film plane at 90°. There result x-ray images on which edges of anatomical structures can be reliably traced in a conventional abstraction of normal anatomy. For instance, two kinds of curves are used—projections of true space curves, and edges of regression of bony surfaces; and landmark "points" may be true anatomical loci or intersections of shadows. Figure 7 shows a stereotyped tracing of the lateral cephalogram, with indications of five landmarks used in the course of the examples. Operational definitions of these points may be found in Riolo et al., 1974.

The data for these four examples are landmark locations from cephalograms taken annually in the course of the University of Michigan University School Study. The sample is of Ann Arbor schoolchildren followed over various age ranges in the 1950's and 1960's.

Single latent variables

Example 1. Change in mean shape of a single triangle. Figure 8a shows the arrow diagram for the analysis of group differences in the shape of a single triangle. So simple a model needs nothing beyond the most elementary methods for its estimation. Application of the soft interpretation in this context, however, will aid in the transition to the second-order LVs which represent nonlinear deformations.

The data for this example represent the form of the triangle Basion-Nasion-Menton in Figure 7. This triangle is often used by orthodontists to summarize the so-called **splanchnocranium**, the whole head below the brain. From the University School Study archive we retrieved the coordinates of these three landmarks for a subsample of 36 males with cephalograms at both age 8 (plus or minus six months) and age 14.

The LV embodying the form of this triangle bears three indicators: the perimeter of the triangle and the coordinates of Menton in a system with Basion at (0,0) and Nasion at (1,0). The scatter of these shape coordinates at the two ages is displayed in Figure 8b. For all these analyses, age is coded by a single bit: 0 for the 8-year-olds, 1 for the 14-year-olds.

We estimate our "soft model" using the covariance matrix between age and the indicators of the LV:

	Age gp	ν_1	ν_2	Size
Age gp	.25			
ν_1	-.00004	.00382		
ν_2	-.01633	-.00003	.00262	
Size	.03312	-.00073	-.00235	.00597

The outer weights for the LV embodying the change of form over time are estimated by mode-A regression of age upon the indicators of its block. They are just the quotients of the entries in the first column by .25: (-.0001, -.0653, .1325), equal, of course, to the differences in means of the indicators between the groups.

As indicated in Figure 8c, the proportion making the shape LV manifest is essentially the aspect ratio of the triangle under consideration, the ratio of its height (distance of Menton from the Basion-Nasion baseline) to its base (the distance Basion-Nasion). The dominance of this direction in facial growth has been known to craniofacial biologists for some time (Bookstein, 1983). Because size information is present as a third indicator for this first-order block, the net rates of growth observed in the two principal directions may be computed separately and indicated directly upon the diagram: .091 along the base, .175 along the "growth axis." The coefficient .132 of change in "size" (perimeter) is very nearly the average of these.

Example 2. Change in mean shape of a polygon. When there are more than three landmarks under study, the first-order LVs representing triangles one by one must be treated as indicators of a second-order LV representing "the transformation as a whole," the smooth deformation to which Thompson was referring. In this example we continue to analyze a mean change of shape over age, so as to ease the assimilation of the findings; but we consider a mosaic of triangles instead of just one.

Figure 9a shows a polygon from **mandibular plane** to **cranial base**, divided into two triangles Sella-Menton-Nasion, Sella-Menton-Gonion (see Figure 7) along a convenient diagonal which happens to be close to the growth direction unearthed in the previous analysis. The arrow diagram for this model is as in Figure 9b: the single exogenous variable Age is presumed to drive a pattern of correlated shape changes throughout the form.

The covariance matrix relating the four shape indicators (two per triangle) and age is:

	Age gp	$\nu_{1,Nas}$	$\nu_{2,Nas}$	$\nu_{1,Gon}$	$\nu_{2,Gon}$
Age gp	.25				
$\nu_{1,Nas}$	-.00484	.00142			
$\nu_{2,Nas}$	-.01196	.00024	.00153		
$\nu_{1,Gon}$	.00144	.00005	-.00021	.00061	
$\nu_{2,Gon}$	-.00524	-.00018	.00037	-.00004	.00078

Again the outer weights are just the mean differences in shape coordinate between the groups: (-.01936,-.04783) for the first triangle, (.00573,-.02095) for the second.

The manifest shape measures corresponding to the LVs for the triangles separately do not appear to be equal. The second-order LV we have just estimated is therefore describing a nonlinear shape change. We visualize it by abandoning the finite triangles for the differential point of view (Bookstein, 1978). The estimated second-order LV explicitly specifies a reconfiguration of the landmark coordinates as drawn in Figure 9c. Reverting to the spirit of D'Arcy Thompson, we treat these points as a sample of the biological homology function throughout the interior, and interpolate their correspondence by a smooth computation, Figure 9d.

At every point of this correspondence there will be a pair of directions which, locally, serve the role of the axes of the ellipse in Figure 4: they are the principal axes of the affine derivative, directions of greatest and least local rate of change of length. We may integrate the arms of these little crosses into a new coordinate system, the **biorthogonal grid**, which is everywhere parallel to one arm or the other in both forms, and thereby lies at 90° in both. Corresponding intersections of curves in the left and right grids are homologous according to the interpolation in Figure 9d. The pair of grids is thus an orthogonal coordinate system customized for representing this particular shape change.

The changes from left to right in the spacing between successive intersections of these grids represent a **symmetric tensor field** distributing the landmark shifts throughout the interior of the form. They depict the **affine derivative** of the map in Figure 9c, estimated as a weighted average of the affine derivatives $O(\theta')DO(\theta)$ representing the shifts at each boundary landmark with respect to its two neighbors. The LV in Figure 9c is equivalent to the construction at every interior point of its own pair of indicators, the weighted averages of the four indicator pairs describing each corner separately.[1]

The depiction in terms of a tensor field, Figure 9e, is much more convenient. The biorthogonal grid indicates the principal features of the shape change independent of the original triangulation: that is, it draws out the second-order LV without further reference to the first-order indicators. The dilatations indicated on the drawing are all relative to growth along the baseline Sella-Menton. We see that the overall shape change is highly directional in the maxilla, but less so in the lower face, and that the horizontal rate of growth is graded from top to bottom.

Several latent variables

Example 3. Forecasting the shape of a single triangle. Consider again the triangle Basion-Nasion-Menton of Example 1. The mean change of shape (Figure 8) is statistically significant (Bookstein, 1984a), but does not appear to explain much of the

[1]This set of eight indicators is of rank four. See Bookstein, 1984b.

data. The "pin plot" connecting corresponding shape coordinate pairs from the first age to the second indicates a considerable stability of relative position in this scatter. It is useful to know, then, exactly how the shape at the earlier age might abet prediction of the shape at the later. The soft model which allows an answer to this question is diagrammed in Figure 10. The correlations among its indicators are as follows:

	$\nu_{1,old}$	$\nu_{2,old}$	$Size_{old}$	$\nu_{1,yng}$	$\nu_{2,yng}$	$Size_{yng}$
$\nu_{1,old}$	1.0					
$\nu_{2,old}$	.0564	1.0				
$Size_{old}$	-.3175	-.1471	1.0			
$\nu_{1,yng}$	.8592	.0266	-.3643	1.0		
$\nu_{2,yng}$	.1305	.6443	-.0884	-.0532	1.0	
$Size_{yng}$	-.2909	.1350	.7891	-.2794	-.0309	1.0

Estimation of this model using only the two sets of two shape indicators results in the LVs shown, with weights (.96118,.27593) at the later age, (.96074,.27744) at the earlier. The correlation between these two LVs is 0.889.[2] (The second dimension of this data set yields a correlation much lower, some .62.) For males, one direction of shape variation is distinctly most reliable, the direction approximately perpendicular to the

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[2]As the correlations between the shape coordinates of a single block are mild, these weights do not differ materially from the canonical coefficients estimating the same model by Mode B.

growth axis. Approximately perpendicular to this gradient is the gradient direction of greatest shape <u>un</u>reliability; here it is aligned closely with the vector from Basion to Menton. Additional information about size makes the optimal forecasting of shape insignificantly more accurate, although size bears its own strong autocorrelation.

Example 4. Forecasting a more complex configuration. As Example 2 generalized the analysis of Example 1, so we can replace the first-order LVs of the preceding model by second-order LVs assembling diverse triangles. In this example, we use the same pair of triangles that was used in Example 2, and attempt to forecast between the ages as in Example 3. The model we are estimating is shown in Figure 11a with all the triangles filled in.

At convergence (Bookstein, 1982b), each LV is the sum of two partial predictors, each involving the indicators of one triangle with a net weight proportional to the strength of that partial prediction. Each partial predictor is the weighted sum of the two indicators for that triangle, with weights proportional to their correlations with the partial predictor. Thus both the combination of indicators into first-order LVs and the combination of the two first-order LVs into each second-order LV proceed without regard for sample correlations: Both pairs are treated as conceptually orthogonal. Estimation of this same relationship by canonical correlations analysis—that is, by a single pair of first-order LVs tapping all four indicators equivalently—results in a correlation of .936 but weight relations which have much less geometrical meaning.

The first-order LVs are approximately parallel between the ages, as shown in the diagram; the weights for the second-order LVs are nearly equal, indicating that predictability is fairly homogeneously distributed over the face. The correlation between the two second-order LVs is .9084.[3] Drawn out in Figure 11b, the second-order LVs appear to have a geometry of fair complexity.

The interpolation which distributes this LV throughout the interior of the landmark polygon is as in Figure 11c, and is summarized by the biorthogonal grid pair in Figure 11d. (Do not be perplexed by the six-sided singularity at the center; it surrounds an **isotropic point** at which the rate of growth is the same in all directions, and always appears when two adjacent sides of a quadrilateral increase in length faster than the diagonals [Bookstein, 1984b].) The distance having the highest covariance with this LV is the distance Sella-Gonion; that having the lowest covariance is the segment Nasion-Menton. The shape measure most sensitive to this change, and thus most stable over normal male growth from age 8 to age 14, is not a ratio of perpendicular distances, as in the previous examples, but the ratio of nearly parallel distances Nasion-Sella:Gonion-Menton. The orthodontist knows this as the ratio of **anterior** to **posterior facial height** or, in another geometric guise, the **mandibular plane angle** between the segment Sella-Nasion and the segment

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[3]Analysis of the triangles separately, each treated as in Example 2, results in slightly lower correlations: .8966 for the triangle on Nasion, .9041 for that on Gonion.

Gonion-Menton.

These analytic strategies may all be generalized from data in two dimensions to data in three. The first-order LV representing the shape change of a tetrahedron is now a combination of five indicators, each one the result of premultiplying the true transformation matrix **DO** (now three-by-three) by an essentially arbitrary vector. Two of these indicators are those we have already been using: the components of the two-dimensional LV for shape change of one face of the tetrahedron. These are augmented by three additional indicators specifying the movement of the tetrahedron's fourth vertex when all three vertices of the face opposite are fixed in position. The visualization of such a LV is carried out by the generalization to three dimensions of the algorithms underlying Figures 9c-e or Figures 11b-d: conversion of outer weights to landmark shifts, interpolation of a continuous mapping consistent with those shifts and linear between landmarks, and interpretation of that mapping by its principal directions of greatest and least ratios of change in length.

IV. Toward a Calculus of Indicators

To further elaborate the role of soft modeling in morphometrics would render this essay arcane. Instead, in these closing paragraphs I wish to recapitulate one particular theme that speaks to a wider arena than the merely biometric: the role of soft modeling in generating schemes of new measurements.

The relation between indicators and latent variables is not a one-way passage. Through the patterns unearthed by covariance modeling and the interpretation of those patterns, soft modeling deals not only with the covariances of the indicators observed but also with the covariances of other indicators, indicators which might have been measured. One returns from a soft model with notions about better measurement, if not for this data set, then for the next.

In morphometric modeling there is an infinitude of indicators, the size and shape measures, but one does not need them all. The crucial link between latent variables and indicators is the biorthogonal grid of principal strains at 90°. Representation of the LV by its grid, as in Figures 9 or 11, closes the loop of soft modeling by directing our attention to explicit new indicators which best adumbrate the LV out of all the indicators which could be assayed. The LV is a filter, in other words, which purifies our measurement scheme. In biometrics, the indicators specified in this way—latent variables made manifest—very often correspond to informal clinical knowledge hitherto untestable, and always seem to suggest new hypotheses and explanations.

Now, by virtue of the finite dimension of its subject-matter, morphometrics is atypically rich in symmetries and analytic elegances. In other disciplines there are partial substitutes for the powerful analytic geometry of the plane that I have been wielding here: the endless idiosyncrasies of individual social indicators, the semantics of attitude probes, the biases of economic series, and so forth. When a LV bears a contrast between contributions with the same presumptive sense of regression (that is, when the modeling reverses the sign of a simple Pearsonian *r*), the investigator ought to imagine new variables that directly capture the discrepancies. This is an extension of the role played in biometrics by the preponderance of shape variables. Shape ratios, as explicit contrasts, tend to have far lower confounding correlations than size variables. Size need not appear more than once in an analysis once we have discovered that it is there; likewise, the general factor of a block of indicators, once discovered, needs to be augmented by the patterned contrasts contributing additional predictive power to the model. One must thereupon return to the real world in order to systematically oversample the indicators contributing to these contrasts.

In either context, biometrics or the social sciences, the closure of the soft modeling loop is a passage from the covariances of the indicators back to their meaning and their own limitations. That reversal of emphasis serves as a <u>renewal</u>, augmenting the information available to the modeler. As such a cycle proceeds, the latent variables will be developed like latent images on a photographic plate: made steadily more manifest, steadily more explanatory. The lesson of biometrics for soft modeling is that one is never finished with measuring.

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Captions for Figures

Figure 1. Cartesian transformation from *Diodon* to *Mola*, after Thompson (1961).

Figure 2. One set of shape coordinates of triangle ΔABC: the coordinates of point C in a Cartesian system with A at (0,0) and B at (1,0).

Figure 3. The geometry of shape variables in small regions of the shape coordinate plot. (a) Example: isopleths of the shape variable ∠ACB are circles through A and B. (b) Approximating a shape variable by a Cartesian coordinate. The variable is represented by *G*, the direction of its gradient. (c) All shape variables with the same gradient near a mean form are statistically equivalent. Dashed lines, isopleths of the angle ∠AQC; solid curves, isopleths of distance to the midpoint of AB. These variables are statistically equivalent only near the one point indicated.

Figure 4. Homogeneous deformation as a symmetric tensor. (a) The uniform shear of triangles suggested by two sets of three landmarks. (b) Rates of change of length in various directions may be represented by the radii of the ellipse into which a circle is deformed. (c) The principal axes of deformation are the principal diameters of this ellipse, and the principal strains are proportional to their lengths. The corresponding diameters of the circle are perpendicular as well. (d) Because the principal axes have only direction, not location, they may be indicated by

using transects through vertices each dividing the edge opposite in a computed ratio. Distances specified in this way are homologous from form to form according to the uniform deformation in (a) above. The ratio between them is the observable proportion most sensitive to this particular shape change.

Figure 5. Constructing the proportion optimally describing a mean difference of position on the shape coordinate plot. The example drawn corresponds to the gradient G at point C of Figure 3c. (a) From the vector between centroids to the principal cross. (b) From the principal cross to a simple proportion of finite measures. The same result would be obtained by applying the construction of the previous Figure to the deformation from $\Delta\overline{ABC}$ to $\Delta\overline{AB}(\overline{C}+\Delta\nu)$.

Figure 6. Scatterplots for shape and shape change. (a) A population of shapes may be represented by the scatter of locations of the third vertex after a registration (to various scales) upon the other two vertices. (b) The "pin plot." A population of shape changes may be represented by vectors connecting the two registered locations of that third vertex. The directions of the vectors may be coded by a symbol (the "pinhead") at one end.

Figure 7. Conventional tracing of a lateral cephalogram, showing the structures and landmarks used in the examples. After Riolo et al. (1974).

Figure 8. Change in mean shape of a single triangle. (a) Arrow diagram with one triangle. The indicators of the LV here,

representing the mean shape change, are the two Cartesian coordinates of the landmark Menton in a coordinate system fixing Basion at (0,0) and Nasion at (1,0). (b) The complete data set: location of Menton in a Basion-Nasion coordinate system, for 36 males at ages 8 (heads of pins) and 14 (tails of pins). The solid vector connects the age-specific centroids; it is the LV we seek. (c) Arrow diagram after estimation Mode A. The vector of mean shape change given by the outer weights has been interpreted as a cross of perpendicular distances across the triangle according to the construction of Figure 5. Size change is restored to the mean ratios of change in distance along these directions.

Figure 9. Change in mean shape of a polygon. (a) A quadrilateral and one triangulation. (b) Arrow diagram for the second-order LV that is the mean shape change, with first-order LVs (the separate triangles), after estimation. Size change is restored to distances in the principal directions as in the previous example. (c) Reconfiguration specified by the outer weights (here, actual mean shifts). The baseline Sella-Menton is fixed by construction; the tensor analysis is independent of this choice of baseline. (d) The second-order LV, a smooth deformation corresponding to this reconfiguration, here drawn as a Cartesian transformation (cf. Figure 1). (e) Biorthogonal grids for this deformation: the coordinate system whose axes intersect at 90° both before and after the deformation.

The decimal numbers are selected rates of growth as the Cartesian transformation imputes them to its principal directions everywhere in the interior.

Figure 10. Forecasting the shape of a single triangle. Arrow diagram, after estimation, for one triangle at two ages. Note the stability of the estimated weights over six years.

Figure 11. Forecasting the shape of a quadrilateral. (a) Arrow diagram with triangles, after estimation, for the relation of two second-order LVs representing the shape of the quadrilateral at the two ages. (b) Reconfiguration (to the baseline Sella-Menton) specified by the outer weights for a small multiple of the indicated latent dimension. (c) Cartesian deformation representing the second-order LV by the relation of the two configurations in the previous frame. (d) Biorthogonal grid pair for the deformation of frame (c), with selected ratios. The most stable measure of shape is not a ratio of perpendiculars but a ratio of approximate parallels, Sella-Gonion:Nasion-Menton.