

Chapter 16

Prospectus: The Future of Morphometrics

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Idea and Aims

The field of morphometrics has transitioned relatively smoothly through several different phases, from D'Arcy Thompson's (1917) extraordinary and influential treatise on growth and form, through the influx of algebraic and statistical methods related to eigenanalysis, cluster analysis, and multidimensional scaling, to direct landmark-based Procrustes and deformation methods that echo Thompson's original intents and insights. In a sense, the discipline is still riding the wave of methodological advances that began in the 1970s (Adams et al. 2004). Although it is difficult to predict to direction of future methodological advances, it is certain that morphometric methods will be extended to areas currently at the periphery of current applications, such as the use of morphometrics to study the effects of quantitative trait loci (Klingenberg et al. 2001; Klingenberg 2003; Leamy et al. 2008) and the sizes and shapes of molecules (Billoud et al. 2000; Bookstein 2004; Rogen and Bohr 2003). However, even given the current level of methodological sophistication, there are still some important technical and conceptual problems to be solved in the shorter term. I will briefly highlight just a few of these here.

Three-Dimensional Analyses

The extension from 2-dimensional to 3-dimensional analyses has been available in principle for many years, and the use of 3D landmarks is becoming standard practice in fields such as physical anthropology and biomedical science. Procrustes methods are easily extended to three (or more) dimensions, and analyses of Procrustes residuals (Berge and Penin 2004; Lockwood et al. 2002; Nicholson and Harvati 2006) and, more recently, application of three-dimensional extensions of thin-plate splines and other morphometric methods are becoming more widely used (Bookstein 1989;

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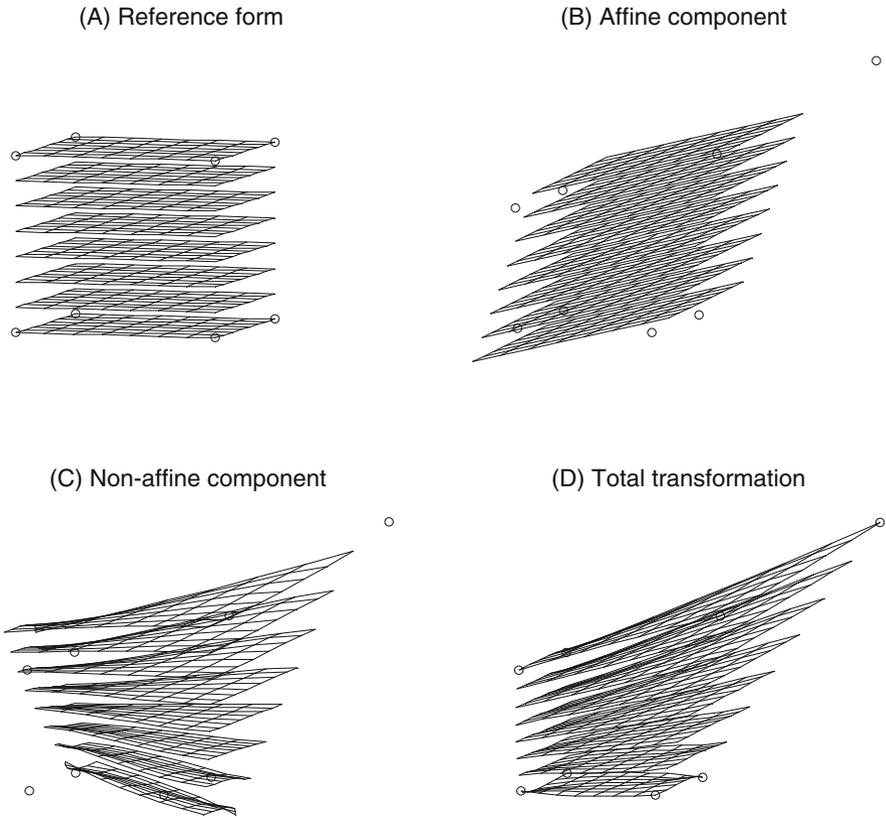


Fig. 16.1 Deformation of a reference form (a cube) to a target form based on the 3D thin-hyperplate spline interpolation. In the target form two landmarks (*top right*) have been displaced, while the others remain in place. The total transformation fits the points exactly, while the affine and non-affine components represent, respectively, global and local components of the total transformation

Gunz et al. 2005; Mitteroecker et al. 2004; Mitteroecker and Gunz 2002; O’Higgins and Jones 1998; Rohlf and Bookstein 2003; Rohr 2001).

Because illustrations of 3D thin-plate splines are rare, a simple example is illustrated in Fig. 16.1. This “thin-hyperplate” spline corresponds to the distortion of a malleable cube. The shift of any arbitrary point is given by a weighted sum of landmark shifts, in which each landmark shift is weighted according to its distance from the point (Bookstein 1989). The weights for interpolated shifts of arbitrary points in three dimensions are $-U(d) = -|d|$, where d is the distance from the point to a landmark. The stacked 2D planar grids for the reference form are a sample of slices through what is actually a solid 3D grid, but the planar grids are useful for visualization. The corresponding layers in the final deformed “cube” are, of course, not necessarily planar even for subsets of landmarks that lie in a plane in both the

reference and target forms. Although, in parallel to the 2D case, the non-affine component of the spline can be decomposed into eigenfunctions in the 3D case, there are a number of computational details that need to be resolved. Bookstein (1989) listed several aspects of the 3D extension that “will require considerable imagination”. In particular, since 2D splines are visualized in 3D, it is not clear how best to draw a thin-hyperplane spline that is a 3D projection of a 4D geometric object.

Landmark Variation

The problem of how to adequately characterize relative amounts and directions of variation at individual landmarks is of interest to many researchers, particularly those utilizing Procrustes analyses of 3D coordinates. Results depend sensitively on the particular method used to superimpose configurations of landmarks (the so-called registration problem). Although several versions of Procrustes alignment are available and their statistical properties have been well characterized (Rohlf 1990; Rohlf and Slice 1990), there are no apparent biological rationales for choosing among them. Minimizing the sum-of-squared deviations among corresponding landmarks on different forms tends to produce circular distributions of coordinate positions, with approximately equal amounts of dispersion for different landmarks, while minimizing the median deviations tends to produce more elliptical distributions and more variation among landmarks. Currently these statistical patterns cannot be distinguished from inherent biological variability.

Allometry

More direct ties to developmental biology are needed (Gilbert 2003; Klingenberg 2002), particularly with respect to allometric scaling. The use of power functions to characterize scaling relationships (Huxley 1932) has a long and venerable history (Brown et al. 2000; Strauss 1993), and in most biological disciplines the term “allometry” is virtually synonymous with use of power functions (and, more recently, with fractal dimensions). In the context of geometric morphometrics, however, shape is defined much more generally as the “geometric information that remains when location, scale and rotational effects are filtered out from an object” (Bookstein 1978; Kendall 1977, etc.). The Procrustes method is used in geometric morphometrics to standardize forms to a common centroid size, which represents an isometric size standardization (Bookstein 1991; Rohlf 1993). Consequently, the concept of allometry has been generalized to *any* variation in shape that is correlated with size (Bookstein 1991; Zelditch et al. 2003). The null hypothesis both for the geometric model and for Huxley’s model is isometry; however, deviation from the null in Huxley’s model represents a particularly constrained form of anisometry. In geometric morphometric analyses the coefficients describing shape differences are not meaningful in terms of specific growth models such as Huxley’s power law (Zelditch et al. 2004). Whereas deformation models are portrayed in the linear

space, Huxley's model is linear in the log-space. The anisometric "shape" variation studied in geometric morphometrics therefore consists of two components: allometric (*sensu* Huxley) and non-allometric. The issue of allometric size-adjustment (*sensu* Huxley) of Procrustes residuals or of deformation grids needs to be pursued further (e.g., Hammer 2004).

Missing Data

Missing data are a frequent problem in morphometrics, as they are generally in multivariate statistical analyses (Reig 1998; Richtsmeier et al. 1992; Strauss et al. 2003; Strauss and Atanassov 2006; Yarooh 1996). If a form is distorted (as in fossils) or has been damaged or broken off (as in delicate skeletal samples), then landmarks can be missing in some specimens. In statistical studies there are two main strategies for dealing with missing data: either the variables with missing data (coordinates of a missing landmark, in this case) must be ignored, or missing values must be imputed (i.e., estimated from the values in complete specimens). Gunz et al. (2002) have summarized how knowledge about the context of missing landmarks can be used to approximate their positions. This would include factors such as bilateral symmetry (landmarks on one side of the body can be "mirrored" to the other side), allometry (regression of Procrustes shape coordinates on centroid size), morphological integration (quantifying patterns of covariation of subsets of landmarks), and curvature smoothness (as quantified by magnitudes of deformation associated with the thin-plate spline interpolation). However, only a few preliminary comparative studies of these different approaches have been carried out, and much additional work needs to be done to characterize the best strategies for dealing with missing data.

Phylogenetics

Because morphometric studies are often carried out within a phylogenetic context, the use of morphometric data in phylogenetic analyses continues to be a contentious topic. MacLeod (2002) discussed this general question and suggested that the hesitation expressed by many at the use of morphometric data in phylogenetics can be traced back to the strong historical connections between morphometrics and phenetics, which was formulated as a philosophy of systematics in the 1960s and 1970s (Pimentel 1979; Sneath and Sokal 1973) and later directly contrasted with the aims and methods of cladistics.

There are three main areas in which morphometrics can play a role: (a) in the generation of characters useful for phylogenetic inference (i.e., estimation of trees); (b) in the interpretation of morphological diversification within the context of a phylogenetic hypothesis produced with other data (typically molecular sequence data); and (c) in "ancestral reconstruction", the inference about morphological states in ancestors. Of these, the first has been the most problematic. Although many systematists argue that there is no inherent reason for disregarding

the use of morphometric data in phylogenetics (Guerrero et al. 2003; MacLeod 2002), others have disagreed (Cranston and Humphries 1988; Crowe 1994; Curnoe 2003; Pimentel and Riggins 1987). But even among those who agree, there is little consensus on the kinds of data that are most appropriate and how they are best to be used. Most relevant to geometric morphometrics have been the arguments by Zelditch et al. (1995), Swiderski (1993), Fink and Zelditch (1995) and Zelditch and Fink (1995) that particular morphometric methods are compatible with the concept of taxic homology. These authors claimed that latent variables such as partial or principal warp decompositions are the only morphometric variables applicable in phylogenetic contexts. Others (Bookstein 1994; Felsenstein 2002; Lynch et al. 1996; Naylor 1996; Rohlf 1998) have challenged or cautioned about the use of geometric morphometric variables for phylogenetic analysis. Additional enlightenment may come from application rather than theory. For example, González-José et al. (2008) have recently shown that when continuous, correlated, modularized morphometric characters are treated as such, cladistic analysis (which is conventionally based on discrete, hypothetically independent characters) can successfully resolve phylogenetic relationships among species of *Homo*.

MacLeod (2001) reviewed the basic principles involved in viewing morphometric variation within the context of phylogenetically structured comparisons. Excellent recent examples of the use of morphometrics to interpret patterns of morphological diversification include Guill et al. (2003), Magniez-Jannin et al. (2004), and Larson (2005). As for ancestral reconstruction, Rohlf (2002) described a method for estimating ancestral states of shape variables using “squared-change parsimony”, and using the inferred states to depicting shape changes between nodes of the tree as deformations and to estimate the image of an ancestor.

Conclusion

The geometric morphometric methods that have been developed over the past several decades to extend beyond the limitations of traditional distance-based methods have become transformed into the new standard research protocol. As the technologies of measurement, analysis and display continue to improve, it will be interesting to see how the current methods evolve over the next few decades.

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