2.1 Rates of Change at a Point

2.1.1 General propositions

1. The measurement of biological form-change is quite different from the measurement of shape. Changes need not be quantified by measuring shapes separately and then subtracting scores on corresponding measures. Rather, form-change is a geometric object in its own right, the deformation of one form into another that accords with biological homology.

2. Of the information relevant to the analysis of shape change, that which is biological is manifested in the homology map, a function that assigns a correspondence between the points of any pair of forms. We generally sample this function at landmarks, points reliably located by anatomical criteria.

3. The choice of the coordinate system to be superimposed over any single form is not important. The computation of shape change is driven instead by the relation between two coordinate systems for two homologous configurations of points.

4. For sufficiently small regions, shape changes may be modeled as uniform. They are described by the rate of change of length, or dilatation, as a function of direction. Dilatation is measured as a ratio, not a difference, of homologous lengths. It is dimensionless.

5. The biorthogonal method summarizes the dilatations at any point by the largest and smallest, called the principal dilatations. The directions along which they lie, the principal axes or biorthogonal directions, are at exactly $90^\circ$ both before and after transformation.

2.1.2 Shape change as a relation of coordinate systems

The measurement of shape change may be thought of as the description of one picture in the coordinate system of another.

2.1.2.1 The Cartesian grid.—Consider the famous transformation between the forms of Diodon and Mola which D'Arcy Thompson uses to introduce his method. (These drawings are really projections onto the midsagittal planes of the fish. The component of deformation that this operation contributes will be ignored until Chapter 5.) From the pair of forms alone, drawn in Figure 2.1.1a, it is clear that they differ a great deal. Thompson suggested that we construe this pair of forms as a transformation of the entire picture (plane projection) making homologous points correspond—taking mouth to mouth, eye to eye, tail to tail. We could have drawn this mapping with any set of points in the picture plane of Diodon.
Figure 2.1.1 Diodon and Mola. (a) Geometric forms, after Thompson (1961), with a sampling of landmarks. (b) A Cartesian grid on Diodon and its transformation according to Thompson. Notice that the grid does not quite conform with the landmark homologies. (c) Alternate graphical representation of the data base: two coordinate systems upon the diagram of Mola.
To us this representation emphasizes numerical features of the form that are altered—lengths, heights, angles. This is a distraction. Thompson suggested that one separate the description of change from the description of the form, by superimposing an artificial structure over the drawing. In the course of deforming the fish, the homology map will deform the abstract structure as well. It is easier to describe the shape change by considering its effect on the abstraction, which is regular, than on the fish, which is not. For his abstraction Thompson chose to use an ordinary square ("Cartesian") grid aligned with the body axis of the left-hand fish. The grid is deformed (Fig. 2.1.1b) into a general curvilinear mesh that has no exact metric regularities. (The replacement of the extended Cartesian grid with one more appropriate to the task at hand, which is the description of shape change, will concern us in Section 4.5.)

Two different coordinate systems may be superimposed over the form on the right. One system is that drawn in Figure 2.1.1b, the deformation of the system that was Cartesian for *Diodon*; the other is the Cartesian system for *Mola* as the starting form, drawn as Figure 2.1.1c. The deformation of *Diodon* into *Mola* can be described as well by the relation between these two coordinate systems on *Mola*; all the information we need, both geometrical and biological, is still present.

The relation of the forms may be described most easily in small regions of the figure within which we can ignore the curving of the grid lines in *Mola*. Sufficiently small squares of a Cartesian grid will be transformed into parallelograms, as in Figure 2.1.2. The smaller the region, the better the approximation. This transformation takes any small straight line of tissue in *Diodon* into the homologous small straight line in *Mola*. These arbitrarily small straight-line segments are called line-elements. It is in terms of their correspondence that we shall describe the whole transformation.

2.1.2.2 Principal axes computed from coordinate mesh.—In the transformation of square into parallelogram both distances and angles are altered. We may begin our inquiry into the quantification of the transform by considering a specific query: Are there homologous pairs of line-elements that are at $90^\circ$ in both forms?

What could we do if we had two such pairs of perpendicular line-elements, one pair in *Diodon*, one pair in *Mola*? We could learn a great deal about dilatations (the ratios measuring rate of change of length) in *every* direction in terms of the dilatations along just those two, as follows.

Let us assign a Cartesian center $(0,0)$ in the middle of the square in the first form, and a local Cartesian coordinate system aligned with the axes we hope to have found, the principal axes, which start and finish at $90^\circ$ (Fig. 2.1.3a). In this coordinate system, when we assign points coordinate pairs $(x,y)$ relative to $(0,0)$, their squared distance from $(0,0)$ is $x^2 + y^2$.

We can assign coordinates on *Mola* that are set to $(0,0)$ at the homologue of *Diodon*'s $(0,0)$ and that are aligned with the two principal axes in *Mola*. Call these coordinates $x'$ and $y'$ (Fig. 2.1.3b). If $d_1$, $d_2$ are the dilatations along the principal axes, then we will have $x' = d_1x$ and $y' = d_2y$, by the uniform nature of the deformation in
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Deformations may be taken as linear over small regions. Successive enlargements of the transformation of Diodon to Mola show how small squares are transformed approximately into parallelograms.

Suppose we take the collection of points \((x,y)\) all at the same distance from the origin in Diodon. These will be the points on a circle (Fig. 2.1.3c) of some convenient radius—call it 1 unit. The coordinates of these points satisfy the equation \(x^2 + y^2 = 1\) or \(y^2 = 1 - x^2\). The squared distance from \((0,0)\) to the homologue \((x',y')\) in Mola becomes, with this substitution,
Figure 2.1.3 Biorthogonal directions bear the maximum and minimum dilatations. (a) Directions that start and finish at 90° for a transformation of the square into a parallelogram (cf. Figure 2.1.2 bottom). (b) Two Cartesian coordinate systems \((x,y), (x',y')\) oriented with these principal directions, and then rotated to an arbitrary vertical. (c) A circle and its deformation. Dilatations may be represented by the lengths into which the deformation takes radii of a circle. This length is greatest along the principal axis of larger dilatation, and least along the principal axis of smaller dilatation.

\[
d_1^2x^2 + d_2^2(1 - x^2)
\]

which is the same as

\[
d_2^2 + x^2(d_1^2 - d_2^2).
\]

Because in \(Diodon\) distances from \((0,0)\) to these points \((x,y)\) were all the same, namely, 1, the distances from \((0,0)\) to their homologues \((x',y')\) explicitly represent the factors by which distance has been expanded in the various directions. Because \(d_1 > d_2\), by assumption, this \(Mola\)-distance will be greatest when \(x^2\) is greatest. That happens for
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$x^2 = 1$, $x = \pm 1$, $y = 0$. These are just the points on the circle in the direction of the line-element we are temporarily considering to be horizontal (Fig. 2.1.3c). *Hence dilatations are greatest in this direction.*

Likewise, the distance from (0,0) to $(x',y')$ is least, and so dilatations are least, for those points on $x^2 + y^2 = 1$ with $x^2 = 0$, the points along the other principal line-element, drawn as vertical in Figure 2.1.3c.

Thus the **biorthogonal** (bi-orthogonal) **directions**—the line-elements that start and finish at $90^\circ$—are the directions of greatest or least local rate of change of length out of all directions at a point. These rates are the **principal dilatations**, lying along the **principal directions** of the deformation for this small region. This dual property accounts for their remarkable descriptive efficiency.

We have explained the reason for desiring these line-elements; it would be very convenient if we were certain that we could find them. Our guarantee is supplied by an ancient theorem, one of the simpler proofs of which we will now present.

Let us consider the relation between angles in *Diodon* and in *Mola* by taking a pair of line-elements at a constant angle in *Diodon* and examining the angle that their homologues make in *Mola*. We take, in particular, the line-elements along our arbitrary Cartesian vertical and horizontal there. These lines are at $90^\circ$ in *Diodon* and make an angle of some value or other in *Mola*, as shown in Figure 2.1.4. We may as well assume this angle is less than $90^\circ$, as drawn.

When we rotate this pair of elements in *Diodon*, keeping it always at $90^\circ$, its homologues in *Mola* will rotate, too, within its little homologous region. As they rotate, the angle between them will change as a smooth function of orientation in *Diodon*.

By the time we have rotated by $90^\circ$ in *Diodon*, we have reverted to the same pair of line-elements with which we began, but now one of them has had its direction reversed. The angle which had been less than $90^\circ$ in *Mola* has now been replaced by its supplement, which is of course greater than $90^\circ$.

Because this angle in *Mola* is a continuous function of the position of the right angle in *Diodon*, however, somewhere in-between it must have had exactly the value $90^\circ$.

This unexpectedly curt line of reasoning proves the existence of the biorthogonal directions. For another version of the same argument, see the Appendix on the Shape Nonmonotonicity Theorem in Bookstein (1980a). A slight extension of the algebraic argument above is sufficient to prove that these directions are unique: see Bookstein (1978a:103–104).

2.1.3 Shape change as a deformation of points considered in one coordinate system

In the preceding exposition we have argued as if the biological substance remained the same—i.e., the homology map was an identity—but the distance function was somehow changed; our task was to describe the directional variation of
Figure 2.1.4 Demonstration of the existence of biorthogonal directions. One corner of the square (a) is deformed into an acute angle, another to an obtuse angle (b). As the pair of perpendicular lines in (c) rotates through $90^\circ$, the homologous lines in (d) rotate at different rates. The perpendicular pair in (c) must pass through one position for which its homologue spans an angle of $90^\circ$ in (d).

those two distance-measures of the “same” line-element. One can arrive at the very same conclusion—the existence of biorthogonal grids at $90^\circ$, one direction bearing the largest dilatation, the other the smallest—by reversing the logical roles of the two coordinate systems. You will see that the use of Cartesian coordinates is entirely dispensable in the discussion of the principal axes and directions.

2.1.3.1 Line-elements in a triangle.—For the previous development, with its emphasis upon Cartesian coordinates, our basic unit of analysis was a bit of abstraction—a little square of coordinate mesh. For the alternate presentation our basic unit will instead be a homologous pair of triangles of landmarks, as in Figure 2.1.5a. In the absence of other information we may take the transformation sampled by these limited data to be uniform between each homologous pair of edges and throughout the interiors of the triangles. The homogeneity of this affine transformation is indicated clearly in the transformation grid Thompson-style (Fig. 2.1.5a).
Figure 2.1.5 The method of biorthogonal directions for two homologous triangles. (a) The sets of landmarks suggest a uniform transformation of the interior. (b) The uniform transformation alters lengths in various directions. (c) Dilatations are proportional to radii of the ellipse into which a circle is deformed. (d) The principal directions are axes of this ellipse, and the principal dilatations are proportional to their lengths. The principal axes upon the circle, left, are along the diameters transformed into the principal axes of the ellipse.
But we may draw the transformation just as clearly in terms of the collection of lines in all directions (Fig. 2.1.5b). The deformation we are observing, driven by the displacements of those landmarks at the corners, will deform these lines into others that divide the edges in the same fractions. That is, the deformation takes edges to edges, median lines (dividing the opposite sides in the ratio 50:50) to medians, and so on.

2.1.3.2 Principal axes computed from triangles of landmarks.—We are interested in the ratios of lengths of corresponding lines in the two triangles, the dilatations. We could compute them explicitly by taking quotients of corresponding lengths, direction by direction. However, it is more elegant to borrow the device of the previous demonstration. Again we may observe the dilatations directly as the lengths of the deformations of lines of constant length, that is, of radii of a circle. In this coordinate-free presentation we have the advantage of our geometric intuition. We can actually draw the circle (Fig. 2.1.5c) whose deformation we wish to observe, and the oval into which the uniform shear takes it. The dilatations of line-elements are proportional to the radii of this oval.

You may be convinced by an accurate drawing that this oval is remarkably like an ellipse. It is possible to prove by entirely non-algebraic (i.e., coordinate-free) means that it is exactly so. The image of the circle, being an ellipse, has two axes of symmetry, which lie at 90°. One is the largest diameter of the ellipse, one the smallest. The diameters of the circle that transform into them are likewise at 90°.

Recall that the lengths of the radii embody the dilatations as a function of direction. Therefore the principal axes of the ellipse into which a circle is taken are the principal directions of the deformation as they lie upon the right-hand form. The diameters that were mapped into them are determined by corresponding fractions of intersection along edges of the triangles. In Figure 2.1.5d we have drawn them without their ovals, showing that the remaining information about dilatations in intermediate directions may be readily reconstructed. The dilatations indicated on the figure were computed by division of lengths of homologous segments; all the other dilatations may be computed from these two alone, according to the formula

\[ d_\theta^2 = d_1^2 \cos^2 \theta + d_2^2 \sin^2 \theta \]

where \( \theta \) is the angle between the direction and the axis of larger principal dilatation.

We thus arrive at the same conclusion by two rather different lines of argument. Our unit of analysis may be the abstract cell of coordinate mesh or the biologically real triangle of landmarks; our line-elements may be bloodless little vectors inside parallelograms or real segments between points lying in fixed relation to those

\[ \text{† By an argument that we will not present here (see Bookstein, 1982c: part ii), dilatations for affine transformations are a function of direction only, so that we may restrict our attention to lines all through a convenient center.} \]
landmarks. The conclusions are the same in either demonstration, because they follow rigorously from the identification of biological homology with geometrical deformation. At every point of a deformation representing biological homology there are two directions that are at $90^\circ$ both before and after deformation; one is along the direction of greatest rate of change of length between homologues, and one of least rate, of all directions at that point. These directions, a description of the form-comparison, involve both forms for their computation, and cannot be determined by consideration of either form separately.

There is one exception to this elegant simplification. The ellipse at the right of Figure 2.1.5d may be a circle—it may not have a unique pair of axes. In other words, the dilatations $d_1$ and $d_2$ in the algebra of the previous section may be equal. In this case, dilatation is not a function of direction. We already know the deformations to which that description applies: they are the simple changes of scale. Such transformations may be represented locally by any pair of lines at $90^\circ$, because all right angles, indeed all angles, are preserved. These special transformations are called isotropic; points at which the transformation is isotropic are called singularities of the biorthogonal description. We shall encounter them from time to time as special cases of the more general deformation.

Appendix A.5.1.1 lists a Fortran subroutine that extracts the principal directions and dilatations relating two sets of three points in the Cartesian plane.

2.2 The Derived Data of Size and Shape

Throughout this book our data are those that conform to an underlying model of smooth deformation or transformation: (1) locations of homologous landmarks, as recorded by their coordinates; or (2) log-transformed straight-line distances between landmarks, taken from samples of organisms of varying sizes. Other types of data, e.g., meristic and qualitative variables, are best treated separately because they are not compatible with the deformation model. In the following sections we will discuss aspects of size variables (and their log-transformations) and aspects of the "adjustment" of shape for size, which follow from their origin in the geometry of the data.

2.2.1 Logarithmic transformations

Since Huxley’s pioneering exposition of 1932, statistical studies of allometry have generally invoked all the common measures of extent—length, area, volume, weight—in terms of their logarithms. So strong is this presumption that the transformation is occasionally applied totally inappropriately, as to Cartesian coordinates (see Sec. 3.1.3). We have found at least five justifications for the resort to log-transformed distances as the basic variables of multivariate morphometric modeling. We believe