Morphometrics is the statistical study of biological shape and shape change. Its richest data are landmarks, points such as "the bridge and the nose," that have biological names as well as geometric locations. This book is the first systematic survey of morphometric methods for landmark data. The methods presented here combine conventional multivariate statistical analysis with themes from plane and solid geometry and from biomathematics to support biological insights into the features of many different organs and organisms.

The book begins with a review of the fundamentals of landmarks and a discussion of the thin-plate spline, a new, statistically tractable implementation of the old model of shape change as deformation. This is followed by a critical survey of conventional multivariate morphometrics (the use of interlandmark distances as separate variables). Coordinates for representing landmark configurations without reference to size are then introduced, and their multivariate statistics explored in full.

The second half of the book is a survey of the most general and powerful new methods for describing the results of these analyses for both simple and complex landmark configurations. Using diagrams linked to biological interpretation, the text explains and interrelates the geometric features by which morphometric findings can be rendered legible. New tools are demonstrated using a variety of data sets from evolutionary biology, micropaleontology, neuroanatomy, and craniofacial growth.

This book should be of value to applied statisticians and geometers, as well as to all biological and biomedical researchers who need quantitative analyses of information from biomedical images.

"...will certainly be a landmark volume in this difficult but important field of shape analysis." -K. V. Mardia, ISI Short Book Reviews

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Preface

1 Introduction

Morphometrics is the study of covariances of biological form.

1.1 Four principles

Four principles underlie the morphometrics of landmark data: (1) archiving biological form by locations of landmark points, (2) converting sets of three locations to pairs of shape coordinates, (3) processing these variables by carefully contrived multivariate statistical maneuvers, and (4) interpreting findings in the picture plane or space of the data.

- 1.2 A typical example: the "phenytoin face" The four principles are exemplified in a study of the effects upon children's faces of prenatal exposure to phenytoin, a maternal anticonvulsant. Diverse algebraic approaches to single triangular shapes and more extensive patterns construe the geometric effects of the drug exposure in diverse, overlapping ways.
- 1.3 Shape features and multivariate analysis The morphometrics of landmark data supplements the covariance-based structure of measurement space usual in multivariate biometrics by a distinctive geometric structure dependent only on the mean form.

1.4 Prospectus

2 Preliminaries

This chapter assembles the fundamental arguments and computational tools that underlie statistical, geometrical, or biological reasoning about morphometric data and morphometric explanations.

2.1 A brief modern history

The morphometric synthesis presented in this book is of full statistical efficiency; it permits explicit tests of the most biologically interesting subspaces and is

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isotropic in its coverage of directions within each of these subspaces. Such methods have been available for landmark data only since the middle 1980s.

2.2 The thin-plate spline

Changes of landmark configuration may be imagined as deformations of the tissue in which the landmarks are embedded. The thin-plate spline, which represents the mapping as a pair of thin metal sheets relating the landmark sets, is a convenient tool for that visualization. The algebra and graphics of this visualization are explored.

2.3 The statistics of "explanation" A discussion of Sewall Wright's path-analytic approach to factors, joint causes of whole collections of observed variables, and a generalization, Partial Least Squares, for analysis of multiple blocks of variables.

2.4 Other kinds of morphometric data Two other types of biological shape data are briefly reviewed, curving outlines and histological textures, and connections or conflicts with the landmark-based style of analysis are noted.

2.5 Other literature

Three reading lists are set out: earlier overviews of morphometrics, introductions to the statistical analysis of multiple measurements in the natural sciences, and the classic literature of nineteenth-century analytic geometry.

3 Landmarks

This chapter explains the usefulness of landmark data for the analysis of biological shape change and introduces the specific data sets that will be the objects of exemplary analyses in subsequent chapters.

3.1 "Distance" and distance

In landmark-based morphometrics, the analogy between "distance" among cases and Euclidean distance in a vector space of arbitrarily high dimension is replaced by a much more careful treatment of ordinary distance as measured between landmarks by ruler.

3.2 Landmarks and explanations

A variety of characterizations of the notion of "landmarks." They link three separate scientific thrusts: the geometry of data, the mathematics of deformation, and the explanations of developmental or evolutionary biology.

3.3 Types of landmarks

There are three principal types of landmarks, corresponding to three basic ways of grounding the explanations they entail: discrete juxtapositions of 2.0

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tissues, maxima of curvature or other local morphogenetic processes, and extremes of algebraic functions of other data at some distance.

- 3.4 Examples of landmark configurations The main data sets underlying the examples of later chapters are introduced, and a typical effect on each configuration is displayed by thin-plate spline.
- 3.5 The medial axis and the limits of landmarks Landmarks are often difficult to descry in organs assembled out of blobby, nondescript parts. This section demonstrates an alternative analytic technique, a quantification of Blum's medial axis or symmetric axis, that often serves some of the same biometric goals.

4 Distance measures

This chapter introduces the distance measures that underlie the statistics of landmark-based shape and reviews some conventional techniques that ignore their origin in landmark locations.

- 4.1 A vector space of distance measures In the vicinity of a mean form, the set of distances between weighted averages of landmark locations can be treated as a vector space spanned by small changes in the distances between pairs of landmarks. The mean square of all these distances, equivalent to the mean squared distance of the landmarks of a form from their common centroid, is called Centroid Size.
- 4.2 General Size and size allometry Size allometry is a form of biological explanation corresponding to a simple factor model for the interlandmark distances. This model is applied in an example of rat skull growth.
- 4.3 Models with two factors: Size and Group Shape Wright's technique of path analysis leads to the interpretation of group differences in a suite of size variables as consequences of joint determination by size and shape factors. Still, the description of shape differences afforded by the distance measures is shown to be incomplete as applied to landmark data.
- 4.4 A comment on "shearing"

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This chapter shows how one single statistical space of linearized shape information underlies the great variety of shape measures for landmark data and supports a fully efficient multivariate analysis that is essentially unique.

5.1 For a single triangle of landmarks For most statistical purposes, the shape of a single triangle of landmarks may be represented by shape coordinates, the coordinates of any one of its 2

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landmarks when the other two are each fixed in position. In the vicinity of a mean triangular form, any shape measure of a triangle of landmarks can be identified with a direction in the plane of the shape coordinates.

5.2 Ratios of size variables for any number of landmarks

For small variation in a configuration of any number of landmarks, a ratio of size variables has the same statistical behavior as some linear combination of the shape coordinates of any set of triangles that rigidly triangulates the landmarks.

5.3 A circular normal model

If individual landmark locations vary independently about mean locations by circular normal noise of the same small variance, then the shape coordinates of any triangle of landmarks are very nearly circularly normally distributed as well. Departures of shapecoordinate scatters from circularity often indicate the presence of factors corresponding to biologically useful explanations.

5.4 Average forms and comparisons of averages Landmark configurations can be averaged by computing sample means for any set of shapecoordinate pairs sufficient to represent them rigidly. When samples are sufficiently numerous, significance tests for mean differences in shape can then proceed by applying Hotelling's T^2 or its generalizations to the vector of shape coordinates. Examples.

5.5 Covariances between size and shape On the null model, Centroid Size is the single size measure that is uncorrelated with all ratios of homologously measured lengths. Even when there is neither size allometry nor any group mean difference in shape, under the null model Centroid Size has the greatest power of all size variables for the detection of true size differences.

5.6 Kendall's shape space David Kendall's approach to the statistical analysis of landmark configurations directly constructs a "shape distance" having the appropriate Euclidean invariances. Although his approach leads to the same statistical tests of group mean difference as those here, it does not support feature subspaces or biological explanations as well as do the shapecoordinate methods.

6 Principal axes of shape change for triangles This chapter introduces geometric techniques for biological interpretation of geometric findings in the simplest context, a single triangle of landmarks. 170

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6.1 Algebraic version

The interpretation of shape change via the symmetric strain tensor is carried out algebraically, beginning with a square of "landmarks" that is deformed into a parallelogram. There are always two directions, the principal directions, that start and finish at 90°. One is the direction of greatest ratio of change of "homologous" length from square to parallelogram, and one the least.

6.2 Geometric version

The same pair of directions may be constructed from two pairs of shape coordinates by ruler and compass. For small changes in the shape-coordinate plane, ordinary Euclidean distance is proportional to log anisotropy, and the principal directions can be approximated by an angle bisection.

6.3 From tensors to variables: measuring a shape comparison

For any direction of change in the space of a pair of shape coordinates, one suggestive description is the ratio of lengths measured along the principal axes when that shape change is interpreted as a uniform deformation. Table 6.3.1 shows how to name the angles or ratios of distances that are the invariants and covariants of particular changes of triangular shape.

- 6.4 Analyses of more than three landmarks The transect theorem is explained: for any two mean configurations of landmarks, the homologous distance measures showing the greatest and least ratios of change are transects of triangles. But the ratios of simple interlandmark distances are not sufficient to produce these extrema; this failure accounts for the inefficiency of many of the distance-based approaches.
- 6.5 Biometric analysis of triangles of landmarks: examples

The methods just introduced are demonstrated in a diversity of data sets. Exemplary analyses are shown, and their interpretations explored, for group mean differences in form, in growth, and in growth allometry; for the correlation of form with exogenous factors; and for the directionality of digitizing noise.

6.6 A comment on "finite elements" The technique of descriptive finite elements is misleading in most biometric applications and should be considered only as a visualization of transformations that are known to involve no nonlinearity. Even when the multivariate statistics of its descriptors are sufficient, the actual coefficients produced are as expressive of an arbitrary

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mathematical model for homology as of the landmark locations that are the only data.

7 Features of shape comparison

This chapter introduces a variety of geometrical features that tie the statistics of landmark locations to familiar types of biological explanations applying to whole forms or their parts.

7.1 Procrustes superposition

Procrustes superposition is the best fit of one set of landmarks to a homologous set, or to an average, by a combination of translation, rotation, and rescaling. Reexpressed using the shape coordinates, the tactic may be seen to be biologically appropriate only under unusual circumstances. Application to the study of asymmetry may be valid. Example.

7.2 The uniform component of shape difference The description of shape change for any number of landmarks is simplest when its effect can be interpreted as geometrically uniform. The characteristic appearance of uniform changes in the shapecoordinate plane leads to multivariate estimators and tests for goodness of fit. A factor model is introduced that supplies corresponding two-dimensional scores for each specimen of a sample. Examples.

7.3 Pure inhomogeneity and transformations of quadrilaterals

Any change of four landmarks encountered in practice will deviate from uniformity. The residual "purely inhomogeneous transformation" may be described as discrepancies between the shifts of different shape coordinates or as a partial deformation with only two parameters. The spline representation underlies the more suggestive visualizations. Examples.

7.4 The quadratic component and other global nonlinearities

This section shows an implementation of "growth gradients," global descriptions of joint changes of landmark position by polynomials of higher than linear order. It is shown how to fit these gradients and how to interpret them, in the quadratic case, by one or two canonical features. Examples.

7.5 Principal and partial warps: components of bending energy

Principal warps are eigenfunctions of the bending energy underlying the thin-plate spline in the vicinity of the mean form. Each has an approximate location and geometric scale. Any shape change can be reexpressed as a sum of partial warps, vector multiples of the principal warps. Examples. 287

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	7.6	Relative warps: components of within-sample variation Relative warps are features of intrasample variation	339	Contents
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A.2 Anisotropy and the Poincaré geometry of triangles

> The fundamental distance measure for triangles and for uniform changes originates in the hyperbolic geometry of a half-plane. Its development by the analytic geometry of circles is instructive.

A.3 A negative comment on morphological "distance"

distance

The scaled-maximum theorem from the literature of random walk implies that regressions upon evolutionary time hardly ever make sense and that when variables are arbitrarily selected from a large pool, the reliability of conventional multivariate measures of "net distance" or "net similarity" is far too low for those values to be of any practical use.

A.4 Data sets

Listings of five archives of raw coordinate data that underlie most of the examples worked in this book.

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