Morphometrics is the statistical study of biological shape and shape change. Its richest data are landmarks, points such as “the bridge of 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.
MORPHOMETRIC TOOLS FOR LANDMARK DATA
Morphometric tools for landmark data
Geometry and biology

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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 
thrists: 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
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 discern 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”

5 Shape coordinates
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
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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 shape-coordinate 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 shape-coordinate 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 shape-coordinate 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.
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
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 shape-coordinate 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 nonlineairities
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.
7.6 Relative warps: components of within-sample variation
Relative warps are features of intrasample variation of landmark shape in order of covariance divided by bending energy. They adapt principal-component analysis to the stringent structure of landmark data. The first relative warp represents the largest-scale pattern of correlated displacements of landmarks beyond the uniform factors of Section 7.2. The technique is exemplified using the running example of rat skull growth.

8 Retrospect and prospect
This chapter reviews Principles 1–4 from Chapter 1 and explores some open questions.

8.1 First Principle: landmark locations
The open questions about landmarks have to do with data of other sorts than clearly defined point locations on rigid, biomechanically integrated organs. Points that represent aspects of curvature (sculpting) of surfaces seem particularly promising.

8.2 Second Principle: shape coordinates
Many open questions about the representation of shape space, especially for three-dimensional data, are related to visualizing the joint distributions of the shape coordinates.

8.3 Third Principle: the form of questions
The shape coordinates support unambiguous tests and estimates for most conventional biometric questions. The more specialized machinery of the warps reinterprets landmark covariances using the mean forms about which they vary. Open questions include new kinds of optimal descriptions, new feature spaces, and new sorts of covariates of shape that are themselves spatially or temporally ordered.

8.4 Fourth Principle: the form of answers
Inexpensive high-speed computer-graphic workstations now transforming the technology of visualization have immediate implications for morphometric studies.

8.5 Envoi

Appendices
A.1 More on thin-plate splines
A Fortran listing of one simple implementation for the splines underlying all the diagrams of deformation in this book; an extension of the spline technology to allow fitting of curving outlines between landmarks; another extension for the averaging of actual discretized images, suitable for medical studies.
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”
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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Preface

No book about methodology is ever finished, really. But after 10 years of major developments in morphometrics, each published (or unpublished) as a separate article, it was time for a coherent overview. My “introductory lecture,” for which there was no text available, would take four hours at the podium. Students complained that my lecture notes, even when not handwritten, were unreadable. I was beginning to mislay some of the explanations of lovely patterns from the earliest examples, while other early work needed triage: Certain changes of position were so blatant as to be embarrassing. And I had grown weary of the endless cross-referencing between papers: Bookstein (1989q) citing (1986x), (1987w, y, z), and (1990e, k, and forthcoming) — many of which cited each other incestuously as well.

Yes, it was time for a 10-year retrospective, if only to simplify the indexing. Yet the principal stimulus for the writing of this book was none of these general intellectual aches and urges, but instead a specific crisis. In 1987 the National Science Foundation instituted a series of workshops on morphometrics for systematic and evolutionary biology. The first took place in Ann Arbor, Michigan, in May 1988. Each instructor was to distribute a text in advance of his lecture. (Most of these are collected in Rohlf and Bookstein, eds., 199.) As they arrived at Michigan through the spring of 1988, these notes ranged from 15 to 40 pages in length; but mine ran to 224. It was thus relabeled the “zeroth edition” of the manuscript for this book. Only a partial draft, it covered Chapters 4 through 7 of this text, without any of the introductory material—without even a bibliography. “That’s all right,” I quipped, “most of the references are to my own work anyway.”

In other words, by 1988 there existed a synthesis of the landmark-based morphometric methods, but no associated pedagogy. For this teaching task there is simply no substitute for a bound volume. I have endlessly shuffled too many slides into the 20- to 40-minute versions of the obviously necessary “four-hour introduction” without ever quite managing to set these techniques in
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an accessible context. My apologies to any of my listeners who were baffled by my experimental lectures at AAAS, AAPA, AIBS, ASA, ENAR, ICSEB, IMS, IPMI, or ISM meetings; apparently the expositions were uniformly more obscure than these initials. This experimentation might have continued indefinitely except that (1) another NSF workshop was approaching (Stony Brook, New York, June 1990), for which I needed another text to distribute, this time one that would be self-contained, and (2) Cambridge University Press had accepted this volume for publication, “pending satisfactory completion.”

Hence the edition you hold in your hand. The newest material is found in the simpler Chapters 1 through 3, while the more technical expositions in Chapters 4 through 7 date from up to eight years ago. Historically, the statistics of simple tensors were developed first, in 1982; then the shape coordinates that linearize them (1983); then the critique of distance-based analyses (1984); then the serious pursuit of feature spaces, both the uniform and the nonuniform (1985); then underlayment of the statistical and geometrical points of view by the spectrum of bending energy of the thin-plate spline model (1987); finally, only yesterday, the language of Chapters 1 through 3 and 8, which speak directly to this unification.

The publication of this book is intended to declare the existence of a new specialty: morphometrics, the biometry of shape (for a more focused definition, see the beginning of Chapter 1). Morphometrics as a discipline should be of interest to anyone in statistics, image analysis, or quantitative biology whose work involves the contemplation of living or fossil form, its causes or its effects. Those are also the fields from which I expect readers to come: professionals and preprofessionals in any of these areas whose problems bear them broadly across the boundary of their own discipline toward one of the other two. Biologists interested in the processes regulating shape over ontogeny or phylogeny need tools for coherent quantitative reports that do not waste data. Computer scientists pursuing features of solid medical images ought to use quantitative form comparisons to guide their parameterizations. Statisticians who have always suspected there might be more structure to some sets of variables than their names and covariances will be challenged by a style of data for which that suspicion is justified. Surgeons, cardiologists, and neurologists need to test and understand covariates of the disproportions they see or correct. All these research purposes, and many, many others, can benefit from the tools taught here.

The new discipline thus deserves a place in several graduate curricula. In biology, it should be required of the student proposing a dissertation in any aspect of morphology. In statistics, it should be offered, like psychometrics, econometrics, or log-linear modeling of tables, as an elective in applied multivariate analysis. In image processing, it should be strongly urged upon anyone
proposing to specialize in medical imaging. In paleobiology, it should be required, period. This book is intended as a main text and reference for such courses in morphometrics and as a supplemental text for lower-level surveys of biomathematics, biometric statistics, quantitative paleobiology, and the like. The examples are not restricted to any single field, but draw widely from medical studies of normal growth and of congenital syndromes and from comparative and evolutionary studies.

To the breadth of coverage intrinsic to the morphometric theme corresponds a commensurate breadth of background. Mastering the material in this book requires that the reader have at least moderate expertise in three different subject areas - geometry, statistics, and mathematical biology. A short course in morphometrics, for which some of this background might be waived, would include Chapters 1 through 3 (except for Section 1.3) and about half the rest of the book: Sections 4.1–4.3 5.1, 5.3–5.5, 6.1–6.5, 7.2–7.3, 7.5.1, and 7.6. For the remainder of the text, the background needed is perhaps the equivalent of a two-semester upper-level undergraduate sequence in multivariate statistics or biomathematics, or the equivalent of a one-semester course in advanced analytic geometry. Of these, only the first, the statistics sequence, is at all common in the American college curriculum. Selections from the reading lists in Section 2.5 can substitute for the syllabus of any of these prerequisites that the aspiring morphometrician has unaccountably missed, but in that case two or three of the books must be read, not browsed, not skimmed.

Beyond this background, the way to learn morphometrics is to think closely and skeptically through dozens of applications, as varied as one can find. Whether beginner or advanced, the student of morphometrics should be careful never to specialize in a particular organism or human organ or particular form of question, but should instead master a large number of specific techniques, such as those emphasized in this book. New morphometric methods introduced for particular applications, like the landmark methods that arose in roentgenographic cephalometrics, usually apply broadly to make sense of data in a variety of biological contexts. It is a good tactic to tailor a method for a particular problem, then see how far afield it can be pushed. In the effort to understand which attempts at generalization succeed and which fail, one may arrive at a clear statement of the tacit assumptions that actually bore responsibility for success in the original context. Exceptions to this metastatic pattern - D'Arcy Thompson's notion of transformation grids, or Blum's invention of the medial axis, each proposed as a general method right from the start - have hitherto not found many specific applications to problems of measurement. Rather, methods carefully developed for particular contexts (growth gradients, for example, or the rubber-sheet techniques for recognizing chromosomes) have proved quite protein. Any model that leads to verifiably meaningful biological expla-
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For any morphometric application should be tentatively considered for every morphometric application, no matter what the literature of the subject finds respectable; but a model must work first in some application, must improve on the routine use of the methods currently “standard” there, before it is worth considering anywhere else.

Many colleagues inadvertently helped me write this book. Those who collaborated on the projects or expositions here include Bernard Crespi, Court Cutting, Barry Grayson, Lewis Holmes, Robert Moyers, Richard Reymont, F. James Rohlf, Paul Sampson, and Elena Tabachnick. Among the many others who asked good questions or supplied good answers are Miriam Zelditch, Richard Skalak, David Ragozin, Stephen Pizer, James Mosimann, Kanti Mardia, Pat Lohmann, William D. K. Green, Colin Goodall, and the late Harry Blum. It is time for me to thank Stephen Jay Gould and Joel Cohen for suggesting, way back in 1973, that it might be possible to be an academic morphometrician. (That phrasing is anachronistic, of course — the vocation of “morphometrician” had not yet been invented.) Two editors — James Tanner of Annals of Human Biology and the late Morris deGroot of Statistical Science — invited me to publish large chunks of not terribly well-digested morphometrics when it was still quite unprecedented to do so. Elena Tabachnick made hundreds of suggestions to improve the comprehensibility of the manuscript. When figures show evidence of balance, the hand is usually Teryl Lynn’s, my illustrator since my dissertation days.

Besides the NSF workshops, two other small groups have borne the brunt of my early attempts at explaining the more technical parts of this material: the Ninth, Tenth, and Eleventh International Conferences on Information Processing in Medical Imaging (Bethesda, Maryland, 1985; Ziest, The Netherlands, 1987; Berkeley, California, 1989), and the two Wilks Workshops on Shape Theory organized by Colin Goodall at Princeton University in 1987 and again in 1990. Thanks to all of you for your patience during the question periods dealing with the thin-plate splines, and special thanks to Goodall and to Kanti Mardia for answering some of the questions, especially those dealing with the ties to Kendall’s shape space, more adeptly than I could. I am grateful to Mardia, also, for so elegantly and expeditiously working out the exact distribution of the complex normal model, Section 5.6, in collaboration with his student Ian Dryden, and yet graciously naming the coordinates after me anyway.

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which earlier “editions” of this text were first distributed were due entirely to the enthusiasm of David Schindel of the Systematic Biology Program at the National Science Foundation. Jennifer Kitchell and Bill Fink urged me to prepare that monstrous hand-out for the 1988 meeting, and F. James Rohlf was similarly tolerant of an inordinate Xerography bill in 1990. My own computer programs run mainly on MTS, the Michigan mainframe. Rohlf has devoted too much time to packaging the spline routines for easy access by the ordinarily perseverant quantitative biologist (see the program TPSPLINE in the disk pack of Rohlf and Bookstein, 1990, and also Rohlf’s 1991 program TPSR); Paul Sampson, the same for the statistician; and Leslie Marcus and Richard Reymert have been spreading the word that there is something in landmark-based morphometrics worth the frustrations of learning it early in its evolution. I thank all of you for your trust that someday these ideas would be not only demonstrated but also explained.

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