

## Aspects of applied morphometrics

RICHARD A. REYMENT\*

REYMENT, R. A. (2005): Aspects of applied morphometrics. [Aspekte der angewandten Morphometrie.] – Z. dt. geol. Ges., 155: 263–274; Stuttgart.

**Abstract:** Biological morphometrics is the science of extracting information on shape variation in organisms. The original analytical work was done in terms of standard methods of multivariate statistical analysis but a growing realisation for the interpretational difficulties introduced by size-confounding led to the development of geometrically oriented morphometrics whereby size could be successfully separated out leaving “pure” shape free to be interpreted by means of some appropriate procedure. Some practical aspects of modern morphometric analysis are reviewed here using examples drawn from several sources.

**Kurzfassung:** Die biologische Morphometrie kann als die Wissenschaft der Zusammenstellung von Information über Formenveränderungen bei Organismen bezeichnet werden. Die ursprüngliche Bearbeitung erfolgte mittels der bekannten Methoden der multivariat-statistischen Analyse. Es wurde jedoch allmählich klar, dass derartige Methoden ungeeignet sind, die Eigenschaften Größe und Form zu trennen. Die Entwicklung der geometrischen Morphometrie erlaubt die Aufteilung der Formenvariation in zwei Komponenten, und zwar in reine Formenveränderungen und in reine Größenveränderungen. Hinzu kommt die Zerlegung der Formenveränderungen in eine affine Verschiebung und in eine nicht-affine Verschiebung. Praktische Fragen der modernen Morphometrie werden durch mehrere Beispiele beleuchtet.

**Keywords:** geometric morphometrics, multivariate statistics, mosasaurs, ammonites, ostracods

### 1. Introduction

Morphometrics may be defined as a more or less informally interwoven set of largely statistical procedures for analysing variability in size and shape of organs and organisms. Some of the concepts have been generalized to encompass non-biological problems. Such areas are not taken up in the following. For a complete account of the subject of generalized shape as a mathematical concept, the most authoritative reference is KENDALL et al. (1999). Attempts at expressing variability in size and shape in quantitative terms have a relatively long history in biology. A convenient starting point may be assigned to the close of the nineteenth century with the work of Karl PEARSON and his associates and the stabilization of the concept of “biometry”. The main contributions of that period were the introduction of the product-moment correlation coefficient and regression. The basic principle of what came to be known as principal component analysis was also presented. However, its development and application were held back owing

to computational difficulties. Some noteworthy biological studies did, however, emerge for material based on just a few variables, for example, the work of PEARCE (1959) on the expression of shape in fruit-trees.

Morphometrics as an organized scientific pursuit arose in the hands of P. C. MAHANOLOBIS in the late nineteen thirties. The formation of the Indian Statistical Institute in Calcutta under the leadership of MAHANOLOBIS led to the development of many avenues of fruitful statistical research. The ISI issues a journal *Sankhya* (meaning “measurement” in Sanskrit) in which the results of much insightful biometric work were published. The unfolding of the basic concepts of what constitutes the biometrics of morphological variation took place in conjunction with the anthropometric survey of the United Provinces of India. The original work centred around the generalized statistical distance definitely proposed by MAHANOLOBIS (1936) some ten years earlier. This distance was used to construct topological diagrams using cranial measurements on samples drawn from various categories of the Hindu class system. The step from using distances computed between all categories to a multivariate generalization followed quickly in the hands of ISI researcher C. R. RAO under the tutelage of M. S. BARTLETT. The generalization was called canonical variate analysis on  $p$  variables for  $k$  groups. Canonical variate analysis is usually interpreted

\* Address of the author: Prof. Dr. R. A. REYMENT (e-mail: richard.reyment@nrm.se), Department of Palaeozoology, Swedish Natural History Museum, Box 50007, S-10405 Stockholm, Sweden.

broadly as encompassing one-way multivariate analysis of variance and multiple group discrimination.

Within the field of experimental biology, R. E. BLACKITH (1957, 1960), in a suite of exceptional papers devoted to polymorphism in insects, in which MAHANOLOBIS distances and canonical variates were handled with great insight, established a foundation for the quantitative study of variation in size and shape. A major problem to be solved in using "distance measures" in the study of variation lies with the fact that size and shape are confounded. This means that a suite of measurements on a locust carapace, for instance, represent not only a component expressing size-differences but also differentiation between variables that arises from differences in shape of the specimens of a sample. BLACKITH could reduce the negative aspect of this by a clever method of linking his distances in relation to known polymorphisms. This could not however hope to provide a general solution to the problem of the analysis of shape. The real nature of the problem was first realized by the mathematically gifted palaeontologist T. P. BURNABY (1966) who devised a mathematical procedure for a transformation that placed "size" in one subspace and shape into another. He named his method "growth-free discrimination". BURNABY's solution is not often used. It is nonetheless a remarkable and foresighted achievement that doubtlessly influenced directly or indirectly the current phase of development of the subject.

While all of this was going on, people were puzzling about how to arrive at a practical and mathematically justifiable solution to the coordinate-based concept of THOMPSON (1917 [1942]) for geometrically illustrating shape relationships in organisms with the emphasis placed on phylogenetic reconstructions. THOMPSON (1917 [1942]) thought it would be possible to represent rela-

tionships between related organisms by means of deformational grids. A typical example taken from his book is shown in Fig. 1. By means of an affine transformation, one genus of fishes can be transformed to another genus, hopefully phylogenetically connected. For years workers puzzled over how this was actually done – what did the mathematics look like? Speculation went on for decades without much light being cast on the subject. This can be checked in Fig. 1 by noting where the intersections of the square grid meet in relation to the left-hand figure and where those of the parallelograms meet in the right-hand figure. BOOKSTEIN (1991) and DRYDEN & MARDIA (1998: 200) noted the subjectivity attaching to the freehand transformations. HUXLEY (1932: 104–110) discussed weaknesses he considered to be inherent in the method of Cartesian coordinates from the aspect of the constancy of growth-gradients. THOMPSON's book was reprinted many times after 1917 but he did not in any of the editions refer to how he had made his figures. In any event, THOMPSON's insight was a major break-through in thought about biological variability but it was not until 1978 that BOOKSTEIN provided a solution for the affine case and then in many later publications, summarized in BOOKSTEIN (1991), for the non-affine case.

## 2. The principal component decomposition of size and shape

As computational facilities became more generally available, so did interest in studying shape variation increase. A rather simple procedure rapidly gained ascendancy that relies on interpreting the latent roots and vectors of a matrix of covariances or correlations in terms size and shape components. The idea seems to

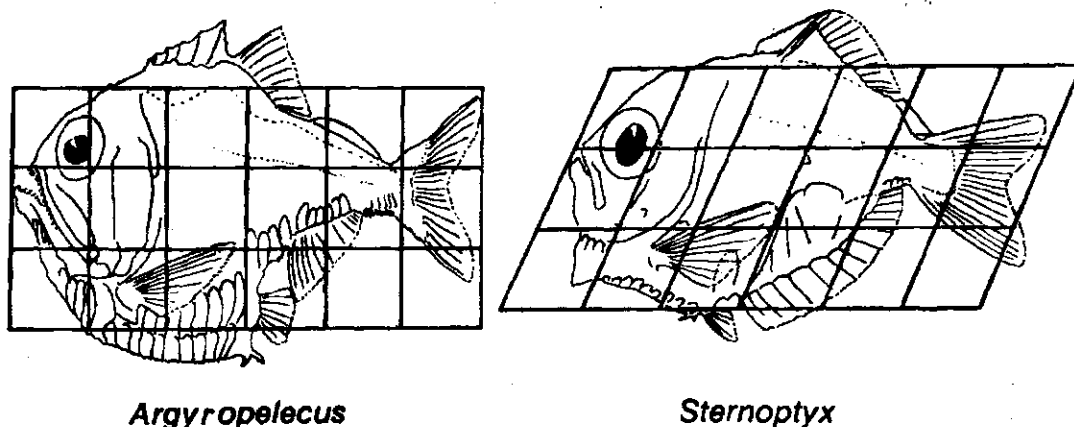


Fig. 1: An example of THOMPSON's use of Cartesian coordinate grids for representing shape-change between related organisms.

Abb. 1: Ein Beispiel der graphischen Methode mit Cartesischen Koordinaten nach THOMPSON (1917 [1942]), wobei eine approximative Formeninterpolation zwischen verwandten Formen dargestellt, d. h. nicht berechnet wurde.

have been formulated by the French marine biologist TEISSIER (1938) and then improved and introduced into the anglophone literature by JOLICOEUR & MOSIMANN (1960) and later provided with a sound mathematical model by HOPKIN's (1966). JOLICOEUR (1963) developed his original idea further by successfully relating the latent vector reification of principal component analysis to an allometric model. HOPKIN's contribution was a significant theoretical improvement to the allometric solution. Although the general "algebraic solution" is usually attributed to JOLICOEUR & MOSIMANN (1960). QUENOUILLE (1952) was, it seems, probably the first worker in the field to give latent vectors a biological shape-oriented interpretation, closely followed by PEARCE, who summarized his work on the growth of trees in a statistical textbook (PEARCE 1965). SPRENT (1972) proposed a formalisation of the prevailing concepts at the time for the analysis of size and shape.

The principal component method for describing size and shape variation relies on an intrinsic property of non-negative matrices known as the Perron-Frobenius theorem which states that the maximum root of the matrix is associated with a latent vector with positive components. The first latent vector of a covariance or correlation matrix of distance-measures observed on some organism is interpreted as indicating variation in size. Subsequent latent vectors are said to be indicative of various factors of shape-variation. This interpretation is rather circumstantial in that it is in part based on an artefact. Nevertheless, the method is still in wide use and there is some evidence that supports the claims for a useful spectral decomposition of variability in size and shape. The same methodology is applied in Geology to the study of sedimentary data, species compositions in palaeoecology, and in the analysis of geochemical data. In these connexions there may be more convincing justification for the interpretation of the latent vectors. The results of multivariate analyses of distances observed on fossils are often presented as ordinations. That is, as bivariate scatter plots of the scores obtained from substituting the columns of the data-matrix into the latent vectors.

Growth and shape-change include a tensorial component in that they are at different rates in different directions at typical locations in a tissue. HUXLEY (1932) was well aware of this distinction. This directionality is not easy to test in a principal component decomposition, but easy of access if a geometrical orientation is adopted. The principal component analysis of size and shape perforce accepts that shape variation is subordinate to variability in size. Whenever it is not a vector will all components unity, the first latent vector of a covariance matrix of appropriately selected distance measures, this vector is an expression of shape variation whereby unequal loadings represent different rates of

extension with respect to general size (i.e. allometry). Hence, for a first latent vector with unequal elements (all positive) the greater the increase in size of the organism, the more will the proportions between the components diverge. MOSIMANN's (1970) paper on allometry and the "identification" of the size vector can be said to mark the starting point for a more geometrical approach to morphometrics and one which lies at the heart of the new geometric morphometrics.

### 3. Measuring outline shape

Distance measures can be arbitrarily constructed around an outline by a simple geometrical method by marking off equi-spaced points. A well known means of describing a curve, such as an outline, is by decomposing the line into a Fourier Series which can be made to approximate the contour of the object by passing through a series of progressively more complex trigonometric functions for the digitised points. Although very good approximations of the shape of an object can be made, the results cannot be linked to homologous relationships between objects. The use of Fourier Series is well known from the sphere of analytical sedimentology.

LOHMANN (1983) applied a result of ZAHN & ROSSKIES (1972) to the study of shape in planktonic foraminifers. This result shows that a complex curve can be expressed as a series of steps around a circle. The underlying mathematical concept of LOHMANN's "eigen-shapes" is conceptually similar to that of BURNABY's decomposition into size and shape spaces. In eigen-shapes, size is represented by the length of the steps around the perimeter of the object and shape by the set of angles estimating the deviation of each step from the expected direction. LOHMANN's work, considered in the context of time and knowledge, is an outstanding achievement. SWIDERSKI et al. (2002) have given a thoughtful appraisal of eigenshape analysis. MACLEOD's (2002) extended eigenshape analysis is a serious attempt at coming to grips with the problem of comparability between objects. BOOKSTEIN (1997) proposed powerful coordinate-based methods for studying forms without landmarks, that is, for accessing the information in curving outlines.

A reasonable case for outline methods can be made for planispirally coiled shells such as those of ammonites. Natural circumferentially located reference points are not available on such shells, even where ornamental features occur, owing to the inherent instability in such properties with respect to the number per whorl and the degree of development. Ammonites are often richly ornamented with tubercles and ribs. These features are, however, seldom stable enough to permit using them as a base for homologous landmark points. Greater availa-

bility is offered by the apertural aspect in which points of intersection of features occur.

#### 4. Reference points (landmarks)

Geometrically based morphometrics is in its current form dependent on the selection of reference points, designated by X-, Y-coordinates and conveniently referred to as "landmarks".

In my personal opinion, the adoption of the term "landmark" may have served to confuse issues in morphometrics in that it tends to conjure up a false impression of exclusiveness. MACLEOD (2002) has drawn attention to this and, for example, pointed out that taxonomic distances in current use are no more than measures between reference points on an object which in turn are just "landmarks". The same distinction has been made by DRYDEN & MARDIA (1998) and BOOKSTEIN (1991). KENDALL et al. (1999: 1) enunciate a rather rigid interpretation of labelled points (they bypass the use of the word "landmark") in their mathematical concept of markers in that they underline that for them, labelled points are basic and determine the objects studied. According to the biologically oriented concept of the "geometric morphometricians" the 'marker points' are selected from a usually two-dimensional or three-dimensional continuum. The biological interest does not encompass cases where markers all lie in lower-dimensional subspace or two or more of them coincide, which contrasts with KENDALL's spaces, which contain the shapes of all possible configurations except those for which all the points coincide (KENDALL et al. 1999: 2). For the mathematically gifted, the book by KENDALL et al. (1999) is the ultimate reference.

Landmarks are specified by pairs of X-Y-coordinates (the usage is originally a borrowing by osteologists from topographical surveying where fixes are located with respect to coordinate pairs). Using simple geometry, distances can be constructed from taxonomic reference points: the reverse procedure is, however, not possible. The arbitrary points on a circumference in eigenshapes are likewise landmarks, denoted by X-Y-coordinates, but they lack the property of homology or point-to-point correspondence from specimen to specimen.

In order to make morphometric use of the biological information embodied in the lateral properties of a planispirally coiled cephalopod shell one requires the specification of pseudolandmarks located around the periphery of the conch. The concept of a pseudolandmark here implies that apart from the initial homologous point, a sequence of points is laid out along the periphery of the last preserved whorl. Such points are constructs of the same type as proposed by LOHMANN (1983) for his method of "eigenshape analysis".

#### 5. Thin-plate spline-based morphometric

One must be sure of what the spline-based morphometrics can do. Exaggerated claims for biological relevance made especially in the earlier stages of applications have not always been useful. The selection of landmarks determines the outcome of the shape-analytical conclusions owing to the fact that the thin-plate spline decomposition is not rooted in covariation in shape-changes in the input-data. Hence, each configuration of landmarks is a unique representation of just the set of points selected on the object (ROHLF 2002: 179). Deletion or addition of points is often found to change the visualization diagram and hence the interpretation. In consequence hereof, it is desirable to make clear that the results of a particular analysis pertain to a particular configuration of reference points on an organism. Biological interpretation must inevitably be made with expert insight.

Palaeontological material consists almost exclusively of fossilised hard parts, the shells encasing the tissues and organs of the animal. Material obtained from living organisms, for example, brains can be related to more than raw morphology which implies that an analysis of an organ can be given a more biological interpretation what can be hoped for by a palaeontologist. For example BOOKSTEIN's (1991) work on schizophrenia. The study of shape-variability in fossilised hard parts must perforce be in terms of "deformations"; this limitation implies that exceptional care must be expended on choosing reference points that really mean something in a palaeobiological context and which can be extrapolated from case to case. In many cases, apart from fossil mammals, it is seldom possible to relate shape-variation in shell details to the anatomy of the animal. It is tempting to view a sequence of spline relationships resulting from the latent-root decomposition as being a kind of microscope-ratchet which successively yields a scale of magnifications of the surface of a fossil as a function of the latent-roots. For different configurations, different impressions of the topology of the surface will be communicated. Hence, there is a very considerable obligation placed on the investigator to select reference points that are of real significance. Large latent roots correspond to latent vectors that describe small-scale features – the deformation of landmarks that are close together. Small latent roots correspond to latent vectors that describe large-scale deformational features.

There is an important field in invertebrate palaeontology, however, that can supply much useful information from morphometric appraisal of shell properties and shape. This is the subject of polymorphism and polyphenism. Interesting results have been obtained for ostracods

and cephalopods, for example, REYMENT & KENNEDY (1990) for ammonites and REYMENT & MCKENZIE (1993) for Ostracoda from southern Australia.

## 6. Remarks on spline-based methods

There are two main openings available for charting differences in form by means of coordinates. One of these takes each form, superimposes it in relation to others, and then computes differences in terms of reference-point displacements relative to this registration. The second tack is concerned with describing differences in point configurations as deformations of a grid produced by mapping one form into the other and visualising the shrinkings and stretchings that are generated by the procedure. The analysis of the registrations of the coordinates may be done in several ways. One may register to a common baseline by translating, rotating, and scaling so that most points fit well, or register by minimising the sum of squared differences between the equivalent landmarks of forms. This is usually referred to as generalised Procrustean fitting. The result is scaled by division by the centroid size. Clearly both of these procedures introduce a constraint the actual effects of which have yet to be subjected to scrutiny.

## 7. Overview of main geometrical concepts

Let  $X_i$  denote the  $2 * p$  data matrix of digitised  $x$ - $y$ -coordinates for the  $i$ -th specimen of a species and let  $X$  be the  $2n * p$  matrix of all  $n$  specimens of the sample. We shall also write  $X_x$  for the  $n * p$  matrix (vector) of  $x$ -coordinates alone and  $X_y$  for the corresponding array of  $y$ -coordinates. It is required to align the  $n$  specimens so that a reference specimen (i.e., an averaged specimen)  $X_p$  can be computed. This can be done by some suitable method of superposition, such as an affine resistant-fit procedure. This is a composite on which all the essential features of a species, morph, or any other taxonomic unit can be displayed and mathematically specified to any degree desired.

BOOKSTEIN's method of shape coordinates (BOOKSTEIN 1991) can be applied to a previously defined baseline. The location of each landmark in the reference specimen can be computed as the mean  $x$ - $y$ -coordinates across the objects. The reference specimen is used to define the principal warps. The bending energy matrix  $L_{p \times p}$  is found for the reference specimen by the following sequence of steps restated from BOOKSTEIN (1991):

Begin by constructing the partitioned matrix  $L$

$$L = \begin{bmatrix} P_k & Q \\ Q^T & 0 \end{bmatrix}$$

where  $P_k$  is a matrix with zeros down its diagonal and with off-diagonal elements defined as

$$U_{(r_{ij})} = r_{ij}^2 \ln r_{ij}^2.$$

The term  $r_{ij}$  denotes the distance between landmarks  $i$  and  $j$  of the reference specimen. The matrix  $Q$  consists of three columns and  $p$  rows, the first of which is a unit vector, the second one is the vector of  $x$ -coordinates, and the third one is the vector of  $y$ -coordinates.

The upper left submatrix of the inverse of  $L$  is often referred to as the **bending energy matrix**. It has latent roots  $\Phi$  and latent vectors  $E_{(p \times p)}$  in which columns correspond to the normalized latent vectors and rows to the landmarks. These were called BOOKSTEIN (1991) the **principal warps**, by analogy with principal components. Because of the way in which  $L$  is constructed (incorporating the lower right matrix of zeros), there can be at most  $p-3$  non-zero latent roots (ROHLF 1993). The latent root of each latent vector can be constructed as a specific bending energy, to wit, that of the partial warp corresponding to the latent vector when each coefficient is regarded as the height above the corresponding landmark. Any deformation can be decomposed as a sum of these principal warps as they apply first to the  $x$ -coordinate of the deformation and then to the  $y$ -coordinate. These components of deformation were named the **partial warps** of the thin-plate spline by BOOKSTEIN (1989). Of the  $K$  warps,  $K-3$  show bending, whereas the last three together represent the affine part of the shape-change. The latent roots corresponding to the affine change are zero in value.

The product  $X_i L_q^{-1}$  yields the affine coefficients, where  $L_q^{-1}$  is the upper right portion of the inverse of  $L$ . The product  $X_i L_q^{-1}$  gives the coefficients for the non-affine part of the thin-plate spline that maps the landmark coordinates of the reference configuration into those of the target specimen.

The next step is to assemble the weight matrix  $W$  of order  $n * 2$  ( $p-3$ ). This is a scaled projection of the  $x$ - and  $y$ -coordinates of the deviation of the  $n$  specimens from the consensus specimen onto the principal warps having nontrivial latent roots. This may be written as

$$W = [W_x | W_y]$$

where  $W = n^{-1/2} V (I_2 \otimes E \Phi^{\alpha 2})$ .

Here,  $I$  is a column vector of  $n$  ones and  $V_x$  is an  $(n * p)$  matrix of the  $x$ -coordinates of the differences between the  $n$  specimens and the reference specimen.  $V_y$  is the equivalent matrix of the  $y$ -coordinates (ROHLF 1993).

The singular value decomposition of the weight matrix yields:

$$W = PDR'$$

where  $P$  is an  $n * 2(p-3)$  matrix having as its columns the contributions of each of the  $2(p-3)$  relative warps to the  $n$  specimens.  $D$  is a diagonal matrix of singular values and  $R$  is a  $2(p-3) * 2(p-3)$  matrix whose columns are distinguished under the designation of the relative warps in terms of the principal warps. The first  $p-3$  rows of  $R$  pertain to the  $x$ -coordinates and the remaining  $p-3$  rows pertain to the  $y$ -coordinates. The matrix of relative warps represents the displacements of the positions of the landmarks on the reference specimen that one would expect if an individual differed from the consensus specimen by an unit change in a specified relative warp. The method of relative warps is an analogue of principal component analysis.

The spectral analysis of the sample covariance matrix of shape coordinates can be taken with respect to the bending energy matrix  $L_p^{-1}$  evaluated at the sample mean shape. Another solution is to confine the analysis to the non-linear part, which is the interesting portion from the aspect of evolutionary analysis. One can then use scores of relative warps for each specimen or species and analyse them by multivariate methods. The weight matrix,  $W$ , of shape-data also can be utilised without going to the spectral decomposition that produces the relative warps.

The concept of affine transformations seems to be due to the celebrated mathematicians MÖBIUS and EULER. In Physics, the idea of affine transformation is known under the name of homogeneous deformation (KLEIN 1925: 75). Decomposition of coordinate-based data by the thin-plate spline technique exhibits a close analogy with the well known decomposition by means of Fourier trigonometric series. The constant term in such a series is a global parameter and the trigonometric coefficients are local parameters at successively smaller scales (DRYDEN & MARDIA 1998: 199).

DRYDEN & MARDIA (1998: 286) point out that the results yielded by distances and coordinates are often similar and the former cannot be dismissed out of hand. For small variations, registration methods and distance methods lead to analogous conclusions about shape. Unfortunately, there is no general rule available to support this belief. Assuredly, this is oft-times found to be the case, but it is not an invariable situation.

## 8. Possible sources of error

Errors can and do arise in the multivariate analytical processing of data generated by geometric morphometric procedures. The otherwise attractive method of tri-

angulating data, BOOKSTEIN coordinates, whereby coordinates are registered on a common edge induces spurious correlations and consequently invalid covariance matrices (DRYDEN & MARDIA 1998: 173). The possibility of applying the theory of compositional data analysis (AITCHISON 1986) to the problem has not yet been more than briefly considered. Another source of error lies with imperfections in the data. This is more likely to be a problem in palaeontological work where deviations from multivariate normality are a cause of misleading results. MCKENZIE (1979) seems to be the first worker who has given serious attention to practical aspects of consistency and repeatability in multivariate analysis, in particular canonical variates and discriminant functions. MCKENZIE's many results are summarized in REYMENT et al. (1984) and REYMENT (1991).

Campbell

## 9. Some illustrations

Fig. 1 is an example of THOMPSON's (1917 [1942]) Cartesian coordinate grids for representing shape-change between related organisms. This is an affine transformational pattern. Affine transformations were the main focus of BOOKSTEIN's (1978) thesis. This figure shows clearly that the transformation was produced by hand and not calculated.



Fig. 2: The computed pseudo-landmarks around the circumference of 13 Iranian ammonites of the genus *Knemiceras* (Cenomanian).

Abb. 2: Die berechneten Meßpunkte rings um die Umrissse von 13 iranischen Ammoniten der Gattung *Knemiceras* (Cenoman).

Fig. 2 illustrates computed pseudo-landmarks around the circumference of Iranian ammonites of the genus *Knemiceras* (Cenomanian). Such data are not very useful for most work but providing the sizes of the objects are identical, some interesting results can be obtained. The arrows for 13 specimens illustrate the spread of the observations which are clearly greater for the right hand side of the figure than for the left hand side. The significance of the unequal spread could be primary in nature but this aspect would need to be given closer attention before any definite conclusions can be drawn.

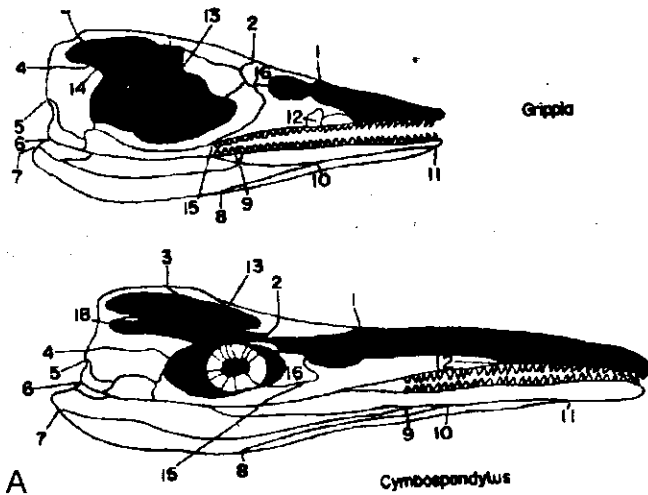


Fig. 3 introduces the method of mapping one form into another by the thin-plate spline technique. The problem is concerned with comparing the skull of an Early Triassic ichthyosaur of the genus *Grippia* from the Spathian of Svalbard with that of a species of *Combylospandylus* of the Middle Triassic. Fourteen landmarks and pseudolandmarks used for the analysis are shown in Fig. 3A. The affine transformation is depicted in Fig. 3B. The total non-affine part of the transformation in Fig. 3C displays well the undulating surface of the mapping (remember that the grid portrays a three-dimensional situation in two dimensions). Not unexpectedly, the strongest deformation occurs in the anterior region of the skull.

Fig. 4 depicts informative partial-warp deformations registered on *Neobuntonia airella* MCKENZIE, REYMENT & REYMENT obtained by the method of principal warps applied to mean configurations. Fig. 4A illustrates a non-affine mapping between female carapaces and moults (left valves). Fig. 4B is an affine transformation for right valves of adult males and moulted shells. Fig. 4C shows the non-affine transformation between right valves of adult males and moulted corresponding to the affine mapping. Fig. 4D shows a non-affine mapping for adult males and moults (right valves) from a deeper stratigraphical level. In the example illustrated in Figs. 3A-3C, the mapping were made between individual

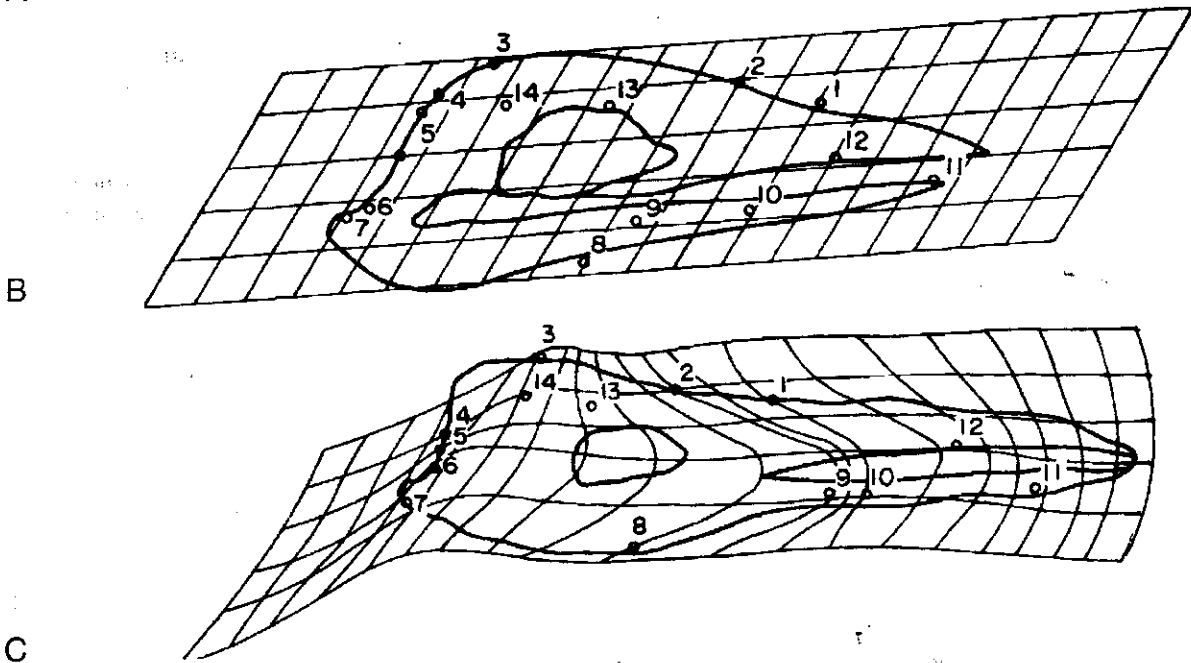


Fig. 3: The mapping one form into another by the thin-plate spline technique illustrated by the Triassic ichthyosaurian genera *Grippia* and *Combylospandylus*. Fourteen landmarks and pseudolandmarks used for the analysis are shown in Fig. 3A. The affine transformation is depicted in Fig. 3B. The total non-affine part of the transformation is shown in Fig. 3C.

Abb. 3: Die Dünnschicht-Splineinterpolation der Merkmale des Schädels von zwei Ichthyosauriern: *Grippia* auf der entsprechenden Ebene von *Combylospandylus* (Trias). 3A: die 14 Meßpunkte; 3B: die affine Interpolation; 3C: die nicht-affine Interpolation.

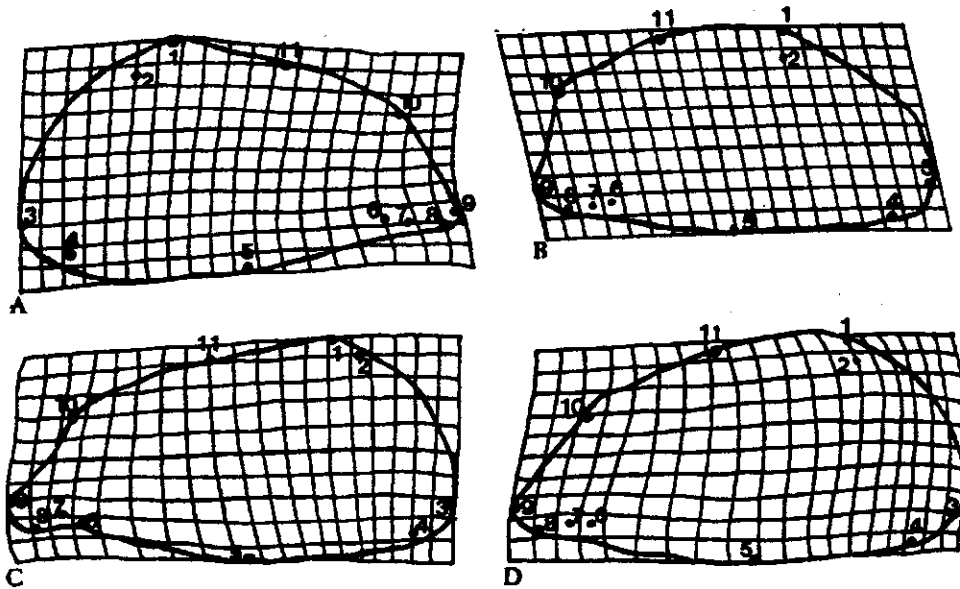
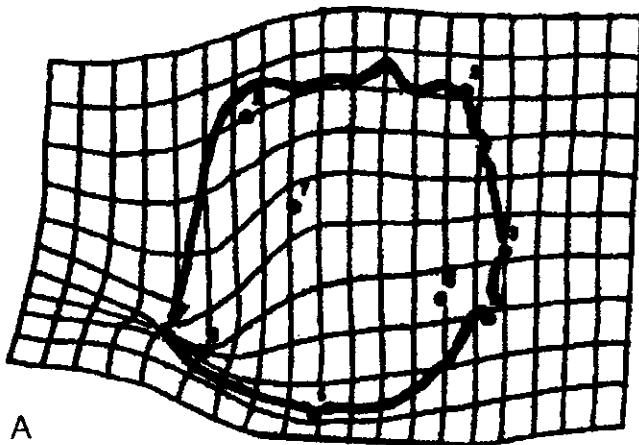
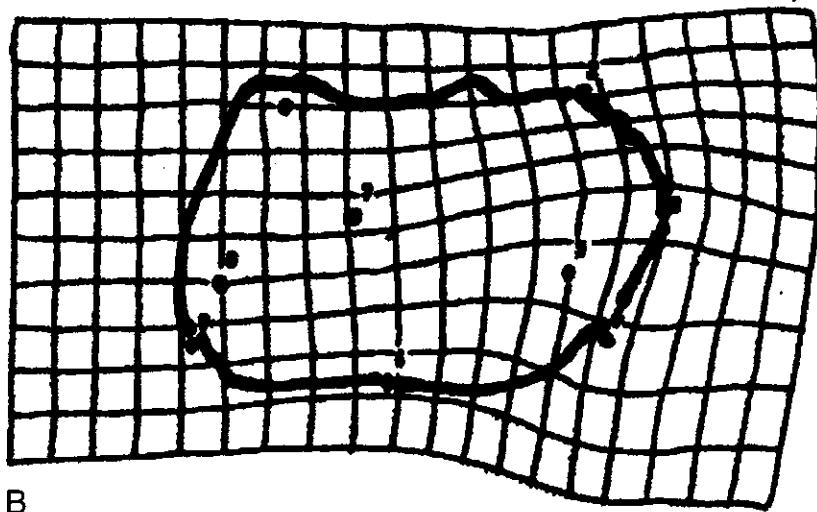


Abb. 4: Verformungsdiagramme der Ostracodenart *Neobuntonia airella* (Miozän), erzeugt mit der Methode der Dünnschicht-Splineverformung, die auf die durchschnittliche Merkmalskonfiguration angewendet wurde. 4A: die nicht-affine Verformung zwischen linken Klappen von Weibchen und der letzten Häutung; 4B: die affine Verformung zwischen rechten Klappen von Männchen und der letzten Häutung; 4C: die nicht-affine Verformung zwischen rechten Klappen von Männchen und der letzten Häutung (aus dem Oligozän); 4D: die nicht-affine Verformung zwischen rechten Klappen von Männchen und der letzten Häutung (aus dem Miozän).



A

Fig. 5: Phylogenetic use of the thin-plate spline technique. 5A: the second partial warp for the transformation from *Quasibradleya momitea* (middle to late Eocene) to *Q. premackenziei* (middle Miocene); 5B: the first partial warp for the transformation from *Quasibradleya momitea* to *Q. praemackenziei*.



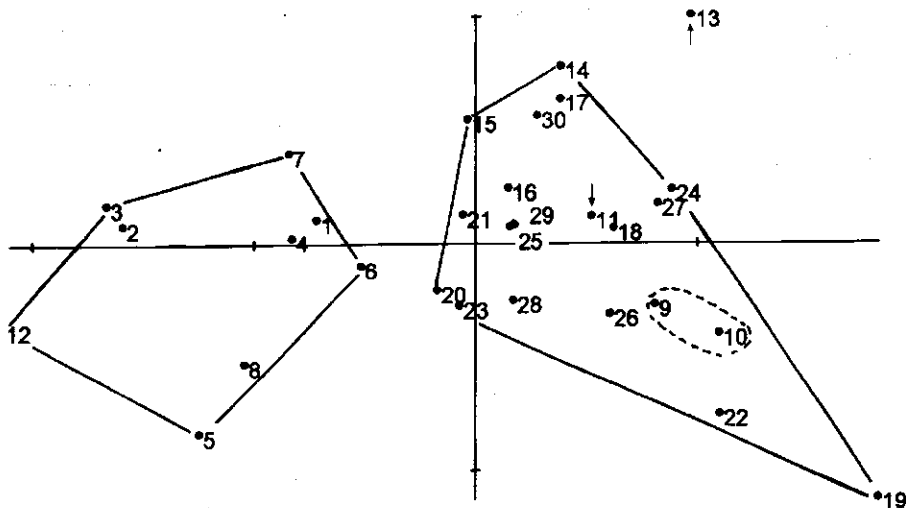
B

Abb. 5: Phylogenetisches Beispiel der Methode der Dünnschicht-Splineinterpolation. 5A: zweite Teilverformung für *Quasibradleya momitea* (Eozän) zu *Q. mackenziei* (Miozän); 5B: Darstellung der ersten Teilverformung.



Fig. 6: The first two relative warps for Iranian (1–13) and Lebanese (14–30) specimens of the Cenomanian ammonite genus *Knemiceras*.

Abb. 6: Streubereiche der beiden ersten relativen Verformungen, bezogen auf zwei geographisch weit getrennte Vorkommen der cenomanen Ammonitengattung *Knemiceras* aus dem Iran (1–13) und Libanon (14–30).



images. In the example considered here, the less usual procedure of using averaged data and averaged outlines was employed. The complete analysis is available in REYMENT & BOOKSTEIN (1993).

Fig. 5 presents examples of the phylogenetic use of the thin-plate spline technique. Fig. 5A shows the second partial warp for the transformation from *Quasibradleya momitea* (middle to late Eocene) to *Q. premackenzeyi* (middle Miocene). The mapping involves global deformation and strong anteroventral pinching; it is connected to a large value of the bending energy. Fig. 5B is the first partial warp for the transformation from *Quasibradleya momitea* to *Q. praemackenzeyi*. Most mapping deformation occurs in the posteroventral region; this is a small-scale deformational feature, connected to a small value of the bending energy. It is interesting to record that the degree of deformation disclosed here is unusually strong for related ostracod lineages. The complete analysis for some Australian Cenozoic ostracods is given in REYMENT & MCKENZIE (1993).

Fig. 6 illustrates the ordination for the first two relative warps for Iranian (specimens 1–13) and Lebanese (specimens 14–30) specimens of the Cenomanian ammonite genus *Knemiceras*. These have been assumed to be the same species but the size-free plot for apertural shape landmarks suggests that there are important differences in the apertural shape properties of the two groups. Two of the Iranian specimens fall centrally in the Lebanese constellation of points and one Iranian specimen lies far from both convex hulls. Inspection of the specimen concerned shows it to be an extreme morphological variant.

Fig. 7 illustrates the relationship between the factor of overall size, as expressed by centroid size and the first relative warp for two populations of the bioluminescent ostracod species *Vargula hilgendorfi* from Tokyo Bay. Misaki and Tateyama are located on facing sides of the entry to Tokyo Bay at relatively close proximity.

This arresting result incites interest since it suggests that there are two largely isolated populations of the species close to each other. The bioluminescence of some species of ostracods has been shown to be an expression of differentiation such that copulation only occurs between males and females displaying the same

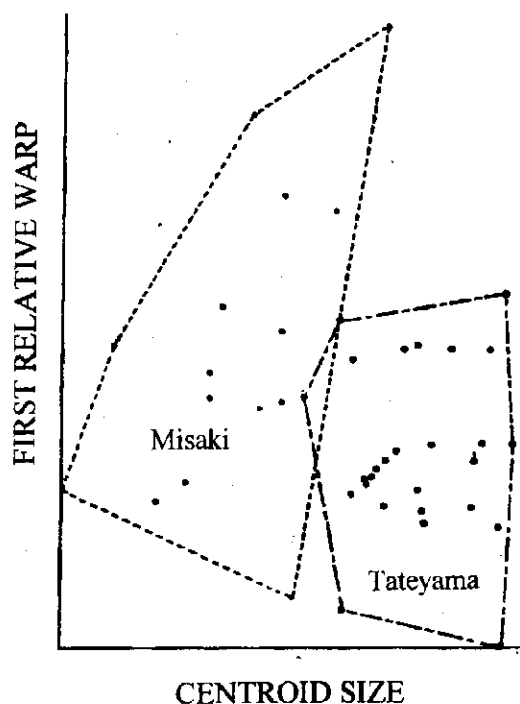


Fig. 7: Ordination for specimens of *Vargula hilgendorfi* from Misaki and Tateyama in Tokyo Bay. The scores for the first relative warp are plotted against centroid size. There is practically no overlap between the distributions.

Abb. 7: Streubereiche der ersten relativen Verformung und Größe in Bezug auf zwei Populationen der Ostracodenart *Vargula hilgendorfi* aus Tateyama und Misaki (Bucht von Tokyo). Die konvexen Hüllen der Punkte überlappen einander kaum.

bioluminescent signalling code. The situation for the Japanese populations has yet to be resolved.

## 10. Concluding remarks

The brief account of morphometrics presented in the foregoing pages can do no more than highlight a few of the most important features of what is a complicated subject caught up in a phase of expansive development. The introduction of advanced geometrical thinking into statistics is not widespread and very few statistical textbooks take it into consideration. The level of mathematical theory involved is certainly beyond the reach and learning of many statisticians and certainly transcends the ability of geologists and biologists. The truth of this statement can be assessed by consulting the magnificent volume by KENDALL et al. (1999). An interesting and promising development in biological shape analysis

has been proposed by BOOKSTEIN (2000) by means of a method called "creases", being an allusion to the pinched features characterizing the associated spline diagrams. The method of crease analysis examines the effect of expansions forwards and backwards in time in phylogenetic reconstructions (BOOKSTEIN 2000). Fig. 8 is an example of crease-analysis for data on the cranial evolution of *Homo* in relation to ancestors and *Pan* in relation to all *Homo* variants (figure kindly supplied by Professor Fred L. BOOKSTEIN).

The crease computation underlying Fig. 8 compares modern Man to the hypothetical common ancestral form and Man to *Pan*. The least bent contrast concerns related forms (varieties of *Homo*), whereas the comparison of forms of Man with chimpanzees is strongly creased. The crease method holds promise of being a means of developing the automated description of diagnostic contrasts between reference specimens of species, that is, image-based taxonomy.

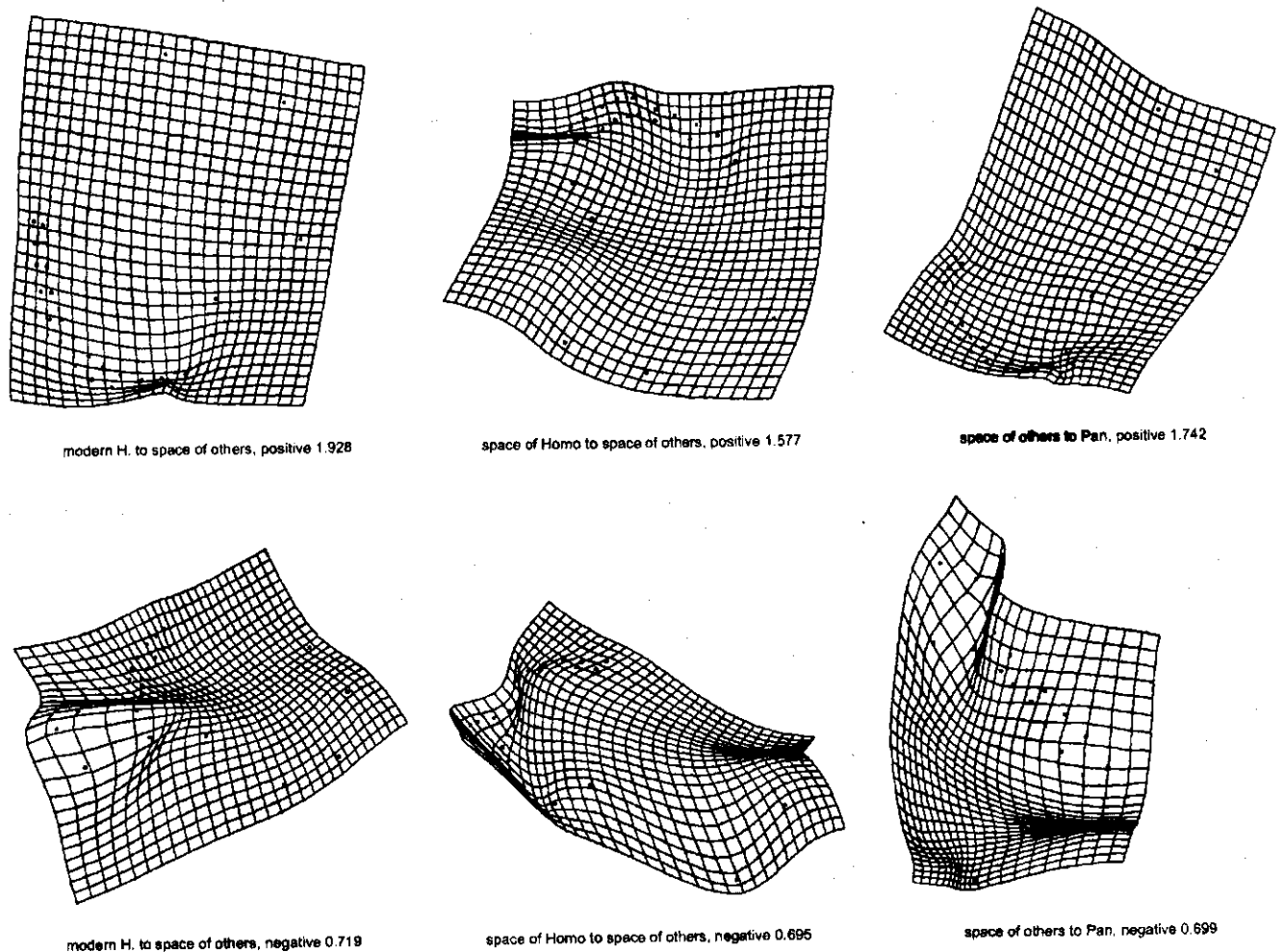


Fig. 8: Example of the method of crease analysis applied to primate evolution (by courtesy of Professor Fred L. BOOKSTEIN).

Abb. 8: Beispiel der Methode der „Faltenanalyse“ hinsichtlich der späteren Entwicklung der Primaten.

## 11. Acknowledgements

I wish to thank the Trustees of the Swedish Museum of Natural History, Stockholm, for providing facilities. I also owe a debt of gratitude to Fred L. BOOKSTEIN for continued advice and for providing Fig. 8.

## 12. References

- Aitchison, J. (1986): The statistical analysis of compositional data: 416 pp.; London (Chapman and Hall).
- Blackith, R. E. (1957): Polymorphism in some Australian locusts and grasshoppers. – *Biometrics*, **13**: 183–196; Washington D.C.
- (1960): A synthesis of multivariate techniques to distinguish patterns of growth in grasshoppers. – *Biometrics*, **16**: 28–40; Washington D.C.
- Bookstein, F. L. (1978): The measurement of biological shape and shape change. – *Lecture Notes in Biomathematics*, **24**: 1–191; New York.
- (1989): Principal warps: thin-plate splines and the decomposition of deformations. – *IEEE Transactions on Pattern Analysis and Machine Intelligence*, **11**: 567–585; Washington D.C.
- (1991): Morphometric tools for landmark data: 435 pp.; Cambridge (University Press).
- (1994): Can biometrical shape be a homologous character? – In: Hall, B. K.: *Homology: the Hierarchical Basis of Comparative Biology*: 197–227; New York (Academic Press).
- (1997): Landmark methods for forms without landmarks: localizing group differences in outline shape. – *Medical image analysis*, **1**: 225–243; Amsterdam.
- (2000): Creases as local features of deformation grids. – *Medical image analysis*, **4**: 93–110; Amsterdam.
- Burnaby, T. P. (1966): Growth-invariant discriminant functions and generalized distances. – *Biometrics*, **22**: 96–110; Washington D.C.
- Campbell, N. A. (1979): Canonical variate analysis: some practical aspects. – Thesis, Imperial College: 242 pp.; University of London (unpublished).
- Dryden, I. L. & Mardia, K. V. (1998): *Statistical shape analysis*: 347 pp.; New York (Wiley & Sons).
- Hopkins, J. W. (1966): Some considerations in multivariate allometry. – *Biometrics*, **22**: 747–760; Washington D.C.
- Huxley, J. S. (1932): *Problems of relative growth*: 276 pp.; London (Methuen).
- Jolicœur, P. (1963): The degree of generality of robustness in *Martes americana*. – *Growth*, **27**: 1–27; Washington D.C.
- & Mosimann, J. E. (1960): Size and shape variation in the Painted Turtle, a principal component analysis. – *Growth*, **24**: 339–354; Washington D.C.
- Kendall, D. G., Barden, D., Carne, T. K. & Le, H. (1999): *Shape and shape theory*: 306 pp.; Chichester (Wiley & Sons).
- Klein, F. (1925): *Elementarmathematik vom höheren Standpunkte aus. Band 2: Geometrie*: 302 pp.; Berlin (Springer).
- Lohmann, G. P. (1983): Eigenshape analysis of microfossils: a general morphometric procedure for describing changes in shape. – *Mathematical Geology*, **15**: 659–672; New York.
- MacLeod, N. (2002): Phylogenetic signals in morphometric data. – In: MacLeod, N. & Forey, P. L. (eds.): *Morphology, shape and phylogeny. – Systematics assoc. spec. vol.*, **64**: 100–138; London (Taylor and Francis).
- Mahanolobis, P. (1936): On the generalized distance in statistics. – *Proceedings of the Indian National Science Academy, series A*, **2**: 49–55; New Delhi.
- Mosimann, J. E. (1970): Size allometry: size and shape variables with characterizations of the lognormal and generalized gamma distributions. – *J. American Statistical Assoc.*, **65**: 930–945; Alexandria VA.
- Pearce, S. C. (1959): Some recent applications of multivariate analysis to data from fruit trees. – *Annu. Rep. Horticulture Research Internat. (East Malling Research Station)*, **1958**: 73–76; Wellesbourne.
- (1965): *Biological Statistics*: 212 pp.; New York (McGraw-Hill).
- Quenouille, M. H. (1952): *Associated measurements*: 242 pp.; London (Butterworths Scientific Publ.).
- Reyment, R. A. (1991): *Multidimensional palaeobiology. With an appendix by L. F. MARCUS*: 377 pp.; Oxford (Pergamon).
- & Kennedy, W. J. (1990): Phenotypic plasticity in a Cretaceous ammonite analyzed by multivariate statistical methods. – *Evolutionary Biology*, **25**: 411–426; New York.
- & Bookstein, F. L. (1993): Intraspecific variability in shape in *Neobuntonia airella*: an exposition of geometric morphometry. – In: McKenzie, K. G. & Jones, P. J. (eds.): *Ostracoda in the Earth and Life Sciences*: 291–314; Rotterdam (Balkema).
- & McKenzie, G. (1993): Quantitative genetics in Palaeontology: evolution in Tertiary Ostracoda. – In: Davis, J. C. & Herzfeld, U. (eds.): *Computers in geology – 25 years of progress*, **13**: 155–168; Oxford (University Press).
- , Blackith, R. E. & Campbell, N. A. (1984): *Multivariate Morphometrics. Second Edition*: 233 pp.; London (Academic Press).
- Rohlf, F. J. (1993): Relative warp analysis and an example of its application to mosquito wings. – In: Marcus, L. F. et al. (eds.): *Contributions to morphometrics*: 131–159; Madrid (Museo nacional de ciencias naturales).
- (2002): Geometric morphometrics and phylogeny. – In: MacLeod, N. & Forey, P. L. (eds.): *Morphology, shape and phylogeny. – Systematics Assoc. Spec. Vol., Ser.* **64**: 175–193; London (Taylor and Francis).
- Sprent, P. (1972): The mathematics of size and shape. – *Biometrics*, **28**: 23–28; Washington D.C.
- Swiderski, D. L., Zelditch, M. L. & Fink, W. L. (2002): Comparability, morphometrics and phylogenetic systematics. – In: MacLeod, N. & Forey, P. L. (eds.): *Morphology, shape and phylogeny. – Systematics Assoc. Spec. Vol., Series* **64**: 67–99; London (Taylor and Francis).

Teissier, G. (1938): Un essai d'analyse factorielle. Les variants sexuels de *Maia squinata*. – Biotypologie, **7**: 73–96; Paris.

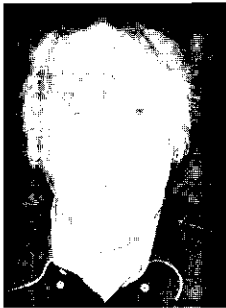
Thompson, D. W. (1917) [1942]: On growth and form: 1116 pp.; Cambridge (University Press).

ZAHN, C. T. & ROSSKIES, R. Z. (1972): Fourier descriptors

for plane closed curves. – IEEE transactions on computers, **C-21**: 269–281; Los Alamitos CA.

Manuscript received: 30.11.2004

Accepted for printing: 09.12.2004



**RICHARD ARTHUR REYMENT.** Born 1926 in Coburg, Australia. – Major Degrees: Fil Dr. Stockholm (1956); Examiners W. J. Arkell and Friedrich Brotzen. D. Sc. Melbourne (1967); Examiner Martin Friedrich Glässner. – Professional employment: Geologist, Kiruunavaara – Luossavaara A.B., Malmberget, Sweden (1949–1950). Geologist, British Colonial Service (1950–1956). Senior Lecturer, University of Stockholm (1956–1962). Professor of Petroleum Geology, University of Ibadan, Nigeria (1963–1965). Associate Professorship of Biometry, University of Stockholm (1965–1967). Professor of Historical Geology and Palaeontology, University of Uppsala (1967–1991).

Current Affiliation: Paleozoologiska avdelningen, Naturhistoriska Riksmuseet, Stockholm.

Academies: Fellow of the Royal Statistical Society. Fellow of the Royal Swedish Academy of Sciences in 1974. Foreign fellow of the Brazilian Academy of Sciences in 1978. Fellow of Kungl. Vetenskapsocieten (Uppsala) and Kungl. Fysiografiska Sällskapet (Lund).

Activities: Leader IGCP project 58 Mid-Cretaceous Events. Prime mover for the International Association for Mathematical Geology (its first General Secretary and subsequently its President). One of the founders of the European Union of Geosciences (Comité de parrainage). Former member of UNESCO committee COGEO DATA. President of the Geological Society of Sweden in 1972–1973.