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The biometrical analysis of invariant relationships ,and a concealed statistical constraint, occurring in Ammonites

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Abstract: The smallest latent root and associated vector of a $k \times k$ positive definite square symmetric matrix is shown to have diagnostic value for finding an invariant linear combination, if and only if the smallest root is very small, almost zero, and much smaller than the k - 1-th root. The matrix must be in the form of a covariance matrix and to derive from a data-set lacking significantly atypical observations. The logarithmic spiral structure of the conch of ammonites introduces a complication with respect to the biometrical interpretation of a multivariate statistical analysis. The reification of the principal component analysis of a positive definite square symmetric matrix (the most commonly occurring model in practical work) is based on an artifact. This, and the problem of the growth/size analysis of coiled shells (ammonites, gastropods, for example) are considered.

INTRODUCTION

The mathematical significance of a zero latent root

The application of multivariate statistical procedures is becoming of greater interest to many workers in the Natural Sciences. In the present note we show that there may be possibilities for producing incorrect analyses if an inappropriate procedure is used. Ammonite shells pose a special problem in that the lateral form of the shell is geometrically controlled by the logarithmic spiral, and hence is not amenable to a simple multivariate statistical interpretation

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Ever since the latent roots and vectors of a positive definite square symmetric matrix were introduced into multivariate statistical analysis interest has been centred on interpreting the first few latent vectors with the end in view of learning as much as possible about those linear combinations of the variables involved that are providing most of the variability in the material.

There is, however, another line of enquiry that ought to be of interest, but which has remained largely neglected. Gnanadesikan and Wilk (1969), Gower (1967), Gnanadesikan (1977), Mardia et al. (1979) have pointed out that the information resident in the smallest (zero, or almost zero) latent root should, logically, be of importance for finding a linear combination of variables which is invariant in the material under study. That is, that combination which is constant, or almost constant, for variables measured in the same metric. The justification for this may not be immediately obvious. Gnanadesikan and Wilk (1969), in a geometrically constructed example, exemplified the manner in which the smallest latent root, and its associated vector, can be invoked for charting an invariant structural relationship.

It is not always understood that the interpretation of principal components is based on an artifact, which is the case in multivariate statistical analysis. The Perron-Frobenius theorem states that among the latent roots of a real positive symmetric matrix **A** there will be a real positive value, $\lambda = x$, the maximum root, the value of which is not surpassed by any other latent root of the matrix and which has a positive latent vector $\mathbf{x} > 0$ (cf. Zurmühl, 1964, p. 219; Gantmacher, 1966). Mardia et al. (1979, pp. 235, 241) noted that there is an indeterminacy involved in reifying principal components, for example, in the case where where *(p-k)* latent vectors are equal or almost equal. Gower (1967) made several pertinent observations of importance in a critique of Principal Components as a statistically relevant tool. Some are obvious; for example: all the variates in the data matrix must be measured in the same units. For many applications, the extraction of the latent roots and vectors is made on the correlation matrix in the belief that this will "stabilize" the data. Another is to work on the logarithms of the observations. In the situations studied in the present note, neither of the foregoing manoeuvres is permissible, granted that we are looking for intrinsic structural information. Hence, the reification of the smallest principal component is only valid for data that have not been adjusted in some arbitrary manner. Geometrically, the components of the smallest principal component vector constitute the best $(n - 1)$ flat (i.e. the multidimensional analogue of a plane which fits the points, the coordinates which are the direction cosines of the normal to the flat (Gower, 1967). Dempster (1969, p. 139) commented on the arbitrariness encapsulated in the method of principal components. He recognized that it makes mathematical good sense that the last latent vector corresponding to the smallest latent root should be the only one of diagnostic value for predicting some scientifically important feature. Empirical information for this conclusion was forthcoming from contributions by Reyment (1978). It is of interest to record here that Izenman and Shen (2009) considered the use of the smallest principal components in outlier detection, which, however, is not of relevance in the present connexion.

The problem posed by the logarithmic spiral

The second part of our considerations concerning the analysis of variability in the ammonite shell is to find a solution for the effect of the constraint imposed by the logarithmic growth spiral. The variables of an ammonite conch in lateral orientation are clearly not free to vary freely if they form part of the spiral growth constraint (Klein,1926, pp. 171-173) . It is obvious that, in effect, all possible selections of variables such as umbilical width, maximum diameter of the conch, whorl-breadths, are constrained and consequently render a standard principal component analysis biometrically redundant.

CASE-HISTORIES

Invariance in Schloenbachia*, *a morphologically complex genus of ammonites

The apertural properties of the conch

The Albian-Cenomanian ammonite genus *Schloenbachia* is remarkable for great variability in apertural shape-dimensions. Ammonites assigned to the genus *Schloenbachia* are conveniently considered to occur in three generalized shapes when viewed in apertural orientation, to wit, an inflated form, a moderately compressed form and a very compressed form. It has been suggested that these shapes in some measure may reflect reactions to palaeoecological factors (Wilmsen and Mosavinia, 2011). Of relevance in this connexion is the very wide geographical distribution of species of the genus.

A sample of 18 well preserved shells of varying provenance from England were subjected to a principal component extraction of the covariance matrix based on six variables observed on the apertural surface, to wit:

1 - maximum diameter of the conch
2- maximum breadth of the last whorl
3 - minimum breadth of the last whorl
4 - diameter at the beginning of the last whorl
5 - breadth of the venter at the beginning of the last whorl
6 - distance across the last whorl to the point of intersection with the second last whorl.

The smallest latent root corresponds to 0.57% of the total variability. The associated latent vector is

1	2	3	4	5	6

(-0.12, 0.33, 0.32, 0.03, -0.87, 0.07)

This vector indicates an invariant relationship likely to exist between variables 2, 3, and 5. That is between two whorl-breadth measures and the width of the venter.

Discoscaphites, a heteromorphic ammonite genus , and a concealed constraint

The constraint imposed by the logarithmic spiral

Ammonites are coiled in approximation to the logarithmic spiral. However, it has not been recognized by workers interested in studying the geometry of ammonite shells that the logarithmic spiral imposes a constraint on the quantitatively appraisable variability of conchs in lateral aspect if the suite of selected variables are part of the spiral growth pattern (Klein, 1926, pp. 171- 173). As an example of this fact, a simple analysis of four lateral measurements of the conchs in Maastrichtian macroconchs of *Discoscaphites conradi (*Morton*)*, to wit, maximum diameter, two whorl dimensions and umbilical width, yielded the latent roots (Landman and Waage, 1993).

Latent roots	(1) 1.0586	(2) 0.0125	(3) 0.0005	(4) 0.0002
Percentages	98.76	1.17	0.05	0.02

There are three very small latent roots of which two are almost zero, whereas the largest latent root accounts for almost all of the variability. In approximate terms, the rank of the covariance matrix from observations in the plane of coiling is almost of unit rank. What does this signify? It is expressing the fact that the logarithmic growth spiral locks the variability in a firm grip and hence the small latent roots cannot be interpreted as natural expressions of morphological variability in a biometrical sense (as was concluded by Landman and Waage (1993, p.248).

Principal components for correlations in the case of Schloenbachia

In this example, we examine the relationships between the apertural breadth of the conch and three variables observed on the lateral aspect of the conch with the end in view of ascertaining whether there is a connexion between selected lateral variables and the aperture, to wit, the problem of interpreting the categorization of shells into three generalized morphotypes. The data used here derive from specimens obtained from the Lower Cenomanian of Bed 30 of the Bezakty section of Mangyschlak, Kazachstan (Marcinowski et al, 1996). (Data generously provided by Professor W. James Kennedy, Oxford University). Interest here centres around the properties of a set of stratigraphically homogeneous data.

The question as to whether the material occurring in the Bed 30 sequence is indicative of a preserved thanatocoenesis or a *köckenmödding* of shells swept together by water and wind is not clear. The shell categories do not seem to come out in favour of an *in situ* situation. The occurrence of glauconite can also be of interest - Wahl and Grim (2008) point out that relatively shallow, agitated water is a pre-requisite for the formation of glauconite as well as the presence of organic material (Degens, 1968).

Summary for the Mangyschlak Data

Number of dimensions = 4, sample-size = 17

Latent roots for correlations

2.30747 1.14871 0.32269 0.22113

percentages of the total variance

57.68683 28.71764 8.06733 5.52821

latent vectors by columns

	1	2	3	4
1	0.0304	0.9114	0.2532	-0.3230
2	0.5832	-0.2724	-0.0625	-0.7627
3	0.5572	0.3021	-0.6773	0.3737
4	0.5904	-0.0629	0.6879	0.4175

correlations between principal components and original variables

1	0.0462	0.9768	0.1439	-0.1519
2	0.8859	-0.2920	-0.0355	-0.3587
3	0.8463	0.3238	-0.3847	0.1757
4	0.8968	-0.0674	0.3908	0.1963

The correlations expressed by the first and second principal components relate to more than 86% of the variability thus indicating that there is an almost zero relationship between the breadth of the conch, an apertural variable, and the three lateral variables, to wit, height of the last whorl (var 2), breadth of the umbilicus (var 3) and the diameter of the shell (var. 4). This result is an inescapable expression of the variational constraint imposed by the logarithmic growth spiral (cf. Klein, 1926, pp. 171-173).

Generality of the Schloenbachia model

The generality of the invariance concept that seems to describe what occurs for *Schloenbachia* needs to be considered briefly. Variability in the conch of *Knemiceras* seems on the surface to resemble what is observed in forms of that genus (Kennedy et al, 2009). Application of the procedure accounted for above yielded the following results for *Knemiceras persicum* (Albian), presented separately for microconchs and macroconchs, using six measurements on the apertural aspect.

For *microconchs*, the smallest latent root corresponds to 0.151% of the total variability (N=12). The associated latent vector is

1	2	3	4	5	6
(-0.0923,	0.0830,	0.0303,	-0.6369,	0.7479,	–0.1621).

which could possibly represent an invariant relationship to exist between variables 4 and 5

However, for *macroconchs,* the smallest latent root accounts for 0.0651% of the total variability (N=8) which is associated with the latent vector

1	2	3	4	5	6
(0.178,	0.2380,	0.1784,	-0.7612,	-0.3703,	0.4412).

The aspect projected by this vector differs markedly from that obtained for the microconchs. We note that the angle between these two vectors is 80.69 degrees.

On the basis of these results, it is not possible to draw meaningful conclusions with respect to invariance in *K. persicum* Collignon. In any event, the homogeneity in invariant shape-relationship that comes to the fore for *Schloenbachia* is not manifested in the admittedly meagre data available for *Knemiceras.*

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COMMENTS ON THE STATISTICAL RESULTS

The examples presented here were selected for their value in illustrating variability in cases where the smallest principal component is of significance for expressing invariance in a set of variables. The concept of mathematical invariance is shown to cast light on the interpretation of seemingly unrelated growth expressions in the *Schloenbachia varians* complex. The second aspect of our study introduces an examples of an imposed constraint, whereby the covariance matrix is virtually of unit rank due to the effect of the logarithmic spiral that controls the shape of the shells of coiled organisms is discussed. This constraint makes the multivariate analysis of, for example, ammonite conchs, questionable when observed in lateral aspect and where all the variables (partly or wholly) are under the dominance of the logarithmic growth factor.

COMMENTS ON THE PHENOTYPICAL ASPECTS OF THE STUDY

The present study of the variability in shell-shape of presumed closely related representatives of a highly variable ammonite "genus" seems to be amenable to mathematical analysis. Reyment and Kennedy (1991) came to the conclusion that the shape of the shell of the Albian genus *Knemiceras* (Iran) displays great variability in the inflation and ornament of conches. It was suggested that this variability could possibly reflect ecophenotypic variation within a single species inhabiting a shallow environment. The variability occurring in the shells of *Knemiceras* has in the past, by traditional reasoning, resulted in a great number of specific names having been erected by workers in the field (cf. Reyment and Kennedy, 1991, fig. 5). It is noteworthy that the range of variants resembles closely that found for *Schloenbachia* which, however, has a very much greater distribution than *Knemiceras*. It is therefore motivated to keep in mind that the distributional factor could account for some of the assumed phenotypicality. It might also be a possibility that feral populations could be influencing morphological evolution. The genetics of feral populations of cichlid fishes of eastern Africa springs to mind, albeit on a much lower level of complexity in the case of the ammonites. In any event, it seems just possible that the *Schloenbachia* problem is not really as baffling as it may seem at first sight.

The concept of niche-polymorphism arising for *Schloenbachia* in the shallow seas of the mid-Cretaceous may be significant (Reyment and Kennedy, 1991). As pointed out by Bulmer (1980, p. 180), a population may become monomorphic for a certain phenotype which is adapted to average environmental conditions. A population may be monomorphic for a certain phenotype which is specialized for the most common kind of environment likely to be encountered by the organism. A population may develop a polymorphic state with each morph adapted to one kind of environment.

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Appendix

In the following text, the central theme of the main problems considered in our note are reviewed.

Spektraleigenschaften unzerlegbarer nichtnegativer Matrizen (nach Gantmacher 1966).

Perron (1907) hat einige bemerkenswerte Eigenschaften der Spektren (d. h. der charakteristischen Wurzeln und Eigenvektoren) positiver Matrizen angegeben.

Eine positive Matrix $A = \|a_{ik}\|$ besitzt stets eine reelle und überdies positive charakteristische Wurzel *r,* die einfache Wurzel der charakteristischen Wurzel übertrifft. Zu einer 'maximalen' charakteristischen Wurzel *r* gibt es einen Eigenvektor $z=(z_1, z_2, \ldots z_n)$ der Matrix A mit positiven Koordinaten $z_i > 0$ ($i = 1,2, \ldots, n$).

Nach dem Satz von Perron sind alle Koordinaten des Vektors *z* von Null verschieden, reell und besitzen dasselbe Vorzeichen.

This property is of crucial importance for the way in which Principal Component results are interpreted. Clearly, the first latent root must be positive, and all subsequent latent roots likewise positive and associated vector must perforce always be positive, secondly all the components of the first latent vector must be positive. This means that the standard interpretation for the first latent vector as expressing variation in size is an artefact of the inherent properties of apositive definite square synmmetric matrix.

Obviously, this property casts a possible shadow of doubt over the invariant vector thesis put forward in our note. If, however, we accept that the first latent vector is , say, also a measure of shape-contrast, then the intepretation of invariance registered in the smallest, near-null, latent vector, would not seem to go logically amiss.

A caveat

The problems analysed in this note are taken from the realm of palaeobiology. However, the invariance theme is quite general in scope and can of course be applied to any topic, from engineering, social sciences to hard-rock geology.