Draft text

2012 – 03 - 12

The biometrical analysis of invariant relationships and a hidden constraint 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, iff 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.

INTRODUCTION

The significance of a zero latent root

It is becoming increasingly more common for palaeontologists to try their hand att using statistical procedures in the study of their material. Most commonly occurring are methods of univariate statistics. It is however the application of multivariate statistical procedures that is becoming of greater interest to ambitious workers.. 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 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 introduction of 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 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, showed 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 appreciated 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). 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 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 lograrithms 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 is mathematically feasible for 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).

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 a umbilical width, maximum diameter of the conch, whorl-breadths, are constrained and consequently render a standard principal component analysis biometrically redundant.

CASE-HISTORIES

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 characteristics. Ammonites assigned to the genus *Schloenbachia* are 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).

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

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

This vector indicates an invariant relationship 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

Ammonites are coiled in approximation to the logarithmic spiral. However, it has not been recognized by workers interested in studying the biometrics 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 assumed by Landman and Waage , 1993, p.248).

Principal components for correlations for 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, recalling 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) and identified for me by Professor W. James Kennedy (Oxford). Interest here centres around the properties of a set of stratigraphically homogeneous data.

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 correlation expressed by the first and second principal components relates to more than 86% of the variability indicates 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 expression of the variational constraint imposed by the logarithmic spiral (cf. Klein, 1926, pp. 171-173).

CONCLUDING COMMENTS

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 variables are under the dominance of the logarithmic growth factor.

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