

18. Archaeological uses of the biplot — a neglected technique?

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18.1 Introduction

Principal component analysis (PCA) is one of the more widely used multivariate statistical techniques in archaeology. Biplots provide an approach to display jointly the rows and columns of a two-way data matrix that arise naturally in the context of PCA. The thesis of this paper is that the biplot is a useful but neglected tool for the exploration and display of archaeological data. After summarising the mathematics of the biplot, applications of PCA in archaeology are reviewed. Areas of use where the biplot is of potential value are discussed and illustrated and the paper concludes with a brief discussion of the relationship to factor and correspondence analysis. A bibliography of 100 archaeological applications of PCA, categorised by subject matter and representative of what I have seen in the literature, is provided. Generalisations in the text about the uses of PCA have been based on a content analysis of these papers, though not all are individually referenced.

Fig. 18.1(a) is based on the component plot resulting from a PCA of a 177 by 19 data matrix of the logged elemental compositions of specimens of Romano-British mortaria. The elements include major, minor and trace components but, in line with most studies, omit silica which is the most abundant component. Such figures occur commonly in provenance studies of pottery and other materials. Less common is a plot such as Fig. 18.1(b) based on the loadings on the leading two components plotted against each other. The joint presentation and interpretation of the two plots constitutes a form of biplot.

There are two clear groups in Fig. 18.1(a). The group to the left will tend to be characterised by high values of those elements to the left of Fig. 18.1(b) and low values on those elements to the right. Groups of clustered variables in Fig. 18.1(b) will, if the representation is a successful one, identify variables with a high degree of positive inter-correlation. Variables opposite each other relative to the origin tend to be highly negatively correlated. Joint inspection of the plots suggests the association of particular groups with particular sets of variables and provides additional information to the separate inspection of plots.

Archaeologists have been aware of the separate merits of both forms of plot at least since the publication of Doran and Hodson (1975) (see also Shennan 1988). Biplots have been discussed in the statistical literature since at least 1971 (Gabriel 1971) and feature in many textbooks on multivariate analysis. The use of PCA in archaeology has been widespread but there are relatively few published uses of the biplot.

This neglect is surprising since the method is a useful one for both exploring data and presenting results. It is also useful for certain common classes of archaeological application where PCA can be applied.

The basis for this view is presented in the rest of the paper.

18.2 The mathematics of biplots

Biplots were introduced and developed by Gabriel (1971, 1981) and his colleagues (e.g. Corsten & Gabriel 1976). The following exposition is based on treatments given in Gower (1984) and Jolliffe (1986) which may be consulted for further discussion of interpretation and fit not covered here.

Let Y be an n by p data matrix. It can be factorised, via the singular value decomposition, as

$$Y = UDV'$$

where U is an n by p matrix; V is p by p ; $U'U = V'V = I$; and D is a p by p diagonal matrix.

It is possible to obtain a two dimensional approximation to Y that may be displayed graphically using co-ordinates for row and column markers held in the first two columns of matrices G and H . Possible definitions of G and H include the following, the first two of which define biplots:

$$\begin{array}{ll} \text{(i)} & G = UD \quad H = V \\ \text{(ii)} & G = U \quad H = VD \\ \text{(iii)} & G = UD \quad H = VD \end{array}$$

A biplot involves the joint graphical presentation of the row and column markers. The attraction of the choices of G and H given above lies in the interpretation of the plots.

In the case of (i) the row plot is just the component plot obtained after a PCA in which inter-point distances approximate Euclidean distance between the rows. The column plot is just a plot of the 'loadings' of variables on the leading two components.

In the case of (ii) inter-point distances on the row plot approximate to Mahalanobis rather than Euclidean distance. The column plot has a particularly nice interpretation. If the plot is a 'good' one then the lengths of vectors from the origin to the column (variable) markers approximate to the variances of the variables. The (cosines of) angles between vectors approximate to correlations so that, for example, an acute angle is indicative of high positive correlation. The column plot by itself is sometimes referred to as an h -plot (Corsten & Gabriel 1976).

Both (i) and (ii) are based on alternative factorisations of Y ; (iii) is not and does not define a biplot in the sense of Gabriel (1971). It does, however, combine what Gower (1984:737) regards as the best features of (i) and (ii). In the case of (i) and (ii) the inner product of G and H reproduces Y exactly. This essentially

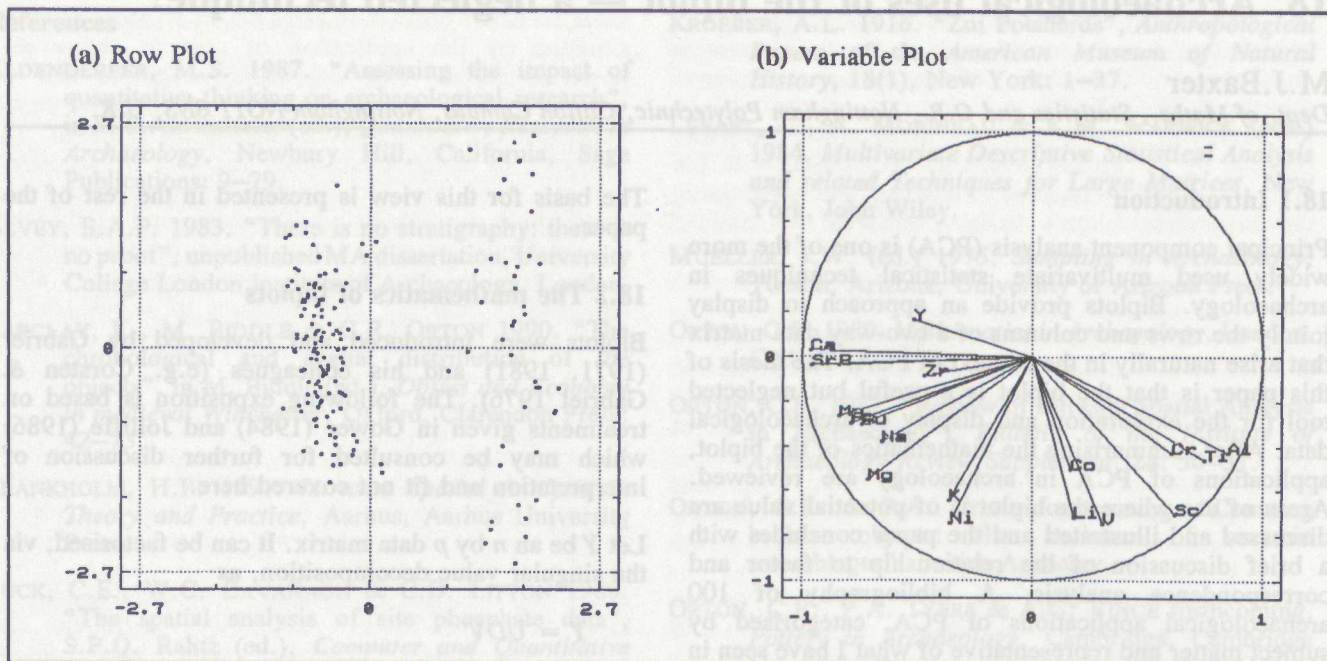


Figure 18.1: 177 specimens of mortaria characterised by the concentrations of the 19 elements used as labels in Figs. 18.1(b) and 18.2(b).

justifies the joint presentation and interpretation of the row and column plots (Jolliffe 1986:79). These exact mathematical relationships are lost with (iii) which can, however, be expected to lead to qualitatively similar results.

Archaeological uses of PCA tend to be based on the use of standardised data. In this case $H = VD$ is a visual approximation to the correlation matrix of the data. In a successful analysis the column markers (on a properly scaled plot) should lie close to the circumference of a unit circle about the origin (since the variances are now unity). This feature can be used to provide an informal assessment of the success of a plot.

18.3 PCA and biplots in the archaeological literature

In this brief survey biplots are viewed as an exploratory technique particularly associated with PCA. The related techniques of factor and correspondence analysis are treated here as distinct and will be considered in the final section.

The bibliography lists 100 references to archaeological uses of PCA classified into four broad subject areas:

- analysis of the chemical compositions of artefacts;
- inter-assemblage comparisons;
- typological/morphological studies;
- varied applications mostly involving biological data.

The bibliography is based on a systematic search through many of the major journals in which multivariate methods have been used as well as a less systematic analysis of conference proceedings and books that I have seen. The ratio of articles in the four categories is 54:14:18:14; this is a reasonable reflection of the distribution within journal articles and within other publications.

Articles in the last category are of a varied kind — many of them ‘once-off’ applications. The first three categories constitute the ‘bread and butter’ of PCA applications in archaeology and I believe that the figures given reflect, qualitatively, their relative popularity. There are technical reasons for doubting the value of PCA in inter-assemblage comparison. These arise from problems associated with the (usually) fully compositional nature of the data (i.e. rows total 100% — see Aitchison 1986) and the problem of defining similarity in terms of correlations with many zeroes in the data. There is not space to discuss these issues in detail here except to note that correspondence analysis may be a more useful tool (Gob 1988). This — if accepted — implies that categories (c) and particularly (a) are the main ‘live’ areas of application of PCA to archaeological problems.

Analyses of chemical compositions typically occur in provenance studies. Almost invariably the elements studied differ widely in their magnitude and standardisation is usual to avoid the dominance of size effects in an analysis. This results in an analysis of the correlation matrix; rare exceptions that use the covariance matrix after data transformation include Bishop and Neff (1989) and Leese *et al.* (1989). Morphological studies often use standardised data for similar reasons or because variables are non-commensurate.

In PCA analyses that result in graphical output presentation of the row plot based on $G = UD$ is common. The use of column plots by themselves is rare (O’Hare 1990 is an example). Biplots, or plots of type (iii) above, are unusual. It can be difficult to determine which form of plot is being used; row and column plots are sometimes presented on separate pages; and they are not necessarily jointly interpreted. On a generous assessment of what constitutes a biplot the following may be noted in each of the categories of use defined

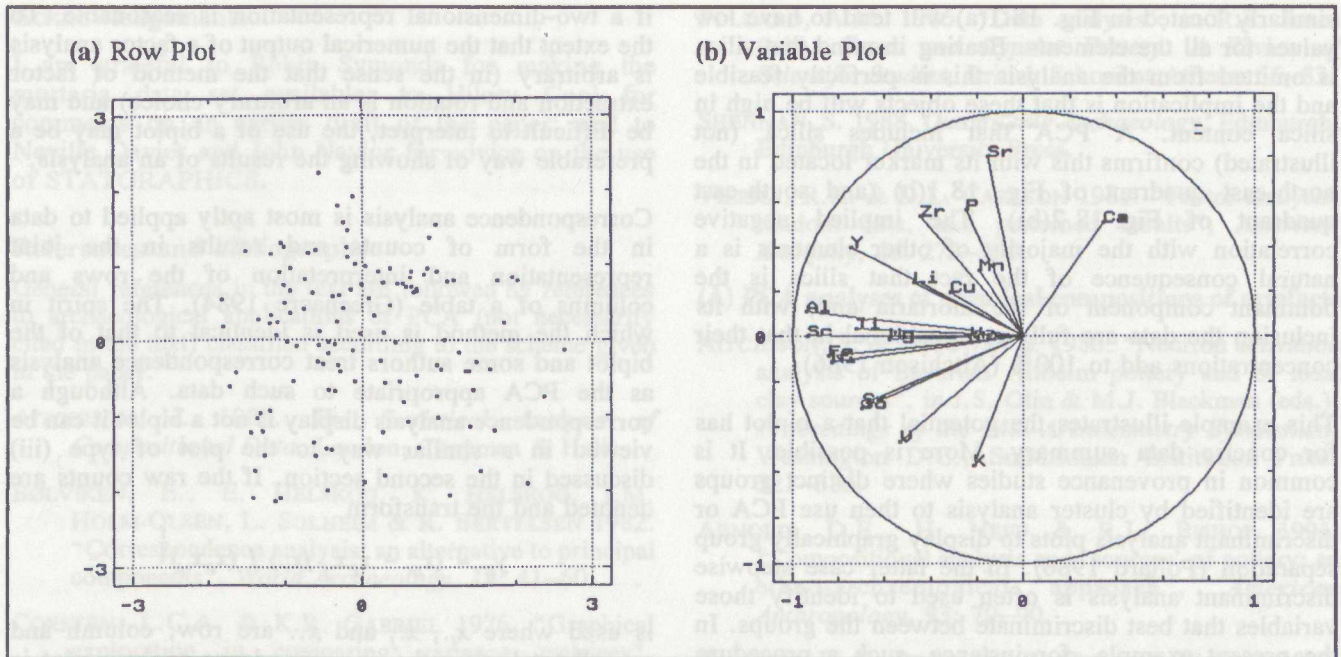


Figure 18.2: 129 specimens in the larger subset evident to the left of Fig. 18.1(a). The construction of the plots is described in the text. Elements that are not close to the unit circle in Figs. 18.1(b) and 18.2(b) are poorly represented.

above: (a) Berthoud *et al.* (1979); Poirier and Barrandon (1983) (b) Tomber (1988); Ringrose (1988a,b) (c) Hinout (1984,1985); Larsen (1988); Speiser (1989) and none in category (d).

A feature of this list, apart from its brevity, is that the references are mainly to scholars on the European mainland and particularly France. Shennan (1988:283) has noted that the related data exploratory technique of correspondence analysis has been much more speedily appreciated by the French — a view supported by Djindjian's (1989) review. (Scandinavian scholars should also be similarly credited — Holm-Olsen (1981); Bølviken *et al.* (1982); Madsen (1988)). This apparent 'cultural bias' in the readiness to use certain kinds of exploratory multivariate technique is, arguably, reflected in the use of biplots as well.

18.4 Possible uses of biplots

The foregoing discussion suggests that biplots have had limited use in archaeology. Is this neglect unjust and surprising? The answer is — I think — yes. Reasons for this assessment include:

- archaeologists writing on the use of PCA have clearly been aware of the separate merits of sample and variate plots (Doran & Hodson 1975; Shennan 1988);
- statisticians working with archaeologists regard biplots as a standard exploratory tool;
- the information needed for a biplot typically comes 'for free' with a PCA;
- some of the current popularity of correspondence analysis is attributable to its capacity for the joint representation of rows and columns of a data matrix — a quality shared by the biplot;
- Shennan (1988:284) notes that the possibility of a joint case/variable representation 'to some extent undercuts the arguments which have raged (on the subject of) ... the definition of archaeological types

and whether they should be treated in terms of correlations between variables or similarities between cases';

- biplots are of potential use in a common (the most common?) area of application of PCA to archaeological data — namely the analysis of chemical compositions in provenance and related studies.

This last point is now pursued in more detail. Figs. 18.1(a) and 18.1(b) form a biplot based on data on the elemental composition of 177 specimens of mortaria found in excavations at Colchester and other sites. Nineteen elemental concentrations were determined by inductively coupled plasma spectroscopy (ICPS); the analysis, in accordance with fairly common practice, uses logarithms of the concentrations subsequently standardised. The biplot is of type (ii). A discussion of computer implementation and scaling is given in the Appendix to this paper.

There are two very clear groups in the data as shown by Fig. 18.1(a). For this data set simple univariate and bivariate analyses will also identify the groups — although PCA is as easy and as quick to implement. From Fig. 18.1(b) groups of highly inter-correlated variables include (Ca, Sr, P); (Mn, Fe, Cu, Na, Mg); (Cr, Ti, Al) etc. This last group is negatively correlated with the other two. These inferences can be (and have been) checked by reference back to the original correlation matrix.

The advantage of joint inspection is that it can be deduced at a glance that the group to the left of Fig. 18.1(a) will have relatively high values for the variables to the left of Fig. 18.1(b), such as Ca, Sr, P etc. and low values for the variables to the right such as Cr, Al, Ti etc. The converse is true of the group to the right of Fig. 18.1(a). These deductions are also easily checked. The implication of the empty sector in the north-east quadrant of Fig. 18.1(b) is that objects

similarly located in Fig. 18.1(a) will tend to have low values for all the elements. Bearing in mind that silica is omitted from the analysis this is perfectly feasible and the implication is that these objects will be high in silica content. A PCA that includes silica (not illustrated) confirms this with its marker located in the north-east quadrant of Fig. 18.1(b) (and south-east quadrant of Fig. 18.2(b)). The implied negative correlation with the majority of other elements is a natural consequence of the fact that silica is the dominant component of the mortaria and, with its inclusion the data are fully compositional in that their concentrations add to 100% (Aitchison 1986).

This example illustrates the potential that a biplot has for concise data summary. More is possible. It is common in provenance studies where distinct groups are identified by cluster analysis to then use PCA or discriminant analysis plots to display graphically group separation (Pollard 1986). In the latter case stepwise discriminant analysis is often used to identify those variables that best discriminate between the groups. In the present example, for instance, such a procedure might identify Ca and Al as the best discriminators. The biplot makes clear that this would be a misleadingly simple summary and that other pairs of variables such as Sr and Ti would do almost as well. In the presence of highly correlated data it is misleading to attribute discrimination to a subset of variables that are highly correlated with others not in the subset. The biplot makes this clear.

In Fig. 18.1 there is clear group structure and the biplot identifies those variables that help to differentiate between the groups. In the absence of group structure the biplot may help identify clusters of variables that characterise a sample of homogeneous material. Fig. 18.2, for example, is a biplot for the separate analysis of the larger subgroup in Fig. 18.1 (four outliers, identified in the original re-analysis of the subgroup, are omitted). There is little obvious group structure. Fig. 18.1(b) suggests that the composition within this group may be characterised by the positively correlated suite of elements to the left Al, Sc, Fe Ni, etc. In studies of glass the biplot may assist in the identification of suites of correlated variables which may, in turn, be informative about the use of raw materials in the glass manufacture (Baxter & Heyworth 1991).

18.5 Biplots, correspondence and factor analysis

It is hoped that the foregoing discussion shows that biplots are a potentially useful tool for data exploration and presentation, worthy of greater use than they have had. In this final section some comments about the related areas of factor and correspondence analysis are made.

Factor analysis in archaeology does not now seem to be as widely used as was once the case. Earlier uses often seem to have been concerned with the identification of clusters of attributes or variables and have taken a PCA analysis, subsequently rotated, as their starting point (Doran & Hodson 1975; Vierra & Carlson 1981). Qualitatively the identification of clusters of correlated variables on the biplot may achieve much the same end

if a two-dimensional representation is reasonable. To the extent that the numerical output of a factor analysis is arbitrary (in the sense that the method of factor extraction and rotation is an arbitrary choice) and may be difficult to interpret, the use of a biplot may be a preferable way of showing the results of an analysis.

Correspondence analysis is most aptly applied to data in the form of counts and results in the joint representation and interpretation of the rows and columns of a table (Greenacre 1984). The spirit in which the method is used is identical to that of the biplot and some authors treat correspondence analysis as the PCA appropriate to such data. Although a correspondence analysis display is not a biplot it can be viewed in a similar way to the plot of type (iii) discussed in the second section. If the raw counts are denoted and the transform

$$y_{ij} = (x_{ij} - x_i x_j / x_{..}) / (x_i x_j)^{\frac{1}{2}}$$

is used where x_i , x_j and $x_{..}$ are row, column and overall totals then the correspondence analysis plot is based on (iii) except that scores for the i 'th row are divided by $(x_i)^{-1/2}$ and for the j 'th column by $(x_j)^{-1/2}$.

Appendix

Statistical packages that allow PCA to be carried out should also provide the ingredients for a biplot. The usual component and coefficient scores and loadings form the basis of plots of type (i). Given this information plots of type (ii) can be based on a simple rescaling. If scores on the first two components are divided by the square roots of their corresponding eigenvalues (information that is usually provided) the necessary coordinates result. Column coordinates are obtained similarly on multiplying component coefficients by the square roots of eigenvalues. Plots of type (iii) are, of course, a mixture of the two.

If scaling of the axes of the plot is not identical, but adapted to a fixed frame (as with screen output in MINITAB), the plots will look the same and may be adequate for interpretation whatever method is used. Points on the column plot, in an analysis of the correlation matrix, should lie close to the circumference of an ellipse rather than circle in a successful analysis. Experience suggests that if there are both positive and negative correlations represented in a plot with a reasonably central origin then the scaling may not be too critical for interpretation. If correlations are mostly of the same sign interpretation is easier if scales are commensurate, with the origin clearly shown.

The plots (of type (ii)) in this paper were obtained by using the MINITAB PCA command, saving scores and coefficients using the SCOR and COEF sub-commands, rescaling them as previously described, writing the rescaled coordinates to an external file, and then reading them into STATGRAPHICS in order to use the superior graphical facilities available for data display. Routine application plots of type (i) in MINITAB can be produced immediately after the PCA but will not be properly scaled. For smaller data sets than that used here STATGRAPHICS can be used directly.

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