MULTIVARIATE ANALYSIS IN ECOLOGY AND SYSTEMATICS: PANACEA OR PANDORA’S BOX?

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INTRODUCTION

Multivariate analysis provides statistical methods for study of the joint relationships of variables in data that contain intercorrelations. Because several variables can be considered simultaneously, interpretations can be made that are not possible with univariate statistics. Applications are now common in medicine (117), agriculture (218), geology (50), the social sciences (7, 178, 193), and other disciplines. The opportunity for succinct summaries of large data sets, especially in the exploratory stages of an investigation, has contributed to an increasing interest in multivariate methods.

The first applications of multivariate analysis in ecology and systematics were in plant ecology (54, 222) and numerical taxonomy (187) more than 30 years ago. In our survey of the literature, we found 20 major summaries of recent applications. Between 1978 and 1988, books, proceedings of symposia, and reviews treated applications in ecology (73, 126, 155, 156), ordination and classification (13, 53, 67, 78, 81, 83, 90, 113, 121, 122, 159), wildlife biology (33, 213), systematics (148), and morphometrics (45, 164,
For the six-year period from 1983 to 1988 (Table 1), we found 514 applications in seven journals. Clearly, it is no longer possible to gain a full understanding of ecology and systematics without some knowledge of multivariate analysis. Or, contrariwise, misunderstanding of the methods can inhibit advancement of the science (96).

Because we found misapplications and misinterpretations in our survey of recent journals, we decided to organize this review in a way that would emphasize the objectives and limitations of each of the 12 methods in common use (Table 2; Table 3 at end of chapter). Several books are available that give full explanations of the methods for biologists (53, 128, 148, 159, 164). In Table 3, we give specific references for each method. In the text we give examples of appropriate applications, and we emphasize those that led to interpretations that would not have been possible with univariate methods.

The methods can be useful at various stages of scientific inquiry (Figure 1). Rather than classifying multivariate methods as descriptive or confirmatory, we prefer to consider them all descriptive. Given appropriate sampling, 6 of the 12 methods can also be confirmatory (see inference in Table 2). Digby & Kempton (53) give numerous examples of applications that summarize the results of field experiments. Most often the methods are used in an exploratory sense, early in an investigation, when questions are still imprecise. This exploratory stage can be a very creative part of scientific work (206, pp. 23–24). It can suggest causes, which can then be formulated into research hypotheses and causal models. According to Hanson (86), by the time the

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**Table 1** Applications of multivariate analysis in seven journals, 1983–1988. In descending order of the number of applications, the journals are *Ecology*, 128; *Oecologia*, 80; *Journal of Wildlife Management*, 76; *Evolution*, 72; *Systematic Zoology*, 55; *Oikos*, 41; *Journal of Ecology*, 35; and *Taxon*, 27.

<table>
<thead>
<tr>
<th>Method</th>
<th>Applications</th>
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<tbody>
<tr>
<td>Principal components analysis</td>
<td>119</td>
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<tr>
<td>Linear discriminant function analysis</td>
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<tr>
<td>Cluster analysis</td>
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<td>Multiple regression</td>
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<tr>
<td>Multivariate analysis of variance</td>
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<td>Principal coordinates analysis</td>
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<tr>
<td>Factor analysis</td>
<td>15</td>
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<tr>
<td>Canonical correlation</td>
<td>13</td>
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<tr>
<td>Loglinear models</td>
<td>12</td>
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<tr>
<td>Nonmetric multidimensional scaling</td>
<td>8</td>
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<tr>
<td>Multiple logistic regression</td>
<td>7</td>
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<tr>
<td><strong>Total</strong></td>
<td><strong>514</strong></td>
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Table 2  General objectives and limitations of multivariate analysis

<table>
<thead>
<tr>
<th>Objectives</th>
<th>Codes to Procedures (see Table 3)</th>
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<tbody>
<tr>
<td>1. Description</td>
<td>All</td>
</tr>
<tr>
<td>2. Prediction</td>
<td>MR, LDFA, MLR</td>
</tr>
<tr>
<td>3. Inference</td>
<td>MR, MANOVA, LDFA, FA, MLR, LOGL</td>
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<tr>
<td>4. Allocation</td>
<td>LDFA</td>
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<tr>
<td>5. Classification</td>
<td>LDFA, MLR, CLUS</td>
</tr>
<tr>
<td>6. Ordination</td>
<td>LDFA, PCA, PCO, FA, CANCOR, COA, NMDS</td>
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</tbody>
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Limitations:

1. The procedures are correlative only; they can suggest causes but derived factors (linear combinations of variables) and clusters do not necessarily reflect biological factors or clusters in nature.
2. Because patterns may have arisen by chance, their stability should be checked with multiple samples, null models, bootstrap, or jackknife.
3. Interpretation is restricted by assumptions.
4. Automatic stepwise procedures are not reliable for finding the relative importance of variables and should probably not be used at all.

Theoretical hypothesis test has been defined, much of the original thinking is over. In the general scientific procedure, descriptive work, including descriptive applications of multivariate analysis, should not be relegated to a status secondary to that of experiments (28). Instead it should be refined so that research can proceed as a combination of description, modelling, and experimentation at various scales (106).

The opportunities for the misuse of multivariate methods are great. One reason we use the analogy of Pandora's box is that judgments about the results based on their interpretability can be dangerously close to circular reasoning (124, pp. 134–136; 179). The greatest danger of all is of leaping directly from the exploratory stage, or even from statistical tests based on descriptive models, to conclusions about causes, when no form of experimental design figured in the analysis. This problem is partly attributable to semantic differences between statistical and biological terminology. Statistical usage of terms like “effect” or “explanatory variable” is not meant to imply causation, so the use of terms like “effects” and “roles” in titles of papers that report descriptive research (with or without statistical inference) is misleading. Partial correlations and multiple regressions are often claimed to have sorted out alternative processes, even though such conclusions are not justified. “If . . . we choose a group of . . . phenomena with no antecedent knowledge of the causation . . . among them, then the calculation of correlation coefficients, total or partial, will not advance us a step toward evaluating the importance of the causes at work” (R. A. Fisher 1946, as quoted in reference 54, p. 432).
Although this idea is familiar to biologists, it seems to get lost when they enter the realm of multivariate work.

The objective of the present review is to help the researcher navigate between the Scylla of oversimplification, such as describing complex patterns with univariate analyses (147), and the Charybdis of assuming that patterns in data necessarily reflect factors in nature, that they have a common cause, or, worse, that statistical methods alone have sorted out multiple causes.

Present understanding of the role of multivariate analysis in research affects not only the way problems are analyzed but also how they are perceived. We discuss three particularly controversial topics, and we realize that not all researchers will agree with our positions. The first is the often-cited "problem" of multicollinearity, the idea that, if correlations among variables could be removed, one could sort out their relative importance with multivariate analysis. The problem here is a confusion between the objectives of the

Figure 1  General research procedure showing stages (double boxes) at which exploratory and inferential* (confirmatory) multivariate analysis may be appropriate (modified from 106).
method and the objectives of the researcher. Second, in the sections on analysis and ordination in plant ecology, we discuss the special problems that arise with indirect ordinations, such as the cases where the data are the occurrences of species in stands of vegetation. The arch pattern frequently seen in bivariate plots is not an artifact of the analysis; it is to be expected. Third, in the section on morphometrics, we explain why we argue that shape variables, which we define as ratios and proportions, should be studied directly. Of course the special properties of such variables require attention. We do not treat cladistics or the various software packages that perform multivariate analyses. In the last section, we give examples of how some basic concepts in ecology, wildlife management, and morphometrics are affected by the ways in which multivariate methods are being applied.

**SUMMARY OF METHODS: OBJECTIVES LIMITATIONS, EXAMPLES**

**Overview**

It is helpful to think of multivariate problems as studies of populations of objects about which information for more than one attribute is available (48, 169). One can describe the pattern of relationships among the objects (individuals, sampling units, quadrats, taxa) by ordination (reduction of a matrix of distances or similarities among the attributes or among the objects to one or a few dimensions) or by cluster analysis (classification of the objects into hierarchical categories on the basis of a matrix of inter-object similarities). In the former case, the objects are usually displayed in a graphic space in which the axes are gradients of combinations of the attributes. Principal components analysis is an ordination procedure of this type. It uses eigenstructure analysis of a correlation matrix or a variance-covariance matrix among the attributes. Principal coordinates analysis is a more general procedure in the sense that it starts with any type of distance matrix for distances among objects. Both principal components analysis and principal coordinates analysis are types of multidimensional scaling. Nonmetric multidimensional scaling uses the ranks of distances among objects, rather than the distances themselves. Correspondence analysis is an ordination procedure that is most appropriate for data consisting of counts (contingency tables). In this case, the distinction between objects and attributes is less relevant because they are ordinated simultaneously. Factor analysis is similar to principal components analysis in that it uses eigenstructure analysis, usually of a correlation matrix among attributes. It emphasizes the analysis of relationships among the attributes. Canonical correlation reduces the dimensions of two sets of attributes about the same set of objects so that their joint relationships can be studied.

When the objects fall into two or more groups, defined a priori, the
problem is frequently to describe the differences among the groups on the basis of a set of attributes. Multivariate analysis of variance, which is often used in the analysis of experiments, can be used to test for differences among groups. Linear discriminant function analysis describes which of the attributes contribute most to the differences between the groups. When it is used as an exploratory ordination procedure, to reduce multigroup data to fewer dimensions on the basis of a set of attributes, it is called canonical variates analysis. Another objective of linear discriminant function analysis, used less frequently in ecology and systematics, is to assign new objects to previously separated groups. Multiple logistic regression permits the prediction of a binary (0, 1) attribute from a set of other attributes, which may be categorical or continuous. Its counterpart for approximately normally distributed data is multiple regression. Loglinear analysis can reveal the relationships among categorical variables. It assumes a multiplicative model, so it is linear after logarithms are taken.

Procedures 1–7 in Table 3 use linear combinations of the variables in some fashion. They are only efficient with continuous data. If the variables being analyzed are denoted by \( X_1, X_2, \ldots, X_n \), then all the linear techniques find linear (additive) combinations of the variables that can be represented by:

\[
L_x = b_1 X_1 + b_2 X_2 + \ldots + b_k X_k
\]

where \( b_1, b_2, \ldots, b_n \) represent coefficients determined from the data. The way the coefficients are found is governed by the method used. For example, in principal components analysis they are chosen to make the variance \( L \) as large as possible, subject to the constraint that the sum of squares of the \( b \)'s must be equal to one.

Linear methods are appropriate when the researcher wants to interpret optimal linear combinations of variables (e.g. principal components in principal components analysis, factors in factor analysis, and discriminant functions in linear discriminant function analysis).

The researcher applying linear methods usually assumes that the values of the variables increase or decrease regularly and that there are no interactions. If this is not the case, one should transform the variables to make them at least approximately linear (55). For example, a quadratic model can be constructed with \( X_1 \) as a variable \( W_1 \) and \( X_2 \) as \( W_1 \) squared, or interactions can be included, in which \( X_3 \) is \( W_1 \) times \( W_2 \) (104, 133). For some of the techniques the analysis of residuals can uncover the need for the inclusion of nonlinear terms or interactions. In multivariate analysis of variance, the nonlinearities appear in the interaction terms and may reveal biotic interactions in experimental results (see below). Presence-absence data, categorical data, and ranks are usually more efficiently handled with nonlinear models. It seldom
makes sense to calculate weighted averages from these types of data, as one does with the linear methods. With nonlinear methods, the variables are combined with nonlinear functions.

The coefficient of an individual variable represents the contribution of that variable to the linear combination. Its value depends on which other variables are included in the analysis. If a different set of variables is included, the coefficients are expected to be different, the "bouncing betas" of Boyce (27).

The term "loading," often encountered in multivariate analysis, refers to the correlation of an original variable with one of the linear combinations constructed by the analysis. It tells how well a single variable could substitute for the linear combination if one had to make do with that single variable (89, p. 221). High positive or negative loadings are useful in the general interpretation of factors. However, the signs and magnitudes of the coefficients should only be interpreted jointly; it is their linear combination, not the correlations with the original variables (cf 220), that must be used to gain a proper multivariate interpretation. Rencher (162) shows how, in linear discriminant function analysis, the correlations with the original variables (loadings) lead one back to purely univariate considerations. This distinction is not important with principal components analysis because the correlations are multiples of the coefficients and their interpretations are equivalent.

Unfortunately, in observational studies, it is often difficult to provide clear descriptions of the meanings of individual coefficients. Mosteller & Tukey (146, p. 394) discuss the important idea of the construction of combinations of variables by judgment, in the context of multiple regression.

Some of the problems we found in our literature survey apply to univariate as well as to multivariate statistics. The first one is that statistical inference is being used in many cases when its use is not justified. The "alpha-level mindset" of editors leads them to expect all statements to be tested at the 0.05 level of probability (175). As a result, our journals are decorated with galaxies of misplaced stars. What the authors and editors have forgotten is that statistical inference, whether multivariate or univariate, pertains to generalization to other cases.

Confirmatory conclusions are only justified with a statistical technique if the study was conducted with appropriate sampling. It is the way the data were gathered, or how an experiment was conducted, that justifies inferences using statistical methods, not the technique itself. Inferences are justified only if the data can be regarded as a probability sample from a well-defined larger population. When this is not the case, probability values should not be reported, and the conclusions drawn should extend only to the data at hand.

The tendency to perform statistical tests when they are not justified is related to the even more general problem of when generalizations are justified. There are too many cases in which results of analyses of single study
plots or single species are assumed to be representative of those for large areas or many species. More caution is warranted even in cases of widespread sampling. For example, if several vegetation variables are measured at a series of regularly spaced sites along an altitudinal gradient, the correlations among the variables will show their joint relationship to altitude, but these will differ from the correlations that would have been found had the sites been randomly selected. A principal components analysis based on the former correlations should not be interpreted as giving information about sites in general, and only limited interpretations are possible, even in an exploratory sense.

A further extension of the tendency to overinterpret data is the unjustified assignment of causation in the absence of experimentation. Papers that report the use of stepwise procedures (automatic variable selection techniques) with multiple regression, multivariate analysis of variance, linear discriminant function analysis, and multiple logistic regression to assess which variables are important are examples of the disastrous consequences of this tendency. Such judgments about the importance of variables usually carry implications about causal relationships. In the section on multiple regression, we defend our position that stepwise procedures should not be used at all.

In summary, when faced with data that contain sets of correlated variables, ecologists and systematists may prefer to interpret each variable separately. In such cases univariate methods accompanied by Bonferroni-adjusted tests (89, especially pp. 7–9, but see index; 150) may be appropriate. Often, however, the joint consideration of the variables can provide stronger conclusions than are attainable from sets of single comparisons. With proper attention to the complexities of interpretation, combinations of variables (components, factors, etc) can be meaningful. Linear methods of multivariate analysis (Table 3, 1–7) should be used when the researcher wants to interpret optimal linear combinations of variables. Otherwise, nonlinear methods (Table 3, 8–12) are more appropriate and usually more powerful. Multivariate statistics, modelling, and biological knowledge can be used in combination and may help the researcher design a crucial experiment (Figure 1).

**Review of Methods**

Our survey of the literature revealed that the methods most commonly applied in ecology were principal components analysis, linear discriminant function analysis, and multiple regression; in systematics the order of use was cluster analysis, principal components analysis, and linear discriminant function analysis. Therefore in this section we devote most of the space to these methods.

We have included both multiple regression and multiple logistic regression even though many statisticians would not classify these methods as multi-
variates, a term they use only where the "response" (Y) variable rather than the "explanatory" (X) variable is multivariate. We acknowledge that, in multiple regression and multiple logistic regression, the outcome variable is univariate, but we include the topics here because many methodological issues in multiple regression carry forward to multivariate generalizations. The intercorrelations among the explanatory variables (X’s) in multiple regression are important to proper interpretation of the results.

MULTIPLE REGRESSION The objective of multiple regression should be either to find an equation that predicts the response variable or to interpret the coefficients as associations of one of the explanatory variables in the presence of the other explanatory variables. The coefficients (b₁, b₂, . . . , bₖ) in Equation 1 have been determined either to maximize the correlation between Y (the response variable) and L (the linear combination of explanatory variables) or equivalently to minimize the sum of squared differences between Y and L. Only in experiments where the X’s are controlled by the investigator can the individual coefficients of a multiple regression equation be interpreted as the effect of each variable on the Y variable while the others are held constant, and only when a well-defined population of interest has been identified and randomly sampled can multiple regression provide statistically reliable predictions. Unfortunately, these conditions are rarely met. “Validation” with new, randomly collected data will be successful only when the original sample is typical of the new conditions under which validation has taken place, and this is usually a matter of guesswork.

Many workers think that, if one could eliminate multicollinearity (intercorrelations) among the X variables in a descriptive study, the predictive power and the interpretability of analyses would be improved (35). This belief has led to the practice of (a) screening large sets of redundant variables and removing all but one of each highly correlated set and then (b) entering the reduced set into a stepwise multivariate procedure, with the hope that the variables will be ranked by their importance. Statisticians have pointed out many times that this is unlikely to be the case. The procedure of screening variables may improve prediction, but it may also eliminate variables that are in fact important, and stepwise procedures are not intended to rank variables by their importance.

Many authors have documented the folly of using stepwise procedures with any multivariate method (99; 100; 139, pp. 344–357, 360–361; 215, p. 177, Fig. 8.1, pp. 195–196). One example is the reanalysis by Cochran of data from a study of the relationship between variation in sets of weather variables and the number of noctuid moths caught per night in a light trap. Stepwise forward and backward variable selection procedures did not give the same best variable as a predictor or even the same two or three variables as the best
subsets of predictors (51). In another case, an investigator analyzing 13 out of 21 attributes of 155 cases of viral hepatitis used the bootstrap procedure to obtain repeated samples of the 155 cases. Of 100 stepwise regressions, only one led to the selection of the same four variables chosen by the initial stepwise regression, and it included a fifth one in addition (139, pp. 356-357). Clearly, stepwise regression is not able to select from a set of variables those that are most influential.

Wilkinson (217, p. 481) used strong language to defend his refusal to include a stepwise regression program in a recent edition of the SYSTAT manual: “For a given data set, an automatic stepwise program cannot necessarily find a) the best fitting model, b) the real model, or c) alternative plausible models. Furthermore, the order variables enter or leave a stepwise program is usually of no theoretical significance.”

The best that can be hoped for, when an automatic selection method like stepwise multiple regression is used, is selection of a subset of the variables that does an adequate job of prediction (188, p. 668). However, this prediction can be achieved more reasonably without the stepwise procedure. The most reasonable solution for observational studies that have a battery of explanatory variables is to combine them into biologically meaningful groups (146), then to examine all possible subsets of regressions. The results may provide useful overall predictions, but even in this case they should not be used to rank variables by their importance. Thus, Abramsky et al (1) need not worry about field tests purported to discover interspecific competition from the values of coefficients in multiple regression equations. The method is statistically inappropriate for this purpose.

Progress toward assessing the relative importance of variables can be made by modelling, a subjective step that incorporates subject-matter knowledge into the analysis. Interactive methods (96) and methods of guided selection among candidate models (4) can incorporate reasonable biological information into the analysis (see, e.g., 37, 153, 182). This step can help develop causal hypotheses, but the testing still requires some form of experiment and outside knowledge. When controlled experiments are not feasible, quasi-experimental designs can be used to provide weak inferences about causes (32, 41, 44, 106, 111). Such designs involve either blocking, time-series models, or both.

We regret to report that, in our survey of recent journals in ecology and systematics, we could not find a single application of multiple regression to recommend as a good example. Even recent attempts to measure natural selection in the wild by means of multiple regression (119) are susceptible to the criticisms mentioned above (47, 136a). Use of a path-analytic model has been suggested as a means of adding biological information to the analysis (47, 136a), but even here, because it is not possible to break correlations
among characters with experiments, it is not possible to discover whether selection is acting on individual characters. For an example of a proper application of multiple regression and subsequent discussion, see Henderson & Velleman (96) and Aitkin & Francis (2).

**MULTIVARIATE ANALYSIS OF VARIANCE**  Multivariate analysis of variance is an inferential procedure for testing differences among groups according to the means of all the variables. It is like the usual analysis of variance except that there are multiple response variables \( (Y_1, Y_2, \ldots, Y_n) \). The relationship with univariate analysis of variance can be understood if MANOVA is viewed as an analysis of linear combinations of the response variables,

\[
L_y = b_1 Y_1 + b_2 Y_2 + \ldots + b_k Y_k.
\]

\( L_y \) is now a single, combined, response variable. A univariate analysis of variance can be performed on \( L_y \) and an F-statistic calculated to test for differences between groups. One of the suggested tests in MANOVA (Roy’s maximum root test criterion) is the same as choosing the \( b \)'s in equation (2) to maximize the \( F \)-statistic and then using the maximized value of \( F \) as a new test statistic. MANOVA requires that each vector of \( Y \)'s should be independent and that they follow a distribution that is approximately multivariate normal. A good nonmathematical introduction is available (85).

In a good example of the application of multivariate analysis of variance in ecology, a manipulative factorial experiment designed to determine processes that affect the numbers of tadpoles of several species of amphibians was conducted in artificial ponds. Predation, competition, and water level were the explanatory variables and were regulated (216). The model incorporated the explanatory variables both additively and as interactions with other variables. In one case of interaction between predation and competition, predation on newts (Notophthalmus) reduced the effects of competition as the pond dried up, allowing increased survival of the toad *Bufo americanus*. This result would not have been apparent from univariate analyses by species. For an application in a more evolutionary context, see Travis (204). In this paper, he used MANOVA to show that families of tadpoles grew at different rates but were not differentially susceptible to the inhibitory effects of population density.

**LINEAR DISCRIMINANT FUNCTION ANALYSIS**  Linear discriminant function analysis can be regarded as a descriptive version of multivariate analysis of variance for two or more groups. The objective is to find linear combinations of the variables that separate the groups. In Equation 2 above they give rise to the largest F-statistics. The researcher wants to understand \( L_y \) and what
determines the groups to which specific data vectors belong. Linear discriminant function analysis does not formally require any assumptions, but it is the best technique for multivariate normal data when variances and covariances are the same in each group. Then the optimal combination of variables is linear. If the attributes are nonlinearly related, or the data are otherwise not multivariate normal (for example, categorical data), variances and covariances are poor summary statistics, and the technique is inefficient. An appropriate alternative, when there are only two groups, is multiple logistic regression (see below).

In a summary of applications of linear discriminant function analysis in ecology, Williams (220) warns that more attention should be paid to the assumption of equality of dispersion within groups. He also emphasizes the special problems that arise if the sample sizes are small or different (see also 34, 201, 210). Williams & Titus (221) recommend that group size be three times the number of variables, but this criterion is arbitrary. Discriminant function axes can be interpreted in either a univariate or a multivariate way (see overview). Again, the elimination of variables before the analysis and stepwise procedures should be avoided (163).

When the data are plotted on axes defined by the discriminant functions, the distances (Mahalanobis $D^2$) are measured in relation to variances and covariances. Population means may be judged far apart in cases in which the groups are similar except in one small but statistically highly significant way. This is not true of Euclidean distances in principal components space, so the two types of distances should not be interpreted in the same way (106, cf 34). Graphic presentation of the results can be clarified by the use of either concentration ellipses (43) around groups or confidence ellipses (105) around means of groups (188, pp. 594–601).

Linear discriminant function analysis can be used to summarize the results of an experiment (e.g. 91), but in both ecology and systematics it is used most often as an exploratory ordination procedure. In such cases it is called canonical variates analysis. Many descriptive uses concern resource use and the ecological niche. In the literature on wildlife management, there are applications that attempt to define the habitat of a species from quantitative samples of the vegetation taken in used and unused sites. These topics are discussed in later sections.

Some early exploratory applications of linear discriminant function analysis have made important contributions to studies of comparative morphology and functional anatomy. A good example is work comparing the shapes of the pectoral girdles (clavicles and scapulae) of mammals (8, 157). The variables were angles and indices based on the orientation of the attachments of muscles, so they were related functionally to the use of the forelimb. In Figure 2, for primates, the first discriminant function (linear combination of var-
variables) separates the great apes, which use the forelimbs for hanging, from the quadrupedal primates. The second variate expresses an uncorrelated pattern of development that separates ground-dwellers from arboreal dwellers, some of which are quadrupedal in trees. Convergences between the suborders Anthropoidea and Prosimii and radiations within them are demonstrated simultaneously (see 164 and Figure 2), and graded patterns within groups are evident. The analysis shows, in a way that could not have been demonstrated with univariate methods or with cluster analysis, that complex adaptations of biomechanical significance can be usefully viewed as a mosaic of positions along a small number of axes of variation. Note that, although the data were unlikely to have been normally distributed, the multivariate descriptive approach was very helpful, and the 9-variable data set for 25 taxa was displayed in two dimensions.

**Principal Components Analysis** Principal components analysis has been used widely in all areas of ecology and systematics. It reduces the dimensions of a single group of data by producing a smaller number of abstract variables (linear combinations of the original variables, principal components). The method is based on maximization of the variance of linear combinations of variables \( L_y \). Successive components are constructed to be uncorrelated with previous ones. Often most of the variation can be summarized with only a few components, so data with many variables can be

![Diagram of discriminant function analysis](image)

*Figure 2* Discriminant function analysis of data for the shape of the pectoral girdle (clavicle and scapula) of primates by genera (redrawn from Figure 2 of 8).
displayed effectively on a two- or three-dimensional graph that uses the components as axes.

If the original variables were not measured on the same scale, the analysis should be performed on standardized variables by the use of the correlation matrix rather than the variance-covariance matrix. Unfortunately, with the correlation matrix, the interpretation of "variance explained" or accounted for by each component is changed, because all the variables have been standardized to have a variance of one. With the variance-covariance matrix, the eigenvalues and percent of eigenvalues are equal to the variances of the components and the percent of variance explained by the components. This interpretation does not hold for analyses using the correlation matrix. When one is presenting the results of a principal components analysis, it is important to give the list of objects and attributes, the eigenvalues, and any coefficients that are interpreted and to state whether the analysis was performed on the variance-covariance or the correlation matrix.

Principal components analysis requires no formal assumptions, but in practice it is important to be aware of some of its limitations:

(a) Because it is based on either variances and covariances or correlations, principal components analysis is sensitive to outliers, and the coefficients of individual components are highly subject to sampling variability. One should not put too much emphasis on the exact values of the coefficients.

(b) When the distribution of ratios or proportions is reasonably near to normal, the analysis can be useful (see, e.g., 103, 125, 176), but without transformations principal components analysis cannot capture nonlinear relationships (135). Investigators whose data consist of counts, ratios, proportions, or percentages should check to see whether transformations might make their distribution more appropriate or whether a nonlinear approach would be preferable. Methods have been developed that incorporate the use of ratios through log transformations (140–142; see section on morphometrics).

(c) Mathematically orthogonal (independent) factors need not represent independent patterns in nature (14), so biological interpretations should be made with care.

(d) Contrary to some recommendations (101, 191), principal components analysis should not be used in a multiple-sample situation, as it then confounds within- and between-group sources of variation (60, 148, 194). In studies of geographic variation, a PCA on means by locality will give the appropriate data reduction.

A particularly interesting example of principal components analysis is its application to data for the genetic structure of present-day human populations in Europe on the basis of a correlation matrix of the frequencies of 39 alleles (5, pp. 102–108). A map on which the scores by locality for principal component 1 are contoured shows a clear gradient from the Middle East
toward northwestern Europe, a pattern highly correlated with archeological evidence for the pattern of the ancient transition from hunting and gathering to agricultural societies. The analysis is compatible with the authors' demic diffusion hypothesis, which states that this major cultural change was associated with a population expansion. The genetic structure of living populations may still reflect the ancient Neolithic transition. In quantitative genetics, principal components analysis has been used to analyze genetic correlations during development (40, 205). In morphometrics, comparisons of congeneric songbirds in a space defined by principal components (123, 151) have led to useful graphic comparisons of complex forms. Little progress would have been made with any of these problems by the use of univariate statistics.

**PRINCIPAL COORDINATES ANALYSIS** Principal coordinates analysis begins with a matrix of distances among objects (159) and, to the extent possible, these distances are retained in a space with a reduced number of dimensions. It is the same as the technique called classical scaling by psychometricians (38, p. 190; 202). If the data are quantitative and the distances are squared distances between units in a coordinate space (Euclidean distances), a principal coordinates analysis will produce the same result as will a principal components analysis on the correlation matrix among the attributes (53).

In a good example in systematics, a matrix of Roger’s genetic distances among colonizing populations of common mynahs (*Acridotheres tristis*) was expressed in a two-dimensional graphic space, and the populations in the graph were then connected with a minimum spanning tree according to their distances in the full dimensional space (16).

Another useful analysis using principal coordinates analysis was performed on a matrix of the number of interspecific contacts among 28 species of mosses (53). The procedure allowed investigators to express the associations in two dimensions, and the species were seen to occur along a shade-moisture gradient in which six habitats were clearly separated.

**FACTOR ANALYSIS** Basic computational similarities lead many people to regard factor analysis as a category of procedures that includes principal components analysis, but historically the two methods have had different objectives. Whereas principal components analysis is a descriptive technique for dimension reduction and summarization, factor analysis explores the resultant multivariate factors—the linear combinations of the original variables (89). The computational distinction is that, in factor analysis, the axes are rotated until they maximize correlations among the variables, and the factors need not be uncorrelated (orthogonal). The usual interpretation of the factors is that they “explain” the correlations that have been discovered among the original variables and that these factors are real factors in nature. Un-
fortunately, factor analysis encourages subjective overinterpretation of the data. A reading of the mythical tale about Tom Swift and his electric factor analysis machine (6) or Reyment et al (164, pp. 102–106) will persuade most people of the dangers of overinterpretation. Some newer versions of factor analysis, such as linear structural analysis (223, 224), avoid some of the problems of ordinary factor analysis.

Applications of factor analysis in systematics through 1975 have been summarized (31, pp. 135–143), and several examples have appeared in the more recent ecological literature (66a, 95, 127, 174). Q-mode factor analysis investigates the correlations among objects rather than attributes. It has been applied in an exploratory way in numerical taxonomy (185, p. 246) and morphometrics (77). The distinction between Q-mode and the more conventional R-mode analysis has been discussed by Pielou (159).

**Canonical Correlation**  Canonical correlation is a generalization of correlation and regression that is applicable when the attributes of a single group of objects can be divided naturally into two sets (e.g. morphological variables for populations of a species at a set of sites and environmental variables associated with the same set of sites). Canonical correlation calculates overall correlations between the two sets. Linear combinations within the first set of variables, \( L_1 \), and within the second set, \( L_2 \), are considered simultaneously, and the linear combinations that maximize the correlation between \( L_1 \) and \( L_2 \) are selected. Further linear combinations are extracted that are uncorrelated with earlier ones. These are uncorrelated between sets except for paired linear combinations. Sample sizes that are small in relation to the number of variables can lead to instability, and the linear constraints imposed by the method can make interpretation difficult (198).

In spite of its limitations, canonical correlation has been useful in an exploratory sense in several ecomorphological and coevolutionary studies. One such study showed that the size of the rostrum of aphids increases and that of the tarsus decreases in proportion to the degree of pubescence of the host plant: these features could easily obscure underlying phylogenetic relationships (137). Another study explored the canonical correlation between bee and flower morphology by comparing eight species of bees according to their choice of flowers (87). Gittins (72) and Smith (183) review other examples.

**Multiple Logistic Regression**  Multiple logistic regression is a modification of multiple regression for the situation in which the response variable (Y) is categorical and takes one of only two values, 0 or 1. Multiple logistic regression models the log of the odds that \( Y = 1 \) (\( \ln (Pr(Y = 1)/Pr(Y = 0)) \)) as a linear function of the independent variables, which can be continuous or categorical. The method can be used either to predict values of the response
variable or to get information about particular $X$ variables and the response variable. These are some of the same goals addressed by multiple regression, and multiple logistic regression is susceptible to many of the same limitations as multiple regression. Inference of causation (e.g. 166) is not justified, and stepwise procedures should be avoided. Multiple logistic regression can be used as an alternative to two-group linear discriminant function analysis when one or more of the variables are not continuous. In this case the response variable is group membership, and the explanatory variables are those used to discriminate between the two groups. If the data are multivariate normal, linear discriminant function analysis is a more efficient procedure (56).

Multiple logistic regression is used frequently in wildlife studies, but most applications (e.g. 108, 115) use stepwise procedures. As discussed previously, this is not a reliable way to rank variables by their importance.

**LOGLINEAR MODELS**  Loglinear analysis is an extension of the familiar chi-square analysis of two-way contingency tables (tables of counts or responses) for which there are more than two variables. If some of the variables are continuous, they must be categorized before loglinear analysis is used. The objective is simply to study the relationships among the variables. When there is a distinction between the variables, one being a response variable and the others explanatory variables, loglinear analysis is not appropriate. Fienberg (64) gives a good introduction to both loglinear models and multiple logistic regression.

There are more examples of loglinear analysis in behavior than there are in ecology (63, 94). Examples of its use in ecology include a study of population attributes in Snow Geese (*Chen caerulescens*), including interrelationships among parental morphs and the sex and cohort affiliations of the goslings (65); a study of interrelations among characteristics of fruits of the entire angiosperm tree flora of southern Africa (114); and a defense of the existence of a previously described (52) nonrandom pattern for the distribution of birds on the islands of the Bismarck Archipelago in the South Pacific Ocean (71). One excellent study combined a loglinear analysis with “causal ordering” of the variables, thereby injecting some reasonable biological information into the model for a competition hierarchy among boreal ants (211). This is a good example of how a problem can be carried forward through the research process as outlined in Figure 1. The next step would be the design of a critical experiment.

**CORRESPONDENCE ANALYSIS, RECIPROCAL AVERAGING, AND DETRENDED CORRESPONDENCE ANALYSIS**  Correspondence analysis, which is the same as reciprocal averaging, is an ordination procedure that decomposes a two-way contingency table of counts of objects and their attri-
The data might be the number of times various plant species occur on different quadrats, the number of times particular behaviors occur among various species, or the number of fin rays on various fish. Scores are calculated for each of the row and column categories of the table, and row and column eigenvectors show the ways in which the rows and columns deviate from what would be expected with independence. These scores are used as axes for dimension reduction, and objects and attributes are ordinated simultaneously. Because the analysis uses chi-square distances (81, p. 54) it should be based on data of counts. Continuous data such as allele frequencies, percentage of ground cover, or percentage of time spent foraging would be more efficiently handled by another method.

An excellent example of correspondence analysis is a summary of data for the distribution of 17 genera of antelope in 16 African wildlife areas (82). With supplemental information about the vegetation in these areas and about the distribution of the same species in the past, the authors were able to make inferences about the distribution of habitats in the past. In another example, an ordination of 37 lakes in the Adirondack Mountains of northern New York was found to be highly correlated with surface lakewater pH (37).

The term indirect ordination in plant ecology refers to the above class of problems, those involving a reduction of the dimensions of a table (matrix) of data for the occurrence of a set of species at a set of sites. The data may be counts, presence-absence data, or percentages. Because the species are likely to be responding in a unimodal way to underlying environmental gradients and each species is likely to have an individualistic response, their joint distribution is likely to be one of successive replacement (13). Phytosociologists have long felt that, in such cases, neither correspondence analysis nor any of the other traditional ordination procedures give reasonable results. In particular, they complain that an arch or horseshoe effect is evident in the pattern of sites in a two-dimensional ordination. Detrended correspondence analysis is an ad hoc technique intended to remove this arch (36, 67). However, it sometimes fails and can even introduce further distortion (112). A recent critique by Wartenberg et al (214) argues that detrending does not contribute to the analysis and that the arch is not an anomaly. Rather, it is an inherent property of data that represent transitions in species abundances as one passes through localities more favorable to some species and later more favorable to other species. Not even nonmetric multidimensional scaling (see below) can provide satisfactory single-dimensional ordinations in this case (214), because the relationships among the variables (species) are both non-linear and nonmonotonic. With the indirect ordination problem, the arch in two-dimensional plots is to be expected. An unambiguous ordering along the arch would be an acceptable result.
NONMETRIC MULTIDIMENSIONAL SCALING  Nonmetric multidimensional scaling is potentially a robust ordination method for reducing the dimensions of data without a priori transformations (see, e.g., 59, 112, 136, 154, and especially 214). The results are often similar to those of principal components analysis.

Like principal components analysis and principal coordinates analysis, it is a scaling technique, but with nonmetric multidimensional scaling, only the rank order of interobject distances is used. Thus the objective is to estimate nonlinear monotonic relationships. A limitation of both principal coordinates analysis and nonmetric multidimensional scaling is that interpretations must be qualitative and subjective. Because the axes are not functions of original variables, they are not very useful for formulating hypotheses about possible causal relationships. In fact with principal coordinates analysis and nonmetric multidimensional scaling, variables do not enter into the analysis; only interobject distances are used.

CLUSTER ANALYSIS  With cluster analysis, objects are placed in groups according to a similarity measure and then a grouping algorithm. The reduction in the data comes from forming \( g \) groups \((g < n)\) out of \( n \) objects. In ecology and systematics, the general term "cluster analysis" usually means agglomerative hierarchical cluster analysis. This is a set of methods that starts with a pairwise similarity matrix among objects (individuals, sites, populations, taxa; see Section on distances and similarities). The two most similar objects are joined into a group, and the similarities of this group to all other units are calculated. Repeatedly the two closest groups are combined until only a single group remains. The results are usually expressed in a dendrogram, a two-dimensional hierarchical tree diagram representing the complex multivariate relationships among the objects.

The most appropriate choice among the various algorithms for agglomerating groups depends upon the type of data and the type of representation that is desired. It has become conventional in ecology and systematics to use the UPGMA (unweighted pair-group method using averages). This method usually distributes the objects into a reasonable number of groups. It calculates differences between clusters as the average of all the point-to-point distances between a point in one cluster and a point in the other (53, 159, 185). There are also algorithms for divisive cluster analysis, in which the whole collection of objects is divided and then subdivided (67).

Cluster analysis is most appropriate for categorical rather than continuous data. It is less efficient than principal components analysis or linear discriminant function analysis when the data are vectors of correlated measurements. It has been the primary method used in phenetic taxonomy (185), in...
which many attributes are considered simultaneously and the objects (operational taxonomic units or OTU's) are clustered according to their overall similarity. Cluster analysis produces clusters whether or not natural groupings exist, and the results depend on both the similarity measure chosen and the algorithm used for clustering. Dendrograms codify relationships that may not really be stable in the data. They are frequently overinterpreted in both systematics and ecology. Nevertheless, as applied by Sokal et al. (186) to the hypothetical caminalcules, cluster analysis can be as robust for the reconstruction of hierarchical phylogenetic relationships as are cladistic methods. Systematics relies heavily on both cluster analysis and cladistics.

RELATED MATTERS

Jackknife and Bootstrap

Jackknifing (146, 148, pp. 31–33) and bootstrapping (57, 58) are statistical techniques that resample the data in order to calculate nonparametric estimates of standard errors. They are particularly effective in two situations that arise frequently in multivariate analysis:

(a) in estimation of standard errors for complicated statistics for which the sampling variability is not well understood and standard formulas are not available (e.g. coefficients of principal components) and

(b) when the distributional assumptions necessary for the use of standard error formulas are not met (e.g. for nonnormal or skewed data).

Jackknifing and bootstrapping differ in the ways in which they resample the data and calculate standard errors. With the typical jackknifing method, each of the observations in a sample, which may be multivariate, is left out of the data set in turn, and the statistic for which one wants the standard error is recalculated. The variability in these recalculated values is used to calculate the standard error. Examples would be applications to coefficients of principal components in studies of morphometric variation (69).

With bootstrapping for a single sample, a random sample with replacement is drawn from the original sample until it is the same size as the original sample. Some of the original observations are likely to occur more than once in the bootstrap sample. The statistic is recalculated from this sample. This process is repeated, typically 200 or more times, and the standard deviation of the recalculated values is used as the standard error. Often, the bootstrap can be applied more easily to complicated situations than can the jackknife, which is mainly a single-sample technique. Applications of the jackknife and bootstrap for estimating population growth rates have been compared (134).
Distances and Similarities

We use the terms distance and similarity to describe various measures of the association between pairs of objects or their attributes. Principal coordinates analysis, nonmetric multidimensional scaling, and cluster analysis require the input of a matrix of such measures. Cluster analysis operates most naturally with similarities, whereas principal coordinates analysis and nonmetric multidimensional scaling are traditionally described in terms of distances (53). With some types of data, such as immunological data (42) or DNA hybridization data (180), laboratory results are in the form of interobject distances so they can be entered directly or transformed to similarities as needed. The various distance and similarity measures have been compared (53; 149, Ch. 9; 159). The proper choice of a measure differs according to the form of the data (measurements, counts, presence-absence, frequencies), the type of standardization desired, and whether or not it is appropriate to use metric distances. The special problems that pertain to genetic distances have been discussed elsewhere (17, 61, 149, 172).

SPECIAL PROBLEMS IN ECOLOGY AND SYSTEMATICS

We think that the present understanding of multivariate analysis among ecologists and systematists is affecting not only how they treat data but how research questions are formulated. To illustrate this point, we discuss in this section some particular issues in animal community ecology, wildlife management, ordination in plant ecology, and morphometrics.

Resource Use and the Niche

Soon after it was proposed that the realized ecological niche be viewed as an area in a multidimensional resource hyperspace (102), Green (79) used linear discriminant function analysis to construct two-dimensional graphic ordinations of the relationships of bivalve molluscs in lakes in central Canada based on physical and chemical properties of the lakes. In many subsequent studies, linear discriminant function analysis has proved useful as a descriptive technique for summarizing, displaying, and comparing differences in resource use among populations (see summaries in 92 and 177).

Green (79, 80) and others have attempted a statistical test for niche size and overlap, but unfortunately, linear discriminant function analysis is not appropriate as a test of niche size. Equality of dispersion matrices is an assumption of the statistical model, but at the same time niche size is being defined by a characteristic of the dispersion matrix. Having been assumed, it cannot be tested (106, pp. 42–44). No one would expect the mean resource use of
different species to be exactly the same, so the test is only of whether sample sizes in the study are sufficiently large to show these differences (see 169).

One can obtain data on resource use for each of a set of species and then express an assemblage as an ordination of their variation (43, 79, 104, and others). Or one can compare used with available resources (34). The former approach has been used to study the regeneration niche of plants (70) and to analyze interspecific associations in plant populations to get a "plant's eye view" of the biotic environment (207). In these cases the data were the species of plants that were neighbors of the species of interest. Grubb (84) used this general approach to show how species-specific "regeneration niches" vary. He suggested that this variation may contribute to the maintenance of the coexistence of both common and rare species in a plant community. This is the kind of new hypothesis, suggested partly by multivariate work, that could be tested with experiments.

**Wildlife Management**

Wildlife biologists have maintained a good dialogue with statisticians about multivariate statistical methods (33, 213), and they are aware of the potential problems with scale, sampling, and linear methods (21). Also, they have been urged to become more experimental (173, 209).

We will give two examples of troublesome areas. First, in recent years the US Fish and Wildlife Service has supported a large program to produce predictive models of wildlife-habitat relations (212). Unfortunately, thus far, few of these models have achieved high predictive power (18, 29, 138). There are several reasons for these problems (130), not all statistical, but the issues of sampling procedures, adjustment for nonlinearities, screening variables to obtain an uncorrelated set, and the use of stepwise procedures discussed above need more attention. Even if predictive models can eventually be developed, there is no guarantee that they will be useful for management (195). That would require the additional step of causal analysis (see previous section).

An additional problem arises with studies of habitat selection, which in wildlife biology usually means the difference between occupied and available (unoccupied) habitat for a particular species. A common procedure is to measure many variables pertaining to the vegetation and its structure both at various localities where a species of interest occurs and at randomly selected locations. Then stepwise discriminant function analysis or stepwise multiple logistic regression is usually applied to examine differences between occupied and unoccupied sites and to rank the habitat variables by their "importance" (129, 165 and citations therein, 167). To see the problem with this approach, excluding the problems with stepwise procedures, recall that the linear discriminant function analysis model tests mean differences between groups. If a
species were highly narrow (selective) in its habitat use, but the mean were the same as that of the average habitat, the species would be judged not to be selective by the model (see Species B in Figure 3a and 107). Also, the characteristics of the poorly defined "unused" group will always affect the result (219). Some of these problems are avoided if sites are located along principal component 1 for variation in randomly selected sites (192). An alternative is to use the first two principal components (131) for randomly selected sites and to depict concentration ellipses (188, pp. 594–601) for occupied and random sites on a graph with those components serving as axes.

![Diagram](image1)

**Figure 3a** Comparisons of habitat used and habitat available for four hypothetical species (A, B, C, D). Four separate two-group linear discriminant function analysis or multiple linear regression tests between used and available habitat, one for each species, would test differences in means but not variances. A and B would not be different from habitat available; C and D would be different. However, this result is misleading because B is as selective (same variance) as D and is more selective (lower variance) than C.

**Figure 3b** Distribution of randomly selected sites in a bivariate graphic space determined by principal components I and II of their habitat characteristics. Concentration ellipses for randomly selected sites and for sites that are occupied by the species of interest indicate both the habitat used and its variance relative to the total variance.
(Figure 3b). This procedure assumes sufficient covariation in the data set for randomly selected sites that two reliable axes can be derived (152). One study that demonstrated the instability that can result otherwise attributed it to interobserver bias (76).

**Ordination in Plant Ecology**

The most general definition of ordination is the reduction of a multivariate data set for a set of objects and their attributes so that their pattern can be seen on a continuous scale (159). Thus linear discriminant function analysis, principal components analysis, principal coordinates analysis, and nonmetric multidimensional scaling all qualify as ordination procedures (Table 2). Ordination procedures are useful for descriptions of the results of environmental perturbations and experiments (53), but they are used most often in purely observational studies. Several particularly useful reviews of the ordination literature are available (53, 112, 159).

In plant ecology, the term ordination usually refers to analyses in which the objects are stands of vegetation at study sites. When the attributes are sets of environmental variables, such as soil nutrients or quantitative measures of the structure of the vegetation, the objective is usually to find a combination of attributes that may suggest an underlying cause for a systematic pattern of the distribution of the stands, one not obvious from the geographic distribution of the stands. Austin et al. (15) present some new extensions of this approach, which is called direct ordination or gradient analysis. The more common approach in plant ecology is to analyze a matrix of data for the presences and absences of species in each stand, or their actual or relative density, biomass, or cover (83), as the attributes. This is called indirect ordination. The objective is to find a systematic pattern of relationships among the stands based on the cooccurrences of their component species. The resultant ordination may subsequently be related to environmental factors (14).

If sites are being ordinated (the usual R-mode analysis), and they have been selected at random, inferences about patterns in a larger area are possible. If the objects and attributes are exchanged (Q-mode analysis), species are ordinated. The biplot (66, 196), a graphical version of principal components analysis and correspondence analysis, can provide a simultaneous view of ordinations of species and stands. The special problems that arise with indirect ordinations when the attributes do not increase or decrease regularly through the data are discussed in the section on correspondence analysis. Previous criticisms of principal components analysis as an indirect ordination technique (e.g. 67) should be reconsidered in the light of these arguments.

In recent years, principal coordinates analysis and nonmetric multidimensional scaling have been popular indirect ordination methods. Phytosociological studies that use indirect ordinations of stands by their species
composition have provided succinct descriptions of stands by their species composition. We agree with Harper (88) that if the objective is to determine causes, the approach of focusing a study on the population biology of species independently and including all interspecific interactions, rather than on studying relationships among communities or among stands, should also be tried. Experiments and quasiexperiments will be required, and multivariate descriptive work at the population level, now a poorly developed field, should be important.

Morphometrics

Morphometrics is the mathematical description of the form of organisms. There are many different kinds of problems in morphometric work, and even for a given problem researchers do not always agree about the best methods of analysis (46). The literature on multivariate morphometrics includes applications in growth (203) and quantitative genetics (118, 208).

For a long time the appealing graphic technique of the transformation of a grid to show its deformation when drawings of two organisms were compared (197) did not seem to be amenable to quantification. However, the study of geometric transformations of forms has been extended, and several techniques have been developed to describe geometric shape change between forms when the data are for \(x, y\) coordinates for homologous landmarks (23–26, 39, 101, 158, 184). Size and shape are considered to be latent unmeasured variables, defined only after the demonstration of a global transformation between forms. Sometimes principal components analysis is used to reduce the dimensions of the result.

Mapping techniques are another set of methods designed to detect shape change among two-dimensional forms (19, 20, 181, 184). In this case the data are interpoint distances between two superimposed forms. Fourier analysis, another alternative for the description of forms that have fixed outlines, can capture shape information without using sets of homologous landmarks (161, 170). Ferson et al (62) applied linear discriminant function analysis to such shape data for two electromorph groups of the mussel *Mytilus edulis*.

A more general problem in morphometrics than the quantification of shape change among two-dimensional objects is the study of allometry, how shape changes with size during growth, or among members of a population, or among populations or taxa. Many systematists prefer conventional linear methods of multivariate analysis for this problem (148, 164). The data are standardized measurements taken on each organism. Atchley et al (12) describe the geometric and probabilistic aspects of distances among individuals (objects) in multivariate morphometric space.

If the variation in the original data is predominantly in size, the coefficients of the first principal component based on a variance-covariance matrix will be
of the same sign, and that component will be highly correlated with the
original variables. Size can be defined variously as this first component, as
any one of the original variables, or as any combination of the original
variables that is biologically reasonable (168). Principal component 1 of the
correlation matrix has also been used as a size statistic (132). It is often
correlated with other reasonable size measures, but we do not recommend it
as a size statistic because differences in scale (size) among the variables have
been removed by the construction of the correlation matrix. Similarly, a
proposed method to constrain the first principal component of the correlation
matrix of the logs of the measurements to be a measure of shape-free size
(189) does not fully achieve its objective, because the residual variation is not
interpretable as shape. A complex method proposed for the removal of
within-group size in a multiple-group principal components analysis (101)
removes size-related shape as well as size, and the residual variation is not
necessarily uncorrelated with size (171).

With a principal components analysis on the variance-covariance matrix of
log measurements, the relative magnitudes of the coefficients can often
indicate whether the component contains shape information as well as size
information (145). Although the first principal component often has been
designated as a general size factor, it usually contains an unknown amount of
allometrically related shape variation (68, 93, 140) and interpretation of the
second component as shape alone is unwise (110, 190). A solution to the
problem of the study of shape independently of size is to study shape directly,
as either ratios or proportions, expressed as the differences between the
logarithms of distances. Of course the proper mathematical treatment of shape
variables requires great care, but the direct study of shape variables should
play a central role in morphometric analyses.

The study of allometry, the covariation of size and shape rather than of size
and size-free shape or shape orthogonal to size, has been emphasized by
Mosimann (140). He shows that, if biologically reasonable size and shape
variables can be defined a priori, and if the data can be assumed to be
lognormally distributed, substantial mathematical theory is available for
morphometric studies. The lognormal assumption can be tested (110). Log
transformations do not always equalize variances (30), but equal variances
among measurements are by no means required for morphometric analysis
(143). Thus shape variables, which are dimensionless ratios or proportions
expressed as differences between logarithms, can be analyzed directly with
either univariate or multivariate methods (144, 145). In a particularly interest­
ing example, Darroch & Mosimann (49) study shape directly in a reanalysis
of Anderson’s classic data set for measurements of the flowers of three
species of iris, originally analyzed by R. A. Fisher. The species are well
Table 3  Objectives and limitations of the 12 multivariate procedures used most commonly in ecology and systematics, with references.

<table>
<thead>
<tr>
<th>Procedure</th>
<th>Objectives and Limitations</th>
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<tbody>
<tr>
<td>1. Multiple Regression (MR)</td>
<td>Objectives:</td>
</tr>
<tr>
<td></td>
<td>1. To predict one variable (Y, response variable) from others (X’s, explanatory variables)</td>
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<td></td>
<td>2. To investigate the association of an X variable with the Y variable in the presence of other variables</td>
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<td></td>
<td>3. If causal models are appropriate (usually with experiments), to investigate cause and effect</td>
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<tr>
<td></td>
<td>Limitations:</td>
</tr>
<tr>
<td></td>
<td>1. Good predictability alone does not allow inference of causation.</td>
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<td></td>
<td>2. Prediction should be carried out only in situations similar to those in which the model was derived.</td>
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<td></td>
<td>3. Stepwise regression is usually inappropriate.</td>
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<td></td>
<td>4. The procedure considers only linear functions of those X variables analyzed.</td>
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<td></td>
<td>5. The procedure is intended for continuous Y variables whose values are independent; errors should be normal and sampling random for statistical inference.</td>
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<tr>
<td></td>
<td>References: 4, 139, 150, 215</td>
</tr>
<tr>
<td>2. Multivariate Analysis of Variance (MANOVA)</td>
<td>Objective:</td>
</tr>
<tr>
<td></td>
<td>1. To test for differences among two or more groups of objects according to the means of all the variables (attributes); mainly an inferential method</td>
</tr>
<tr>
<td></td>
<td>Limitation:</td>
</tr>
<tr>
<td></td>
<td>1. The procedure is intended for continuous, multivariate normal data; each vector of observations must be independent.</td>
</tr>
<tr>
<td></td>
<td>References: 85, 89, 109, 128, 148</td>
</tr>
<tr>
<td>3. Linear Discriminant Function Analysis (LDFA)</td>
<td>Objectives:</td>
</tr>
<tr>
<td></td>
<td>1. To describe multigroup situations; finds linear combinations of variables (attributes) with maximal ability to discriminate groups of objects; when used to reduce the dimensions of data, called canonical variates analysis</td>
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<td></td>
<td>2. A linear discriminant function (equation) can be used to classify current observations or to allocate new observations to the groups</td>
</tr>
<tr>
<td></td>
<td>Limitations:</td>
</tr>
<tr>
<td></td>
<td>1. The procedure is intended mainly for continuous data; it is inefficient for data not well summarized by variances and covariances.</td>
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<tr>
<td></td>
<td>2. With linear discriminant functions, the researcher assumes equal variance-covariance matrices (identical orientation and size of concentration ellipses).</td>
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<tr>
<td>Procedure</td>
<td>Objectives and Limitations</td>
</tr>
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<tr>
<td>3. Only linear combinations of the variables are considered, so the analysis will not discover nonlinear combinations.</td>
<td></td>
</tr>
<tr>
<td>4. Groups must be defined a priori.</td>
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</tbody>
</table>

**References:** 89, 109, 148, 220

4. **Principal Components Analysis (PCA)**

**Objectives:**
1. To describe a matrix of data consisting of objects and attributes by reducing its dimensions, usually for graphical display; to fit uncorrelated linear combinations of the original variables (attributes) with maximal variance.
2. To suggest new combined variables for further study.

**Limitations (see text):**
1. The procedure is intended mainly for continuous data; it is inefficient for data not well summarized by variances or covariances.
2. The procedure considers only linear combinations of the variables, so it will not discover nonlinear combinations.

**References:** 53, 89, 109, 148, 159

5. **Principal Coordinates Analysis (PCO)**

**Objective:**
1. To describe the data by reducing the dimensions of a distance matrix among objects, usually for graphical display; a generalization of PCA in which non-Euclidean distances are used.

**Limitations:**
1. Results depend on the distance measure chosen.
2. The procedure produces a new coordinate system but cannot indicate combinations of variables (attributes), because only the distance matrix among objects is used.

**References:** 53, 148, 159

6. **Factor Analysis (FA)**

**Objectives:**
1. To reproduce a correlation matrix among original variables by hypothesizing the existence of one or more underlying factors.
2. To discover underlying structure in a data set by interpreting the factors.

**Limitations:**
1. Exploratory factor analysis methods are so unstructured that interpretations are subjective.
2. The procedure is inefficient for data not well summarized by correlations, so it is not ideal for nonlinear relationships in categorical data.

**References:** 54, 89, 109, 148
7. Canonical Correlation (CANCOR)

**Objective:**
1. To analyze the correlation between two groups of variables (attributes) about the same set of objects simultaneously, rather than calculating pairwise correlations

**Limitation:**
1. The procedure is inefficient for data not well summarized by correlations or linear combinations, so not ideal for nonlinear relationships or categorical data.

**References:** 54, 89, 109, 148

8. Multiple Logistic Regression (MLR)

**Objectives:**
1. To model a dichotomous (0,1) variable (Y, response variable) as a function of other categorical or continuous variables (X’s, explanatory variables), which may be categorical or continuous
2. To investigate the association of an X variable with the Y variable in the presence of other X variables
3. If causal models are appropriate (usually with experiments), to investigate cause and effect
4. To serve as an alternative to two group linear discriminant function analysis when the variables are categorical or otherwise not appropriate for DFA

**Limitations:**
1. Good predictability alone does not allow inference of causation.
2. Stepwise logistic regression is usually inappropriate.
3. The procedure considers only linear functions of those X variables analyzed.
4. Prediction should be carried out only in situations similar to those in which the model was estimated.

**References:** 64, 148

9. Loglinear Models (LOGL)

**Objective:**
1. To investigate the joint relationships among categorical variables

**Limitations:**
1. Variables must be categorical or made to be categorical.
2. When there are response and explanatory variables, techniques like logistic regression may be more appropriate.

**References:** 64, 148

10. Correspondence Analysis (COA)

**Objectives:**
1. To describe data consisting of counts by reducing the number of dimensions, usually for graphical display
2. To suggest new combined variables for further study
Table 3  (Continued)

<table>
<thead>
<tr>
<th>Procedure</th>
<th>Objectives and Limitations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Limitations:</td>
<td></td>
</tr>
<tr>
<td>1. The procedure is inefficient for data that are not counts because they will not be well described by chi square distances.</td>
<td></td>
</tr>
<tr>
<td>2. The procedure is not suitable for nonlinear data; it will not discover nonlinear relationships.</td>
<td></td>
</tr>
<tr>
<td>References: 81, 120, 159</td>
<td></td>
</tr>
<tr>
<td>11. Nonmetric Multidimensional Scaling (NMDS)</td>
<td>Objective:</td>
</tr>
<tr>
<td>Objective:</td>
<td></td>
</tr>
<tr>
<td>1. To describe data by reducing the number of dimensions, usually for graphical display; to discover nonlinear relationships</td>
<td></td>
</tr>
<tr>
<td>Limitation:</td>
<td></td>
</tr>
<tr>
<td>1. The procedure uses rank order information only.</td>
<td></td>
</tr>
<tr>
<td>References: 53, 54, 116, 148</td>
<td></td>
</tr>
<tr>
<td>12. Cluster Analysis (CLUS)</td>
<td>Objectives:</td>
</tr>
<tr>
<td>Objective:</td>
<td></td>
</tr>
<tr>
<td>1. To classify groups of objects judged to be similar according to distance or similarity measure</td>
<td></td>
</tr>
<tr>
<td>2. To reduce consideration of ( n ) objects to ( g ) (( g ) less than ( n )) group of objects</td>
<td></td>
</tr>
<tr>
<td>Limitations:</td>
<td></td>
</tr>
<tr>
<td>1. Results depend on the distance measure chosen.</td>
<td></td>
</tr>
<tr>
<td>2. Results depend on the algorithm chosen for forming clusters</td>
<td></td>
</tr>
<tr>
<td>References: 53, 54, 75, 148, 159</td>
<td></td>
</tr>
</tbody>
</table>

discriminated by shape alone. Although these methods were developed for morphometric studies, they are applicable in other situations (e.g. 22). We think that authors who have objected to the direct use of ratios in morphometric studies (3, 9–11, 101, 160, 164, 199) have been overlooking some powerful techniques for the direct study of shape and its covariation with size.

**CONCLUSIONS**

Ecologists and systematists need multivariate analysis to study the joint relationships of variables. That the methods are primarily descriptive in nature is not necessarily a disadvantage. Statistical inference may be possible, but, as with univariate analysis, without experiments even the most insightful applications can only hint at roles, processes, causes, influences, and strategies. When experiments are not feasible, quasiexperimental designs, which involve paired comparisons or time-series analysis, may be able to provide weak inferences about causes. As with univariate work, statistical inference (tests and \( p \)-values) should be reported only if a probability sample is taken.
from a well-defined larger population and if assumptions of the methods are met. Interpretations of multivariate analyses should be restricted to the joint relationships of variables, and stepwise procedures should be avoided.

We did not expect our review to have such a negative flavor, but we are forced to agree in part with the criticism that multivariate methods have opened a Pandora’s box. The problem is at least partly attributable to a history of cavalier applications and interpretations. We do not think that the methods are a panacea for data analysts, but we believe that sensitive applications combined with focus on natural biological units, modelling, and an experimental approach to the analysis of causes would be a step forward. In morphometrics, few workers are taking advantage of some precise mathematical methods for the definition of size and shape and their covariation.

ACKNOWLEDGMENTS
We thank D. Burr-Doss, F. R. Gelbach, J. Rhymer, L. Marcus, L. E. Moses, R. F. Johnston, H. F. James, J. E. Mosimann, P. Frank, D. H. Johnson, J. Travis, and F. J. Rohlf for comments on various drafts of the manuscript.

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