

Chapter 2

Exploratory Multivariate Techniques and Their Utility for Understanding Ancient Ecosystems

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Abstract Elucidating the ecology and evolution of the early biosphere is a critical area of research in geobiology. Indeed, the number of described species and data sets from early ecosystems has increased rapidly in the last few decades. Such data-sets lend themselves well to more complex multivariate analyses. The purpose of this contribution is to serve as a primer for commonly used multivariate ordinations. I review data characterization, as it is critical to selecting the proper ordination. Then I discuss principal components analysis, principal coordinates analysis, non-metric multidimensional scaling, detrended correspondence analysis, and canonical variate analysis. For each ordination I discuss the purpose of the procedure, how it manipulates the data, which types of data are appropriate, and examples of how these procedures have been used to better understand the ecology and evolution of ancient life.

Keywords Multivariate Ordinations • Proterozoic • Ecology • Evolution

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2.1 Introduction

Let us begin with a consideration of the most commonly applied dichotomy to the history of life, those histories before and after the dramatic events of the Early Cambrian. People have considered the Phanerozoic (>540 mya) fossil record for hundreds of years (albeit sometimes in ways very different from the way many view it today (da Vinci 1939) owing to the broad geographic coverage of Phanerozoic-aged fossil-bearing rocks, the conspicuous size of many Phanerozoic fossils, and because Phanerozoic fossils are often quite similar to modern organisms. Indeed, vast amounts of data are available for this latest chapter in the history of life in the published literature and in large databases from which workers have gleaned much about macroevolutionary and macroecological patterns and processes (Alroy et al. 2008, 2001; Bambach 1983; Bambach et al. 2007; Boyce 2005; Briggs et al. 1992; Foote 1995; Huntley and Kowalewski 2007; Jablonski 1993; Jernvall et al. 1996; Madin et al. 2006; Payne et al. 2009; Raup 1972; Sepkoski et al. 1981; Thomas et al. 2000).

Our rich knowledge of the Phanerozoic has often been contrasted with that of older Eons (Proterozoic and Archean, or collectively with the Hadean known informally as the Precambrian). This apparent discrepancy was of course a thorn in the side of Darwin when he considered the seemingly rapid appearance of so many phyla, given that nothing was known at the time about fossils in older strata. Large and complex organisms seemed to appear very rapidly with no precursors, and geologists set out to address this issue. The seeds of Precambrian paleontology were sown from the 1860s through the early decades of the twentieth century (not without mistakes and setbacks), though it was not until the 1960s that the search for knowledge of early life began to produce fruit (Schopf 2000, 2009). The decades since have been witness to a rapid growth in the amount of data pertaining to the evolution and ecology of early life.

A cursory survey of the published literature through the Science Citation Index Expanded database reveals that Precambrian paleontology is indeed a vital and thriving discipline and confirms Schopf's (2000) assertion of rapid growth. A search of research articles using the keywords "Fossils" and "Precambrian" demonstrates that there has been a dramatic increase during the past 20 years in our knowledge of Precambrian life and early ecosystems (Fig. 2.1a, b). Searches utilizing proper, and higher-resolution, geochronological terms (Archean, Paleoproterozoic, Mesoproterozoic, and Neoproterozoic) reveal similar patterns of rapid growth, though with few pre-1990 citations (Fig. 2.1c). This discrepancy is likely an artifact of recent advances in geochronological methods producing higher resolution correlations. It should also be noted that though the SCIE database contains references back to 1900 it has the most complete coverage from 1990 to present; however the post-1990 increase in publication activity should not be interpreted as a spurious result of a biased database. The amount of literature published for each Era (as well as for the lone Eon, Archean) increased over the last 20 years. The rate of increase seems to be greatest for the youngest Era, the Neoproterozoic. Older Eras seem to

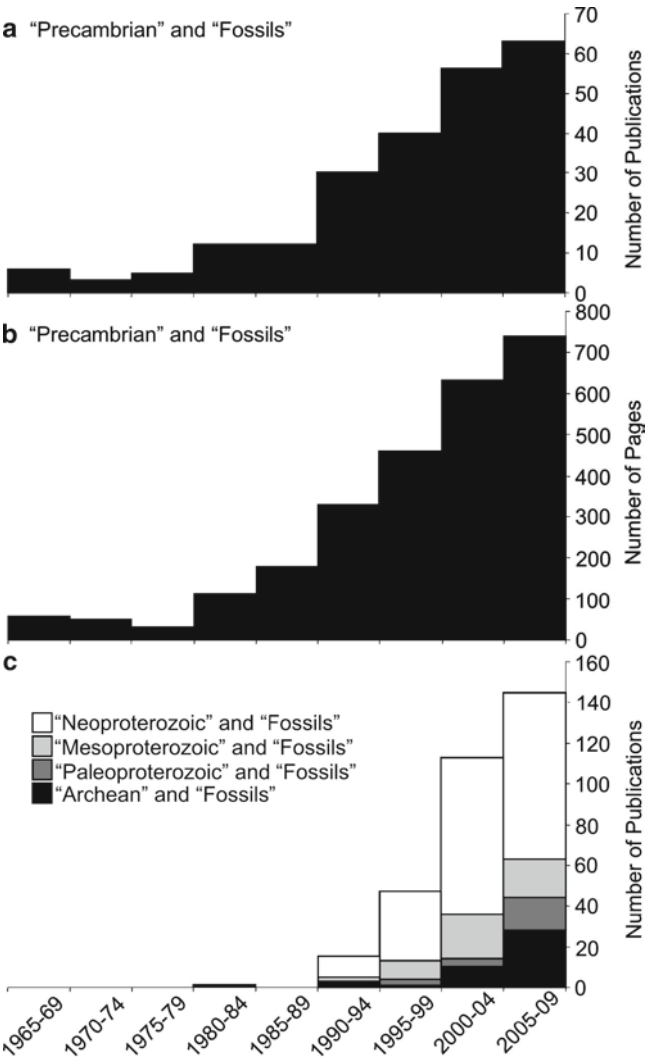


Fig. 2.1 Time series results from Science Citation Index Expanded database search for article citations between 1900 and present. (a) Number of articles published with the topics “Precambrian” and “Fossils”. (b) Number of pages published with the topics “Precambrian” and “Fossils”. (c) Number of articles published with the following sets of topics: “Archean” and “Fossils”, “Paleoproterozoic” and “Fossils”, “Mesoproterozoic” and “Fossils”, and “Neoproterozoic” and “Fossils”. Database accessed on 19 Sept 2009

display less dramatic growth. This pattern could be driven by the relative amount rock available from each Era. The notable exception, of course, is the Archean. Though there are fewer Archean rocks, the prospect of finding evidence of the oldest life is indeed tempting and perhaps attracts more researchers per unit rock than other times in the Precambrian.

Given the dramatic growth in our knowledge of early life, large paleobiological datasets are now becoming more common and it is even possible to conduct “big picture” analyses of macroevolution and macroecology in the Precambrian. These datasets contain many important attributes: presence/absence or abundance counts of species, presence/absence of morphological traits among species, mode of fossil preservation, taphonomic indices, environmental indicators from lithologic data and geochemical proxies, paleolatitude and paleogeographic reconstruction data, etc. Such datasets can be built from both original field and laboratory work as well as constructed through data collection from the published literature.

The purpose of this chapter is to provide an introduction to a few of the more common exploratory multivariate ordination techniques that might be particularly useful for the investigation of Precambrian life. These methods are useful for simplifying multidimensional datasets and for clarifying the relationships among large set of variables. Among many other uses, they can be used to elucidate community or paleobiogeographical structure, construct an empirical morphospace, aid in detecting extinction selectivity and recovery dynamics, recognize subtle shifts in morphology, and identify changing taxonomic composition of samples along one or more environmental gradients. It should be pointed out that these methods are not confirmatory in that one cannot use them by themselves to test a null hypothesis of significant differences among the samples or variables under investigation. They are fundamentally exploratory in nature, but can nevertheless produce outcomes that can then be used in non-parametric and parametric confirmatory statistical testing.

2.2 Characterization of Data

Following the terminology described in Sokal and Rohlf (1994) let us first define and describe a few terms. Data (singular: datum) are comprised of observations or measurements on the smallest sampling unit. These sampling units can include such objects as individual fossils, collections of fossils, thin sections, rock hand-samples, individual mineral grains, etc. Multiple observations or measurements, termed variables or characters, can be taken from each smallest sampling unit. Such variables could include species names, morphological characters, size data, taphonomic scores, mode of preservation, mineral identification, roundness of sediment grains, paleocurrent direction, stable isotope ratios, etc.

These observations and measurements are taken from a subset, or sample, of the total number of observations existing anywhere within space or time, or the population. For instance, there are likely many billions of acritarchs in Mesoproterozoic-aged rocks on Earth. The totality of these acritarchs makes up the population (or sampling universe). Clearly it is not feasible, nor advisable, to collect and observe all of these acritarchs; therefore, a sample of a few tens of thousands of individuals from various workers will have to suffice for characterizing acritarchs during the Mesoproterozoic. This is a primary function of statistical methods; to analyze samples and make meaningful statements with some degree of certainty

about the population. Were we able to observe the population of Mesoproterozoic acritarchs, we would have no need for confirmatory statistical tests since we would know with 100% certainty the descriptive statistics (e.g., mean, median, mode, skewness, kurtosis, etc.) of any variable we may choose.

Variables can be classified into several different categories. It is important to be aware of the specific nature of the variables in your dataset as these may govern which ordination should be used. As is common with classification schemes there are various approaches for categorizing types of variables (Stevens 1946, though see Velleman and Wilkinson 1993; Sokal and Rohlf 1994; Reyment 1991). I will not discuss at length the arguments and multiple points of view; rather I will adopt the scheme that is in my opinion the most suitable for the investigation of early life and ecosystems. To quote Stevens (1946) from his landmark paper on the topic, “Any particular scale, sensory or physical, may be objected to on the grounds of bias, low precision, restricted generality, and other factors, but the objector should remember that these are relative and practical matters and that no scale used by mortals is perfectly free of their taint” (1946, p. 680). We will consider four main categories of variables: measurement, ranked, attributes, and derived.

By definition, **measurement variables** are expressed in a numerically ordered fashion (Sokal and Rohlf 1994). We can further sub-divide these variables based on continuity and the nature of zero in the scale. Theoretically, there is an infinite number of potential values between any two fixed points in the case of *continuous variables* (Sokal and Rohlf 1994). The width of an acritarch vesicle is an example of a continuous variable. Practically, it is impossible to obtain the true value of continuous variables. Our measurements must serve as an approximation of the true value. To return to our acritarch example, we may measure a vesicle diameter of 15 μm under a light microscope. This is a reasonable approximation of acritarch size, but we would have more precision by measuring the acritarch under an SEM, perhaps obtaining a value of 15.015 μm . Since there is an infinite number of possibilities between two points along the continuous variable scale, our accuracy is in part a function of our chosen methodology for data collection. One must make trade-offs between accuracy and resources (such as time and money) to determine what is necessary to collect the data needed for the question at hand. *Discontinuous variables* (also known as discrete or meristic) are expressed as whole numbers; values between these whole numbers are not possible (Sokal and Rohlf 1994). The number of individual *Chuar*ia vesicles on a bedding plane or the number of quartz grains from a thin-section point count are examples of discontinuous variables. The accuracy of this type of measure is contingent upon our ability to count, and not necessarily by the accuracy of calipers or other instruments, as would be the case for continuous variables. We can also characterize measurement variables by the nature of zero in the scale. *Ratio scale* measurements have a constant interval size as well as a true zero. For example, a measure of temperature in degrees Kelvin is a ratio scale measure. The difference between 1 and 2 K is the same as the difference between 240 and 241 K. In addition 0 K is a true value of zero. *Interval scale* measurements also have a constant interval size, but do not have a true zero. A corresponding example is measuring temperature in degrees centigrade. The difference

between 1°C and 2°C is the same as 240°C and 241°C. However, 0°C is an arbitrary zero value as negative values in degrees C are possible. Time of day and directional data (e.g. N 20° E) are also examples of interval scale data as they have zeros with arbitrary values.

Ranked variables cannot be measured *per se*, but are ranked in a meaningful order. The difference between two adjacent ranks is not necessarily equal or proportional to the difference between two other adjacent ranks on this type of scale. A ranking scheme wherein the quality of preservation of a fossil specimen is ranked is an example of a ranked variable. With such a ranking scheme, low values might represent low taphonomic alteration and high values represent high alteration. These scores are quantitatively meaningful inasmuch as they indicate relative values along a qualitative scale. Another example of a ranked variable is Moh's scale of hardness. Moh's scale is based on the relative hardness of specific minerals, though the differences between adjacent ranks are not necessarily equal.

Attribute variables cannot be measured. Coding in a database for such variables is an attempt to quantify qualities for the sake of data analysis. Examples of attribute variables are colors (e.g., red=0, blue=1, yellow=2, etc.), differing growth forms (e.g., as a result of sexual dimorphism or ecophenotypic plasticity), or species, etc.

Derived variables are based on two or more independently-measured variables. These are often expressed as ratios, percentages, and rates. Care should be taken when using derived variables. Much of the time derived variables can be considered redundant and should not be used in multivariate ordinations if one or more of their parent variables are also included in the ordination. If the parent variables are not included in the ordination, one should take care to properly transform the variable prior to analysis (e.g., logit-transformation for proportional data; this transformation is used because proportional data are typically not normally distributed and are bounded by the values of 0 and 1).

2.3 Common Multivariate Ordinations

The following sections will review various multivariate ordinations including Principal Components Analysis, Principal Coordinates Analysis, Non-metric Multidimensional Scaling, Detrended Correspondence Analysis, and Canonical Variate Analysis. These methods differ in purpose and in the types of data required for their proper use. The purpose and data requirements for each method are outlined in each section.

2.3.1 *Principal Components Analysis*

Principal components analysis (PCA) is one of the most commonly used ordinations for projecting the hyperspace of many variables to two or three dimensions.

PCA calculates new “hypothetical” variables or principal components as combinations of the original variables; therefore each observation is assigned a principal component score (PC score) for each of the newly-derived principal components. The scales on principal component axes are unit-less, but can be related to the original variables.

PCA works by extracting eigenvectors and eigenvalues from a matrix of variance–covariance (or correlation) values among the variables in a given data set. Principal components are defined by a linear equation based on the original variables. The coefficients for each original variable in this linear equation are called *eigenvectors* or *loadings*. Therefore each principal component will be defined as some combination of all the original variables through a simple linear equation. The magnitude of the eigenvector (whether positive or negative) will serve as a quick reference as to the importance of different variables in a particular principal component. These equations can also be used to calculate the principal component scores for each observation (Reyment 1991; Hammer and Harper 2006). The PCA ordination will also produce a measure of the variance for each principal component called an *eigenvalue* or *latent root*. The sum of eigenvalues for all principal components is equal to the variance amongst the original variables. By dividing the eigenvalue for a given principal component by this sum we can determine the relative amount of variance explained by that principal component (Reyment 1991; Hammer and Harper 2006). The matrix algebra involved in PCA is beyond the scope of this contribution, but see Jolliffe (2002) and McCune et al. (2002) for more specific descriptions of the procedure.

PCA essentially identifies the direction of maximum variance in the multivariate hyperspace of the data set. A commonly used visual depiction of PCA posits that once the axis of maximum variance is identified the data undergo an orthogonal rotation wherein the distances between the data points in the hyperspace are preserved. This image is useful for understanding the end result of PCA, but is not an accurate description of the actual procedure. This axis of maximum variance is known as the first principal component. Additional principal components are identified in the process of the ordination and are all at 90° to one another in the hyperspace. Each subsequent principal component accounts for the majority of the variance unaccounted for by previous principal components. The number of principal components produced by the ordination can, in theory, be equal to the number of original variables. The expectation in a highly structured data set is that the large majority of the variance will be accounted for with the first few axes.

The data matrix should be constructed such that observations occupy rows and variables occupy columns (as it should for all ordinations). A proper use of PCA requires continuous measurement variables (though Jolliffe (2002) relaxes this assumption when it is used as a purely descriptive technique) and more observations than variables. Interpretation of PCA works best when the dataset displays a multivariate normal distribution. There should be some correlation amongst the variables for PCA to be useful. If none of the variables are correlated, then the data hyperspace will take the form of a hypersphere with no possibility of diagnosing a direction of maximum variance.

One must consider the variances of the original variables when performing PCA. Variables with higher variances can artificially dominate the first principal component and confound interpretations. If variables are measured in the same units and have similar variances then the PCA should be performed on the *variance–covariance matrix* (a matrix consisting of covariance values between the original variables). A dataset characterized by variables in different units (e.g., mm² and K) and/or divergent variances (e.g., morphometric measurements of bottlenose dolphins and blue whales) needs to be standardized in order to prevent spurious results. This is accomplished by instead performing PCA on the *correlation matrix* (conversely, a matrix of correlation values between the original variables; Reyment 1991; Hammer and Harper 2006).

I culled data appropriate for PCA from the acritarch meta-analysis reported in Huntley et al. (2006a). The data were collected from the peer-reviewed literature of acritarch occurrences ranging in age from Paleoproterozoic to Cambrian. The original dataset contains a wide variety of variables including body size (continuous variable), presence/absence of 31 morphological characters (attribute variables), and best estimate age of deposition (derived variable from the maximum and minimum age estimates) among others. In this example we will consider the following variables from species descriptions (all in μm): minimum reported vesicle diameter, maximum reported vesicle diameter, process length, and process width. These are continuous variables and there are no missing values. Typically, one should have no missing values for PCA, however some software packages will substitute the mean value of the variable for the missing datum. The data matrix is therefore comprised of four variables and 62 observations (acritarch occurrences) ranging in age from Mesoproterozoic to Cambrian. This analysis is focused on acanthomorphic (process-bearing) acritarchs and overlooks sphaeromorphs. The measurements were log-transformed. Log transformation is important because of the assumption of PCA that variables display a linear relationship with one another; however a pattern of allometric growth (change in shape with growth) is more common. Log transformation will linearize the relationships between body size dimensions. PCA was performed in PAST 1.94b on a variance–covariance matrix (Hammer et al. 2001; Hammer and Harper 2006) (Fig. 2.2).

The eigenvectors for the PCA of acritarch body size data are presented in Table 2.1. These values are the coefficients in the linear equations that define PC scores. For example, to calculate the PC1 score of a particular variable one would solve the following equation: $\text{PC1 score} = (-0.51 * \text{minimum}) + (-0.56 * \text{maximum}) + (-0.40 * \text{process length}) + (-0.51 * \text{process width})$. We can see from the eigenvalues that in this example PC1 accounts for 61.7% of the variance (Table 2.2).

Once the ordination has been performed and the observations have been assigned PC scores, one must determine how many principal components are actually useful. One method for doing so is a qualitative examination of the scree plot, or descending curve plotting the percentage of variance (or log of the eigenvalue may be plotted as well) for each principal component (Fig. 2.2c). The scree plot from the acritarch PCA indicates that most variance is explained by the first three principal components. The curve begins to flatten after the third PC and little explanatory

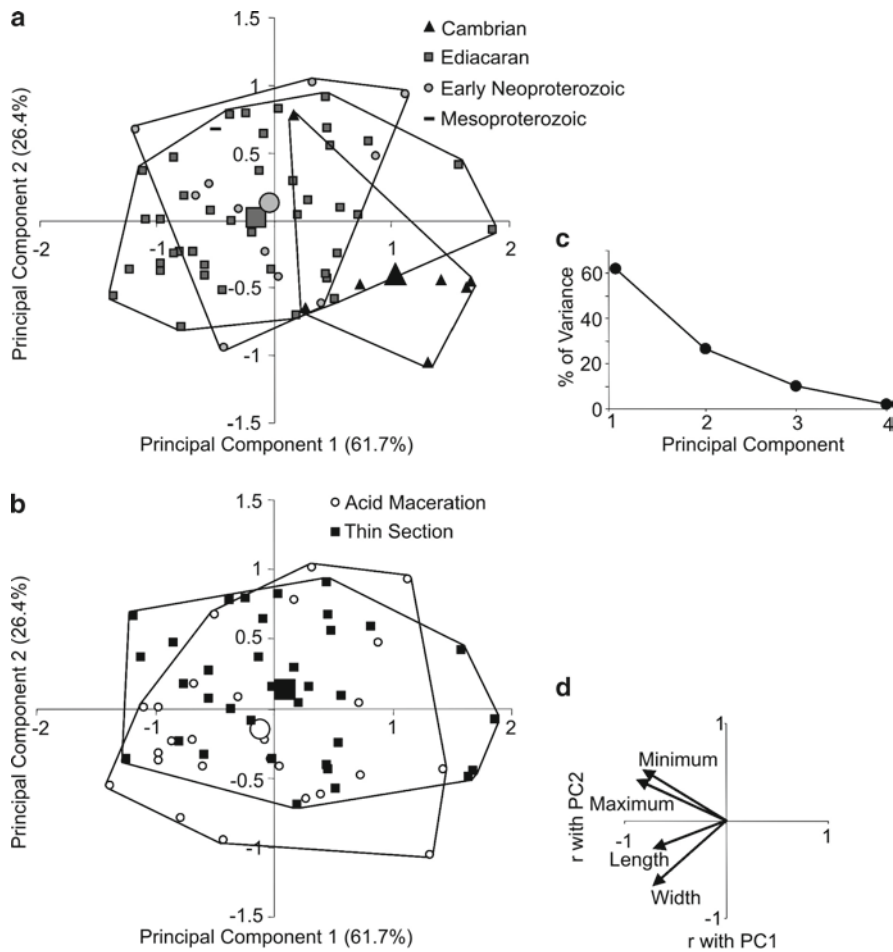


Fig. 2.2 Principal components analysis of acritarch body size metrics. **(a)** Scatter plot of PC1 vs. PC2 with convex hulls classified by age group. **(b)** Scatter plot of PC1 vs. PC2 with convex hulls classified by sample preparation technique. The large symbols in scatter plots **(a)** and **(b)** represent the centroid value for the respective groups. **(c)** Scree plot for percent of variance explained by the principal components. **(d)** Loadings chart for PC1 vs. PC2

Table 2.1 Eigenvectors of PCA of acritarch body size variables				
	Minimum diameter	Maximum diameter	Process length	Process width
PC1	-0.51	-0.56	-0.40	-0.51
PC2	0.49	0.40	-0.23	-0.73
PC3	0.19	0.06	-0.88	0.44
PC4	-0.68	0.72	-0.11	-0.02

Table 2.2 Eigenvalues and percentage of variation explained by the principal components

	Eigenvalue	% Variance
PC1	0.625	61.7
PC2	0.267	26.4
PC3	0.101	9.9
PC4	0.019	2.0

power is likely to be derived (Hammer and Harper 2006). As an alternative method, Reyment (1991) cites an *ad hoc* approach outlined by Jolliffe (1986) based on the following equation: $l^* = 0.7(\Sigma l)/p$ where l is the eigenvalue and p the number of dimensions. In our case $\Sigma l = 1.0127$ (calculated from Table 2.2) and $p = 4$; therefore $l^* = 0.177$. The cut-off eigenvalue of 0.177 falls between the eigenvalues of PC2 and PC3 (Table 2.2), suggesting that only the first two principal components should be considered. See Jolliffe (2002) for an expanded discussion on determining how many to principal components to retain for analysis.

Once the ordination has been completed and we have an idea of how many principal components are potentially interpretable, how shall we actually interpret the results? Loadings charts are useful guides for interpreting the principal component space in terms of the original variables. A loadings chart plots the correlation coefficients between the principal components in question and the original variables. It serves as a qualitative visual guide for interpreting the principal component scatter plot. For example, in Fig. 2.2d we can see that minimum vesicle diameter has an $r = -0.82$ with PC1 and an $r = 0.52$ with PC2 placing the arrow in quadrant I of the loadings chart. Process width, on the other hand, has an $r = -0.71$ with PC1 and an $r = -0.66$ with PC2, locating the arrow in quadrant II of the loadings chart. From the loadings chart we can infer that acritarchs with larger minimum diameters tend to fall toward quadrant I and acritarchs with wider processes tend to fall toward quadrant II. However, there is a more conspicuous pattern that we must first address. All of the original variables are significantly and negatively correlated with PC1. As is often the case, the first principal component is a strong indicator of overall body size (whether by a positive or negative correlation). Indeed, many times PC1 scores are ideal indices of body size as they are derived from many measures of size. In this case, a negative PC1 value indicates larger vesicle diameters and process dimensions while positive PC1 values indicate overall smaller body size. Subsequent principal components are often reflective of differences in shape (PC1 having removed most of the variance related to size). It is possible to remove the factor of body size before using PCA in order to focus primarily on differences in shape (see Chap. 3).

Equipped with an understanding of the relationship between the principal component space and the original variables one can now begin to address important questions. Perhaps we want to know if acritarch size or shape changed through time or if taphonomy and sample preparation techniques can bias size estimates. By classifying the observations by group (e.g., age or sampling technique) we can

identify patterns and potentially test hypotheses through non-parametric or parametric confirmatory statistical techniques. Figure 2.2a presents the results of the PCA with the observations grouped by age and distinguished by convex hulls (a convex polygon which encloses the minimum area required to contain all data points of a given group). The large symbol for each grouping variable represents the centroid, or multivariate mean value. We can see that, on average, Cambrian acanthomorphic acritarchs were smaller (positive PC1 values) than their Precambrian counterparts and, for a given size, had shorter and narrower processes. These assessments can be rigorously tested via non-parametric tests (e.g., bootstrapping (Kowalewski et al. 1998; Efron 1981) and randomization (Huntley et al. 2006a; Huntley et al. 2008)) and parametric tests (e.g., MANOVA) (for more information about hypothesis testing in morphometrics see Chap. 3).

Precambrian acritarchs are typically preserved in one of two ways: compressions in shales or three-dimensional preservation in cherts. These differing modes of preservation necessitate very different modes of sample preparation which can bias estimates of size and morphology. Shale specimens are macerated in HCl, thus dissolving the non-organic content and liberating compressed vesicles. Chert specimens are thin-sectioned to reveal the acritarchs. Thin-sectioning will randomly cut across acritarchs; therefore, one will rarely measure the full diameter of an acritarch, but will, on average, underestimate size. Perhaps, then, we can predict that macerated specimens will display a larger body size and display less variation than thin-section specimens. Figure 2.2b suggests, as reflected by the relative position of the centroids, that acid maceration specimens are, indeed, slightly larger (more negative PC1 score) than thin-section specimens, but *F*- and *t*-tests show that the variance and mean values of size for the two groups are statistically indistinguishable ($p=0.95$ and $p=0.32$, respectively; $\alpha=0.05$). In this limited data set, there is therefore no indication that taphonomy and sample preparation techniques, which are difficult to disentangle in this case, significantly affect our perception of acanthomorphic acritarch body size. Of course one should keep in mind that this is merely a limited example, and not a broad statement about acritarchs in general. A more rigorous study would require one to address other potentially confounding factors such as the exclusion of sphaeromorphs, the age structure of each group, and secular trends in size (Huntley et al. 2006a).

There is much potential for the use of PCA in the study of early life and ecosystems, though primarily for morphometrics of organisms with similar baupläne, given the suggested constraint to continuous variables. Laflamme et al. (2004) applied PCA to clarify the taxonomy of the Ediacaran frond *Charniodiscus*; first in an ordination examining the differences among two species co-occurring on bedding planes in the Mistaken Point Formation of Newfoundland and then in multiple ordinations based on different combinations of variables including global occurrences of the genus (all ordinations confirmed the distinct morphologies of *C. procerus* and *C. spinosus*).

Laflamme et al. (2004) provide a good example of how one should consider principal component scores from different ordinations separately and not mix their results. Principal component scores are derived solely from the original variables in

a given ordination; therefore scores from different ordinations are not comparable. However, the data matrices used in multiple ordinations by Laflamme et al. (2004) were comprised of various combinations of continuous measurement variables (linear body size measurements), a discontinuous measurement variable (number of primary branches in the frond), and an attribute variable (presence/absence of a terminal spine). A principal coordinate analysis (see below) would probably have been a more suitable ordination for this dataset of mixed variable types, but would most likely produce similar results (see Chap. 3).

For more information and discussion about PCA see Hammer and Harper (2006); Jolliffe (2002); Reyment (1991) and references therein. Hammer et al. (2001) provided a very user-friendly and, perhaps just as important, free software called PAST (Paleontological Statistics). This freeware is compatible with Excel spreadsheets and can perform many of the statistical operations commonly used by paleobiologists including PCA. For those interested in having more flexibility in programming their procedures, SAS and R are commonly used software packages. The supplementary information section of Reyment (1991), authored by L.F. Marcus, provides the code for principal components analysis written for SAS. R software, like SAS, is also a highly flexible and powerful platform; however, unlike SAS, R is freeware and available for download at <http://www.r-project.org>.

2.3.2 *Principal Coordinates Analysis*

Principal coordinates analysis (PCO) is another eigen-based method for reducing dimensionality by projecting multidimensional datasets to a smaller number of dimensions. To better understand the difference between PCA and PCO, it is instructive to distinguish *R*-mode analyses from *Q*-mode analyses. *Q*-mode analyses focus on the association between individual observations in a dataset while *R*-mode analyses address the relationships among the variables. PCA is an *R*-mode analysis of a matrix based on similarities (correlation or covariance). PCO is a *Q*-mode ordination based on measures of dissimilarity (with the flexibility to select from a broad family of dissimilarity coefficients, see Hammer and Harper (2006)) (Gower 1966; Reyment 1991). In PCO, the multivariate data do not undergo a rigid rotation (as associated with PCA), but the ordination does aim to preserve the relative distances between data points.

Principal coordinates analysis has less stringent assumptions about the data than PCA. PCO will work with continuous variables, discontinuous variables, ranked variables, attribute variables, or any combination thereof; though there should be no missing values. PCO will sometimes return negative eigenvalues which are typically associated with coordinates which explain very little variance. However, one should be wary of an ordination that produces large numbers of negative eigenvalues (Hammer and Harper 2006). As PCO produces only an estimate of the original distances between points (i.e., similar objects are found closer to one another in the projection), interpreting the ordination in terms of the original variables can be problematic.

However, due to the loosened assumptions about variables in PCO, one has more freedom with the analysis. An empirical morphospace can be produced based on a broader range of characters, and, thus, more dissimilar observations can be included (perhaps organisms of varying baupläne) than in PCA.

Principal coordinates analysis is not one of the more commonly used ordinations in ecology and paleoecology. Wills (1998) coupled PCO with cladistic analyses of modern and Cambrian priapulids to address evolutionary relationships and secular trends in occupied empirical morphospace. Specifically, Wills addressed Gould's assertion (1989) that morphological disparity peaked in the Cambrian and was subsequently greatly reduced. Even though there were more priapulid families in the Cambrian than in the Recent, Wills (1998) found that Recent priapulids actually occupy slightly more morphospace than their Cambrian forbearers. Moreover, the morphospaces occupied by the Cambrian and Recent groups were predominantly adjacent rather than overlapping.

For more information about PCO see Gower (1966), Hammer and Harper (2006), and Reyment (1991). PAST offers users the ability to perform PCO and the freedom to choose from a large number of similarity indices (Hammer et al. 2001; Hammer and Harper 2006). Reyment (1991) provides a SAS code for PCO written by L.F. Marcus. PCO is also sometimes referred to as metric multidimensional scaling (mMDS).

2.3.3 *Non-Metric Multidimensional Scaling*

Non-metric multidimensional scaling (nMDS or MDS) is a numerical technique whose function is to produce a "map" from a dissimilarity index data matrix. Kruskal and Wish (1978) presented the example of performing nMDS on a matrix of distances between ten US cities to produce an ordination that successfully reproduced the relative positions and distances between the cities. nMDS is different from an ordination like PCA where the axis of maximum variance is identified and the data hyperspace is rotated accordingly. nMDS is an iterative process wherein configurations of the data points are produced sequentially with the goal of preserving the original distances between the points. nMDS calculates a stress value for each iteration by comparing the ranked distances between observations in the original data with the ranked distances between nMDS scores from the ordination. Low stress values (~0.10 or less) indicate a close agreement between the ordination and the original data (Hammer and Harper 2006). This procedure runs until it reaches a minimum stress value. As nMDS is an iterative mathematical technique, multiple runs of this procedure will produce multiple results with differing stress values. I will borrow an illustration of nMDS from Kruskal and Wish (1978). One can imagine a landscape with hills and valleys that represents an infinite number of solutions for the nMDS procedure. The vertical dimension, or elevation, of this landscape represents the stress value. Hills represent solutions with high stress values and valleys represent low stress solutions. The nMDS procedure is like a sky

diver who parachutes onto a random point in the landscape; this point represents the initial solution of the nMDS. The sky diver's goal is to reach the lowest point in the landscape, so she begins to walk down slope. With each step the sky diver finds herself at a lower elevation; in the same way each iteration of the nMDS produces a solution with a lower stress value. As this landscape could potentially have multiple hills and valleys, a single nMDS procedure could settle in a local minimum and not the global minimum (the lowest point in the landscape). For this reason software packages will often perform multiple runs of the nMDS procedure with different starting configurations to maximize the likelihood of approaching the global minimum. Moreover, the stress of an nMDS can vary based on the number of dimensions to which the data are reduced. This is another difference between nMDS and PCA. One defines the number of dimensions to which the data are reduced *a priori* with nMDS while the number of dimensions produced in PCA is a function of the number of variables. It is important to examine the effect of the number of dimensions on stress value. Some software packages do this automatically while others require the user to define the number of dimensions. Shepard plots are visual guides for conveying the amount of stress in an nMDS solution. These scatter plots compare the ranked distances between each data point from the original data matrix with the ranked distances between each point from the ordination. A perfect linear correlation indicates zero stress and lower r values indicate higher stress (Fig. 2.3).

Similar to PCO, interpreting nMDS axes in relation to the original variables can be problematic as the ordination axes do not necessarily correspond to the maximal directions of variance and are not likely to be orthogonal to one another. One can subject the nMDS scores to a PCA (as the nMDS scores are continuous variables) to sidestep this problem.

nMDS is commonly used in paleoecological studies and is well-suited to the vicissitudes of data collection from the fossil record. One can use any combination of continuous, discontinuous, ranked, and/or attribute variables with nMDS which also accommodates missing observations in the data matrix. Let us continue to use the acritarch body size data from the PCA example for nMDS. I subjected the four log-transformed body size variables to nMDS using PAST 1.94b with a Euclidian similarity measure (Hammer et al. 2001). PAST gives the option to reduce the data to either two or three dimensions while other software packages have different options. PC-ORD automatically calculates solutions for one to six dimensions (McCune and Mefford 2006) and SAS allows the user to define the number of dimensions (see Huntley et al. (2006b) for a SAS code for nMDS). PAST reported a stress value of 0.098 for the two-dimensional ordination and a stress value of 0.024 for the three-dimensional ordination. These stress values are quite low and indicate that both ordinations were successful in reconstructing the dissimilarities between the variables in the original data. Such low stress values are not surprising because we are considering a small number of continuous variables. One might not necessarily expect stress values this low with larger and more complicated data matrices of mixed variable types. Due to its lower stress value, let us continue the example with the ordination of three dimensions. The distribution of nMDS scores appears similar to the PC scores in Fig. 2.2 when categorized by age (Fig. 2.3a). The tight distribution

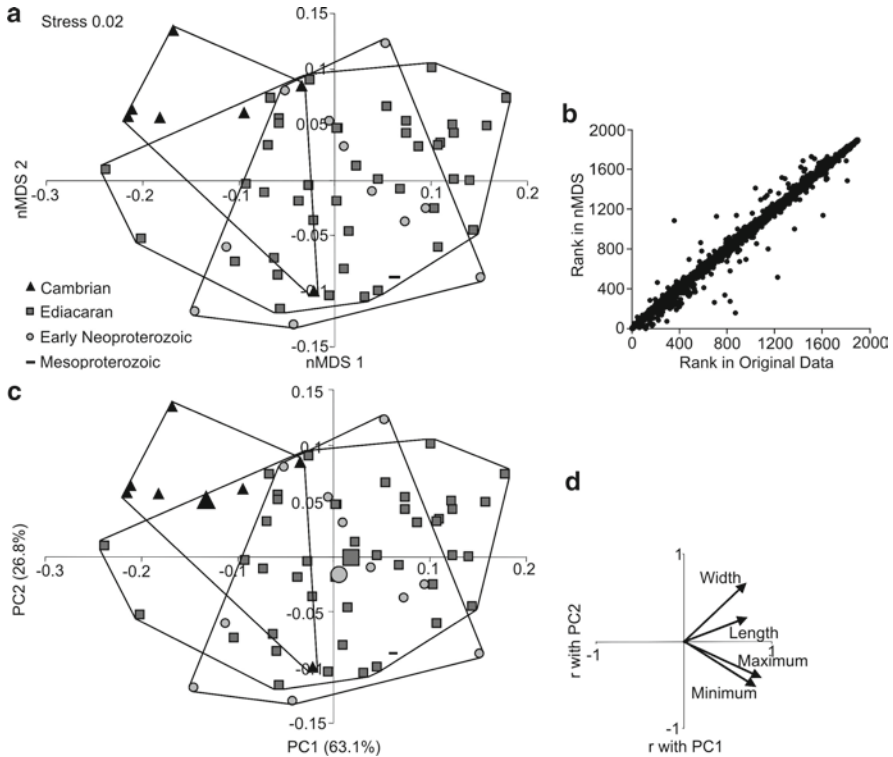


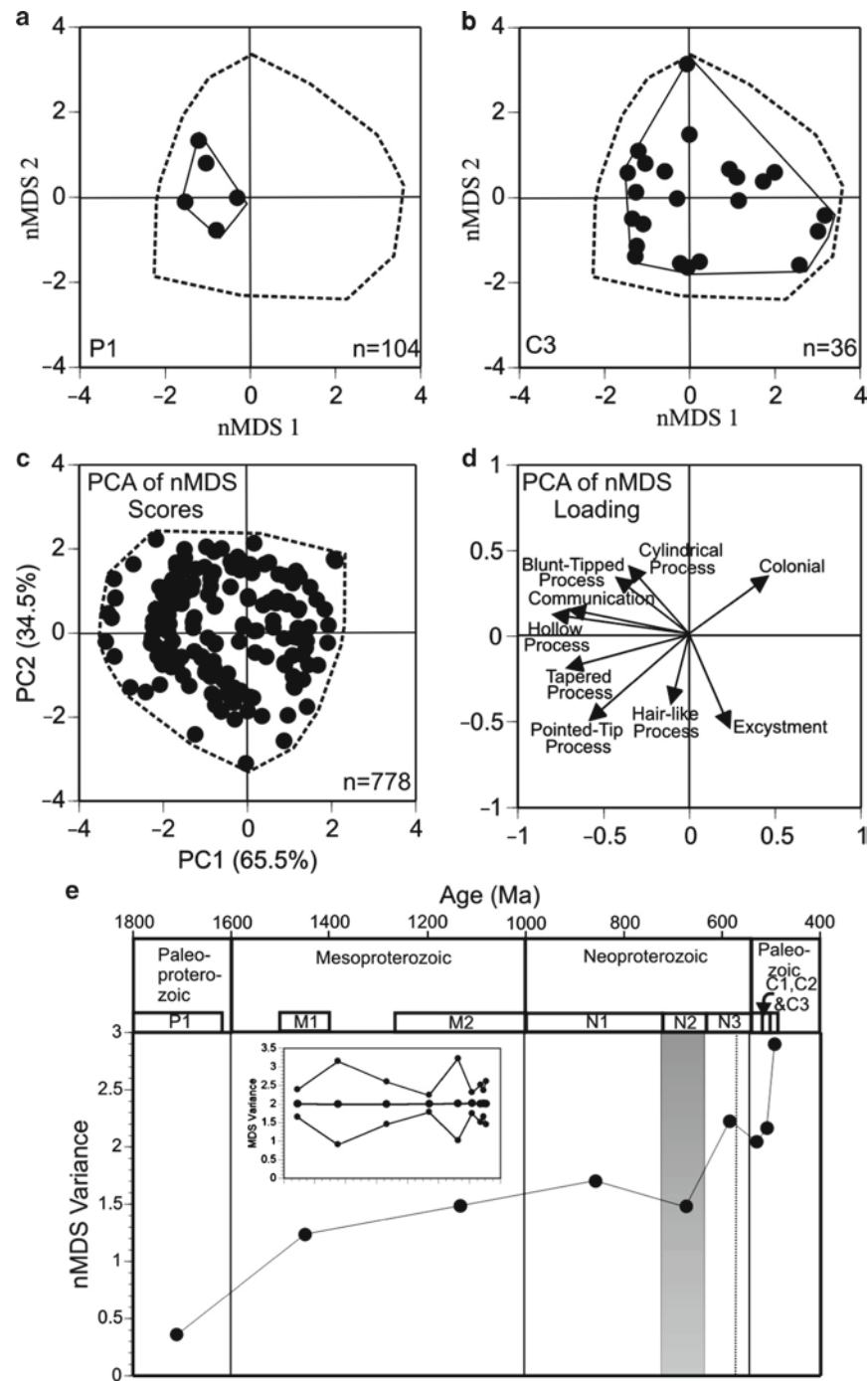
Fig. 2.3 Non-metric multidimensional scaling of acritarch body size metrics (scaled to three dimensions). (a) Scatter plot of nMDS1 vs. nMDS2 with convex hulls classified by age group. (b) Shepard plot for the nMDS ordination. The close association of data points with the line $x=y$ indicates that there is a high agreement between the distances between observations in the original data set and the distances between observations in the ordination. This close association indicates a low stress value. (c) Results of PCA of nMDS scores (MDS1, MDS2, and MDS3): scatter plot of PC1 vs. PC2 with convex hulls classified by age group. Though similar in appearance, the nMDS values were slightly rotated by the PCA. Note how these PCA results are nearly a mirror image of those in Fig. 2.2a; though PC1 and PC2 explain slightly more variation in Fig. 2.3c than in Fig. 2.2. (d) Loadings chart for PC1 vs. PC2

of points about the $x=y$ line in the Shepard plot confirms the low stress value (Fig. 2.3b). One should be suspect of ordinations with high stress values, but the stress values in this example are low and we can proceed with the assumption that the ordination accurately describes the data. As discussed earlier, one should not relate nMDS scores to the original variables; rather one should first subject the continuous nMDS scores to a principal components analysis and then proceed with interpreting the ordination space (see below for a broader example from my own work). One can see that the PCA results (Fig. 2.3c) are quite similar to the nMDS ordination (Fig. 2.3a). Though they appear identical, the PCA did rotate the nMDS values slightly. Using the loadings chart as a guide (Fig. 2.3d) we can interpret the morphospace and draw conclusions that are similar to the PCA example (Fig. 2.2).

Keep in mind that in this example the data are rather simple with four continuous variables and we might expect similar results between the two ordination types. PCA would be the preferred ordination for a data set composed of continuous variables (since it does not distort the distances between the data points); however I use these data in this example for the sake of continuity. nMDS proves its utility when one has a large number of variables of different types as we will see in the following examples from the published literature.

Huntley et al. (2006a) utilized nMDS to construct an empirical morphospace of Proterozoic- through Cambrian-aged acritarchs to elucidate the morphological history of this group, which is wrought with taxonomic inconsistencies. Their global acritarch database was compiled from the published literature and was composed of 778 species occurrences coded for the presence or absence of 31 morphological characters. Huntley et al. conducted a two-dimensional nMDS in SAS 9.1, classified the observations by age bin *a posteriori*, and calculated the variance of nMDS scores for each age bin as a measure of morphological disparity (Fig. 2.4). They further refined these results by performing a randomization to determine the range of temporal trends in nMDS variance likely to occur due to random chance, revealing a significant increase in morphological disparity through time (Fig. 2.4). Huntley et al. (2006) also subjected the nMDS scores to a PCA to interpret the scores in terms of the original variables. The PCA scatter plot is essentially a mirror image of the nMDS scatter plot. The dramatic expansions in occupied morphospace between the Paleoproterozoic and middle/late Cambrian is primarily driven by the diversification(s) of process-bearing acritarchs (Fig. 2.4a–d). This approach enabled Huntley et al. (2006) to address questions in a way not possible with a purely taxic approach. They concluded that the first major expansion of occupied morphospace preceded the first burst of taxic diversity by a half billion years (a pattern common amongst many Phanerozoic eukaryotes) and the occupation of morphospace through time was broadly correlated with major geological and biological events such as Snowball Earth, the first appearance of the large Ediacara organisms, and the Cambrian Explosion.

Fig. 2.4 nMDS of Paleoproterozoic- to Cambrian-aged acritarchs. (a) Occupied morphospace in the Paleoproterozoic. (b) Occupied morphospace in the middle and late Cambrian. (c) PCA of nMDS scores for all species occurrences. (d) Loadings chart for PC1 vs. PC2 of nMDS scores. (e) Temporal trend of nMDS variance (variance of nMDS1 plus variance of nMDS2). Inset is result of 1,000 iteration randomization of nMDS variation. The *center line* represents the mean value of randomization for each bin, and the *upper* and *lower lines* represent the 95% confidence intervals. nMDS variance values which fall outside the confidence intervals display either higher or lower morphological disparity than expected by random chance. Huntley et al. (2006) interpreted the overall trend as displaying a significant increase in morphological disparity. The *dashed lines* in (a–c) represent the convex hull of the total realized morphospace of all acritarchs considered in the study. The *vertical dashed line* in (e) represents the first occurrence of Ediacara organisms (Modified from Huntley et al. (2006))



Xiao and Dong (2006) coupled nMDS with an analysis of surface area to volume ratio to elucidate the evolutionary and ecological history of Proterozoic macroalgae. The meta-analysis of 578 carbonaceous compressions from 17 monographs allowed Xiao and Dong to code for the presence or absence of 19 morphological characters. The results from their nMDS and randomization displayed a pattern similar to that reported in Huntley et al.'s (2006a) analysis of acritarchs. The morphological disparity of macroalgae was low in the Paleoproterozoic, increased dramatically in the Mesoproterozoic, plateaued through the early Neoproterozoic, and increased significantly in the Ediacaran Period. Xiao and Dong suggested that the broad similarity between the evolutionary patterns of these two ecologically distinct groups (acritarchs are generally interpreted as planktonic photoautotrophs while macroalgae are interpreted to be benthic photoautotrophs) is suggestive of an external forcing (whether environmental or through ecological interactions) of their morphological evolution. In addition, Xiao and Dong (2006) illustrated a significant increase in surface area to volume ratio in the Ediacaran, suggestive of an increase in growth rates and primary productivity. They suggested that the increase in surface area to volume ratio could have been driven by a decrease in $p\text{CO}_2$ following the Snowball Earth events or by the origination of herbivory in the Ediacaran Period.

Shen et al. (2008) utilized nMDS to compare Ediacara fossil morphological disparity with diversity through time. Their data matrix coded for the presence or absence of 50 morphological characters from 272 occurrences of a morphologically diverse group of organisms from 60 publications and one museum sample. The ordination data were sorted *a posteriori* into Waggoner's (2003) three assemblages: the Avalon (575–565 Ma), the White Sea (560–550 Ma), and the Nama (550–542 Ma). Diversity estimates, corrected for uneven sampling, were low in the Avalon Assemblage, significantly higher in the White Sea Assemblage (concurrent with geographic expansion), and lower again in the Nama Assemblage. Despite the differences in diversity and taxonomic composition between the three assemblages, the size and positions of occupied morphospace of the three assemblages were quite similar. The full range of occupied morphospace was realized in the earliest appearance of Ediacara organisms in the Avalon assemblage, reminiscent of the rapid evolution of metazoans in the Cambrian Explosion.

For more information about nMDS see Kruskal and Wish (1978), Schiffman et al. (1981), Marcus (1990), Roy (1994), and references therein. PAST, PC-ORD, SAS, and R can perform nMDS.

2.3.4 Detrended Correspondence Analysis

The purpose of detrended correspondence analysis (DCA) is to discover taxonomic groupings among samples distributed across environmental gradients. DCA is a member of a family of related ordinations (see below) which assign scores to both species and samples. One can imagine the distributions of many species along an environmental gradient such as temperature or water depth. Some taxa will have

narrow distributions and other taxa will have wide distributions according to their environmental tolerances. Many taxa will overlap spatially with one another, but typically the species at either extreme of the gradient will likely not overlap with one another. In a sense, DCA works to reconstruct this distribution. Species that commonly co-occur in samples will have similar ordination scores. Ordination scores are calculated for samples based on the weighted-average ordination scores of their component taxa.

DCA is an iterative analysis similar to Reciprocal Averaging (RA; also called Correspondence Analysis or Analyse Factorielle des Correspondances) which begins by selecting an arbitrary set of scores for the species in the data matrix. These arbitrary scores for species are used to calculate scores for the samples in which they occur (by calculating a weighted average). New scores are then calculated for each species as the average score from each sample in which they occur. These new species scores are used to refine the sample scores which are then used to further refine the species scores. This process continues until the scores stabilize (Hill 1973). DCA improves upon RA by addressing two of its key related flaws: (1) RA tends to warp the first ordination axis into an arch or horseshoe shape and (2) RA does not preserve ecological distances well; such that intermediate scores are widely spaced and peripheral scores are spaced closely together (Hill and Gauch 1980). DCA incorporates detrending to eliminate the arch effect and rescaling in order to preserve ecological distances within the iterative calculation process (Hill and Gauch 1980).

Detrended correspondence analysis requires only a few assumptions about the data. Samples comprise rows and species comprise columns. Species occurrences can be coded as counts, percentages, or presence/absence. DCA will not work well if most or all species co-occur in all samples or, conversely, if few or no species co-occur in samples.

Detrended correspondence analysis and related techniques are commonly used for analyzing gradients in ecological studies and in paleoecological studies. Holland et al. (2001) applied DCA to faunal occurrences (1,337 samples and 46 taxa) in the Ordovician Kope Formation and demonstrated shifting ecological structure along an inferred depth gradient that was not reflected by lithological changes. Holland et al. were able to model preferred depth, depth tolerance, and peak abundance of the most common species in the Kope Formation based upon DCA scores (though not absolute depth). Using the same ordination, Miller et al. (2001) produced a meter scale correlation between five localities based on faunal composition as this was not possible using lithologic characters. Indeed Miller et al.'s DC1 scores were indicative of environmental variables related to water depth. High DC1 scores were associated with species previously interpreted as occurring in shallow water facies and low DC1 scores were associated with the interpreted deeper water species. By ordering sample level DC1 scores according to stratigraphic position Miller et al. (2001) were able to produce a relative water depth curve for each of their five localities. These curves, based solely on taxonomic composition, allowed for high-resolution correlation between locations and revealed a dynamic seafloor where relative water depth changed between locations through time. Scarponi and

Kowalewski (2004), following a similar method, applied DCA to Plio-Pleistocene molluscan associations from the Po River Plain. In this case, Scarponi and Kowalewski were able to interpret absolute (rather than relative) depth estimates by relating DC1 scores to the bathymetric preferences of the modern counterparts living in modern coastal environments of Italy. High resolution sampling coupled with the sensitive environmental proxy provided by DC1 scores allowed the authors to further refine independently-derived lithologically-based sequence stratigraphic interpretations of these Quaternary sequences. Bonelli and Patzkowsky (2008) utilized DCA (in addition to nMDS and ANOSIM) on matrices of faunal occurrences in the Late Mississippian (Chesterian) of the Illinois Basin. From this work they were able to deduce that taxa were more strongly sorted along an environmental gradient prior to the onset of the Late Paleozoic Ice Age (LPIA) than after. Bonelli and Patzkowsky's (2008) conclusion that generalist species fared better during the LPIA at the regional scale rings true with Powell's (2005) conclusion that brachiopods with narrow geographic ranges were selected against during the LPIA at the global scale. However, it should be noted that Bonelli and Patzkowsky did not find evidence of selective extinction of environmentally-restricted species in the Illinois Basin. McFadden et al. (2009) used DCA, in addition to correspondence analysis and canonical variate analysis, to biostratigraphically sub-divide the Ediacaran Doushantuo Formation of South China. The DCA of 1,082 acritarch occurrences from 84 horizons suggested that the taxonomic composition of the samples was not related to environmental gradients or to taphonomic processes, but was dependent upon whether the sample came from the lower or upper Doushantuo Formation, indicating that the acanthomorphic acritarchs are useful index fossils. These results are an important step toward a global biostratigraphic subdivision and correlation of the Ediacaran.

Detrended correspondence analysis can be performed in PAST and PC-ORD. See Hill (1973), Hill and Gauch (1980), Ter Braak (1986), Hammer and Harper (2006), and references therein for further discussion of DCA and related techniques.

2.3.5 *Discriminant Analysis and Canonical Variate Analysis*

Discriminant analysis (DA) and canonical variate analysis (CVA) are related ordinations, which project multivariate data sets to a smaller number of dimensions as well as maximize the differences between pre-defined groups (Albrecht 1980; Blackith and Reyment 1971; Hammer and Harper 2006). DA projects a multivariate data set to one dimension and maximizes the differences between two pre-defined groups. CVA is used with a multivariate data set with three or more groups defined *a priori*. The number of dimensions to which the data are reduced in CVA is equal to the number of pre-defined groups minus one. DA and CVA are useful tools for discovering the combination of variables that account for the differences between

groups. DA and CVA report eigenvectors (or loadings; similar to PCA) which relate the DA axis or CVA axes to the original variables. Using the eigenvectors in a linear function allows one to attempt to classify new specimens into a pre-defined group. See Hammer and Harper (2006) for a brief discussion on applying DA to problems of taxonomic classification and testing the reliability of the discriminant function. Though they are useful for questions of taxonomy, one should take care when using DA or CVA because one chooses the groups *a priori* and because these ordinations maximize the differences between the pre-defined groups (for example, as compared to PCA). On these grounds, circular reasoning may come into play when arguing for the veracity of certain groups (e.g., genera, subspecies, sexual dimorphism, etc.). As the two methods are quite similar, the rest of this section will focus only on CVA.

Canonical variate analysis is composed of a series of rotation and rescaling procedures related to within-group and between-group variation (Albrecht 1980). By expanding on examples provided by Albrecht (1980), Fig. 2.5 gives a schematic representation of the CVA procedure. Panels a–d illustrate a successful CVA on data that are multivariate normal and have equal variance–covariance matrices (i.e., the relationships between the variables must be similar among the pre-defined groups). This schematic is of course a simplified two-dimensional illustration of what occurs in a more complex multivariate hyperspace. The first step in CVA can be seen as a rigid rotation of the original coordinates such that the within-group variation is maximized (Fig. 2.5a–b). Within-group variation is standardized in the second step (rescaling; Fig. 2.5c). In the third step between-group variation is maximized or aligned with the primary axis (CV1) (Fig. 2.5d). In this sense CVA can be viewed as two PCA procedures with an intervening rescaling of variation. The primary axis, CV1, explains the majority of the variation in the data and should display the most distinction between the pre-defined groups. Subsequent axes explain the majority of the remaining variation. It is important to stress that CVA works best when the data have a multivariate normal distribution and equal variance–covariance matrices. Figure 2.5e–h illustrate an example of what can occur when the data do not meet these assumptions. Variables 1 and 2 have similar variances in groups A and C but do not covary in the same way. Variables 1 and 2 display a much larger variance in group B than in groups A and C with similar and dissimilar covariances, respectively. The hypothetical end result for the CVA of these groups results in very little distinguishing power along CV1. One can find better distinction among the three groups along CV2 (though still not that great), and of course this should not be the case. Canonical variate analysis works best with continuous variables, but other variable types are allowed. There should be as many (or more) observations as variables. PAST and SAS can perform CVA.

Kowalewski et al. (1997) used CVA to analyze the morphology of seven populations of four *Glottidia* species (lingulid brachiopods). Considered “living fossils”, lingulids are morphologically very simple organisms and interpreted to display very slow rates of evolution. By subjecting a data matrix of 162 specimens

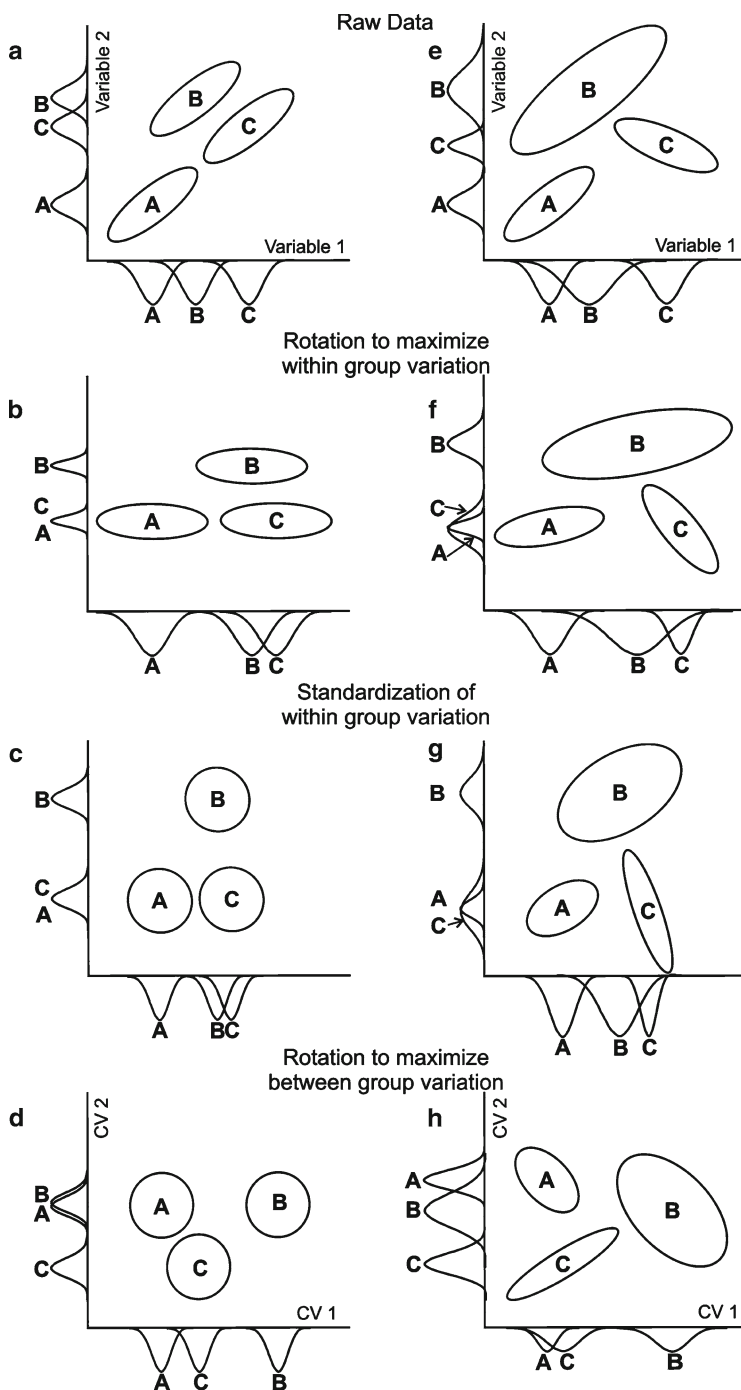


Fig.2.5 Schematic representation of the stages of Canonical Variate Analysis (CVA). Panels (a–d) depict the proper use of CVA on a matrix with three pre-defined groups, whose distribution is multivariate normal, and have equal variance–covariance matrices. Panels (e–h) depict the problems which can arise when data with unequal variance–covariance matrices are used with CVA (Modified and expanded after Albrecht (1980))

and six linear measurements to PCA and CVA Kowalewski et al. performed a size free morphological analysis and recognized five distinct morphogroups. Their findings went against the commonly held assertion that lingulid morphology is too simple to preserve useful taxonomic information. McFadden et al. (2009), as previously mentioned (see DCA section) utilized CVA in their biostratigraphic investigation of Ediacaran-aged Doushantuo Formation acanthomorphic acritarchs. So as to take a more conservative approach, McFadden and others performed CVA on the DCA scores (continuous variables) and classified the observations *a priori* according to lithology of the samples. This approach maximized the differences in taxonomic composition between the different lithologies. Even so, the CVA scores grouped according to biozone and not lithology, further strengthening their case for two assemblage biozones.

2.4 Conclusions

I have reviewed a few of the more common types of multivariate ordinations, discussed their utility and limitations, highlighted the data requirements for their proper use, and discussed a few examples of how these ordinations have been utilized in the study of early life. The selection of examples highlighted here, including some Precambrian examples when available and appropriate, is intended to motivate readers to ask new questions about their projects and research interests. Moreover, it should help to demonstrate that there is much work to be done in the study of early life and ecosystems. As the body of published literature on early life grows there will be more and more opportunity for meta-analysis and multivariate ordinations to address both “small-picture” and “big-picture” questions alike. It is my hope that my selection of examples will quickly become dated as this body of work continues its rapid growth.

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