A COMPARATIVE STUDY OF RECIPROCAL AVERAGING AND OTHER ORDINATION TECHNIQUES

H. G. GAUCH JR, R. H. WHITTAKER AND T. R. WENTWORTH*

Ecology and Systematics, Cornell University, Ithaca, New York 14853, U.S.A.

SUMMARY

Reciprocal averaging is a technique of indirect ordination, related both to weighted averages and to principal components analysis and other eigenvector techniques. A series of tests with simulated community gradients (coenoclines), simulated community patterns (coenoplanes), and sets of vegetation samples was used to compare ordination performance of reciprocal averaging (RA) with non-standardized and standardized principal components analysis (PCA) and polar or Bray-Curtis ordination (PO). Of these, non-standardized PCA is most vulnerable to effects of beta diversity, giving distorted ordinations of sample sets with three or more half-changes. PO and RA give good ordinations to five or more half-changes, and standardized PCA is intermediate. Sample errors affect all these techniques more at low than at high beta diversity, but PCA is most vulnerable to effects of sample errors. All three techniques could ordinate well a small (1.5 × 1.5 half-changes) simulated community pattern; and PO and RA could ordinate larger patterns (4.5 × 4.5 half-changes) well. PCA distorts larger community patterns into complex surfaces. Given a rectangular pattern (1.5 × 4.5 half-changes), RA distorts the major axis of sample variation into an arch in the second axis of ordination. Clusters of samples tend to distort PCA ordinations in rather unpredictable ways, but they have smaller effects on RA, and none on PO. Outlier samples do not affect PO (unless used as endpoints), but can cause marked deterioration in RA and PCA ordinations.

RA and PO are little subject to the involution of axis extremes that affects non-standardized PCA. Despite the arch effect, RA is much superior to PCA at high beta diversities and on the whole preferable to PCA at low beta diversities. Second and higher axes of PCA and RA may express ecologically meaningless, curvilinear functions of lower axes. When curvilinear displacements are combined with sample error, axis interpretation is difficult. None of the techniques solves all the problems for ordination that result from the curvilinear relationships characteristic of community data. For applied ordination research consideration of sample set properties, careful use of supporting information to evaluate axes, and comparison of results of RA or PCA with PO and direct ordination are suggested.

INTRODUCTION

Research on ordination has led to a dilemma of choice between the two most-used techniques, polar ordination and principal components analysis. The polar technique (Bray & Curtis 1957; Loucks 1962; Cottam, Goff & Whittaker 1973) can produce effective ordinations for a wide range of properties of the data ordinated, but it requires choices of endpoint samples that affect its results. Principal components analysis (Orlóci

* Present address: Department of Botany, North Carolina State University, Raleigh, North Carolina 27607, U.S.A.
A comparison of ordination techniques

1966, 1973, 1975) seems preferable for its objective definition of axes, but is not mathematically appropriate for ordination of the curvilinear and non-monotonic relationships with which ecologists often must deal (Beals 1973). Given such data, principal components analysis produces ordinations that are increasingly distorted with increasing range of compositional difference among the samples (Jeglum, Wehrhahn & Swan 1971; Gauch & Whittaker 1972b; Kessell & Whittaker 1976). An ordination technique that offers the objectivity of principal components analysis without its limitations for ordinating ecological data would be welcome.

Recent publications (Benzécri 1969; Guinochet 1973; Hill 1973, 1974) present a new technique, reciprocal averaging or correspondence analysis, that may offer partial solution of the dilemma. This paper first considers some of the characteristics of reciprocal averaging, secondly evaluates it in comparison with polar ordination and principal components analysis, and thirdly offers some observations on the use of ordination techniques. Our purpose is to provide understanding of the behaviour of, and choices among, these techniques.

RECIPROCAL AVERAGING

Reciprocal averaging (RA) originated in work of Hirschfeld (1935) and Fisher (1940); it has since then been rediscovered by others (Guttman 1959; Hill 1973, 1974). Its general use is to reveal correspondences, for a number of observations, between two kinds of information (Benzécri 1969) such as, in our application, species and samples.

Hill (1973) described RA as a weighted-average ordination effected by successive approximations. In the direct iteration algorithm (Hill 1973, Appendix 2) species are weighted by positions along a rough initial gradient and the weights are used to calculate sample scores. These sample scores as weights are then used to calculate a new and improved calibration of the species. The new species weights provide further improvement in sample calibration and so on. Back and forth, iterative calculations lead to a stable, optimal solution that does not depend on the initial arrangement. RA is thus an indirect ordination related to techniques of direct ordination—weighted averages (Whittaker 1967; Goff & Cottam 1967) and elective means (Ramensky 1930; Sobolev & Utekhin 1973).

RA is also an eigenvector technique related to principal components analysis (Hill 1973, 1974). The eigenvector calculation of correspondence analysis or reciprocal averaging (Benzécri 1969; Hill 1973, 1974) differs from the calculations of principal components analysis in: (1) simultaneous double standardization of the primary data matrix, (2) an additional division step ($\xi$ versus $x$ in Appendix 1 of Hill 1973) and (3) employment of chi-square (rather than covariance or correlation) distances (Chardy, Glemarec & Laurec 1976). These differences appear to give RA better properties for ordination, particularly tolerance of non-monotonic rises and falls of species scores (Fig. 1), compared with other eigenvector techniques (Noy-Meir, Walker & Williams 1975; Noy-Meir & Whittaker 1976; Chardy et al. 1976).

RA relates also to traditional phytosociological matrix arrangement, as shown in Fig. 1. RA can be used to arrange phytosociological tables into community-types or syntaxa (Češka & Roemer 1971; Guinochet 1973), but RA also produces an optimal sequence of samples and species in relation to each other. The production of simultaneous ordinations of samples and species, approximately co-ordinate with each other (on scales of 0 to
100), is an especially attractive feature of RA. Finally, RA can be applied as the 'index iteration' of Goff & Cottam (1967) to secondary data matrices (of sample, or species similarity values). We term this 'secondary reciprocal averaging' (SRA). SRA becomes a mathematical optimization of another classic technique of phytosociology—ordination by manoeuvring high similarity values toward the secondary matrix diagonal (Motyka 1947; Matuszkiewicz 1948; McIntosh 1973).

METHODS

Three ordination techniques were compared: RA, principal components analysis (PCA), and polar (Wisconsin comparative or Bray-Curtis) ordination (PO). For PCA a variance-covariance matrix from species-centred data was used; this corresponds to simple geometric projection into fewer dimensions while maximizing variance retained (Gittins 1969). This will be referred to here as 'non-standardized PCA'. For PO, the true end-

![Fig. 1](image-url)  
**Fig. 1.** A primary data matrix of species-by-sample scores arranged at random (a), according to species and sample ordination values from reciprocal averaging (b), and values from centred, non-standardized principal components analysis (c). Note that RA arranges the matrix to concentrate higher values along the matrix diagonal. The data matrix is a simulated coenocline with Gaussian species distributions and a beta diversity of 5 HC (the same as in Figs 2–4), having twenty species and twenty-four samples. Absence is indicated by a dash (–) and scores are rounded into ten equal classes marked ‘+’ and ‘1’ to ‘9’.

points were specified as the endpoint pair to be used, and the distance measure was percentage difference obtained by subtraction of percentage similarity values from 100. Supplementary tests with a few sample sets were carried out with secondary reciprocal averaging, PO with coefficient of community and Euclidean distance, simple ordination (Orlóci 1966), and eight variants of PCA: non-centring, standardization (of species to unit variance, data previously centred by species), relativization (of sample totals to 100), Wisconsin double standardization (Bray & Curtis 1957; Cottam et al. 1973), and data transformation by logarithm, square root, cube root and presence/absence. Several variants on the PO algorithm were also tested.

The direct iteration algorithm (Hill 1973, Appendix 2) is simple and efficient for solving RA for 1 axis, and reasonably efficient to about three axes. For more than three RA
axes, we compute the cross products matrix $BB^T$ of Hill’s (1973) Appendix 1, with prior centring to eliminate a trivial first eigenvector (Orlóci 1975), then reduce this cross products matrix to tridiagonal form, and solve for eigenvalues and eigenvectors by the QL method (routine adapted from subroutines TRED2 and TQL2 of the EISPACK package by B. S. Garbow of Argonne National Laboratory). This appears to be a very efficient algorithm (Wilkinson & Reinsch 1971). The RA, PO, and PCA programs are in the Cornell Ecology Programs Series (Gauch 1976a).

Simulated data of one-dimensional vegetation gradients (coenoclines) were made using Cornell Ecology Program CEP-1 (Gauch & Whittaker 1972a), based on a model with Gaussian species distributions scattered along the gradient. Two-dimensional vegetation patterns (coenoplanes) were simulated by CEP-21 (Gauch & Whittaker 1976), based on Gaussian solids corresponding to the Gaussian curves of the preceding one-dimensional simulation. To simulate field conditions, sample sets were varied in the following features: beta diversity or floristic heterogeneity, number and relative importances of compositional gradients, level of sampling errors or noise, presence of sample clusters, outlier samples, complete or partial disjunction, and variability in species amplitude and sample equitability. A repertory of sixty sample sets representing experiments on effects of these variables was submitted to RA, PO, and standardized and non-

standardized PCA. Smaller numbers of sets were used for other ordinations, and additional sets were used to answer particular questions.

Six field data sets were studied: (1) a topographic moisture transect for altitudes between 1830 and 2140 m in the Santa Catalina Mountains, Arizona (Whittaker & Niering 1965; Whittaker 1967) using the full forty-nine sample set; (2) the ten composite samples of a transect for the same samples; (3) ravine bottoms to upland slopes in Tompkins County, New York, sixty-three samples (Lewin 1973, 1974); (4) coastal terraces in Mendocino County, California, redwood through mixed evergreen and Bishop pine forest to pygmy cypress forest, sixty-one samples (Westman 1971, 1975); (5) Chihuahuan desert on limestone, Mule Mountains, Arizona, seventy-two samples between 1400 and 1860 m altitude, data of Wentworth (1976); (6) woodlands on acid soils, Mule Mountains, Arizona, sixty-nine samples between 1460 and 1920 m elevation, data of Wentworth...
Direct gradient analyses by weighted averages are available for all these except 3, and sets 1, 2, 5 and 6 have also been ordinated by Gaussian ordination and directly by topographic positions of samples.

Ordination results are evaluated by comparing recovered structure (sample and species locations) against the original structure, which serves as a null hypothesis or expectation. Original structure is known precisely for simulated data sets (Swan 1970). For field data, comparisons with results of direct gradient analyses may permit judgments on the realism of different ordinations (Jeglum et al. 1971; Westman 1971, 1975). Graphing (Noy-Meir & Austin 1970; Austin & Noy-Meir 1972) and measurement of sample displacements (Gauch & Whittaker 1972b; Kessell & Whittaker 1976) facilitate comparisons.

FIG. 3. (a)–(c), ordination of a simulated community gradient or coenocline in three dimensions by centred, non-standardized principal components analysis (PCA). The coenocline, with a beta diversity of five half-changes, is represented by twenty-four evenly spaced samples. The expected or correct result is a straight line in axis 1, and no structure in higher axes. (d)–(f), ordination of a simulated community pattern or coenoplane by PCA. The coenoplane had forty samples in an $8 \times 5$ grid with a beta diversity of $2.5 \times 1.5$ half-changes. Arrows are drawn to help show the configurations. A perfect ordination would give a rectangle with sides $2.5$ units on axis 1 to $1.5$ units on axis 2 and no sample displacements from the origin on axis 3.

RESULTS

Beta (sample set) diversity

Beta diversity, the degree of floristic difference among samples of a set, has major consequences for ordination performance. Beta diversity was measured in half-change (HC) units as numbers of $50\%$ changes in percentage similarity along a coenocline (Whittaker 1960; Gauch 1973b). Twelve coenoclines were simulated ranging in diversity from 0.3 to 20 HC. Each used about twenty simulated species, and twenty-four sample positions placed uniformly along the gradient. Given this one-dimensional input, an ideal ordination should recover this structure in evenly spaced sample positions on the first ordination axis and should have no sample displacements into higher dimensions.

Figure 2 shows the structure recovered by RA, standardized PCA, and non-standard-
ized PCA. At 3 HC and above, non-standardized PCA involutes the ends of the coenocline, producing extensive reversals of sample positions on the first ordination axis. The corresponding non-standardized PCA species ordinations (not shown) are also involuted. RA gave effective ordination to 10 HC, with correct sample sequences, but with bending of the coenocline into the second and higher axes that increased with increasing beta diversity, and with some displacement of samples toward the ends of the first axis. Standardized PCA displaced samples more strongly than RA but did not involute. Displacement was measured as mean percentage separation between true sample positions on the coenocline and ordinated sample positions on the first axis, giving both coenocline and axis a total length of 100% (Kessell & Whittaker 1976). For a 5 HC coenocline these displacements were 5·0% for RA, 3·4% for PO, 8·8% for standardized PCA, and 17·6% for non-standardized PCA. Above 10 HC, RA and PO lose sequencing distinctions for samples in the middle of the gradient.

The ‘arch’ distortions of Fig. 2 are due to a quadratic dependency of the second ordination axis on the first (Hill 1973, 1974). Figure 3 (top) shows sample configuration to three dimensions for the 5 HC coenocline ordinated with non-standardized PCA. The shape indicated is a helix of about 3/4 turn. Note that axis 2 is quadratic on axis 1, and axis 3 is cubic. Figure 4 and the results of Gauch (1976b) show that this pattern continues through several axes (until computational limitations are reached). For RA and standardized and non-standardized PCA axis N is an N-power polynomial (except that non-standardized PCA with beta diversity above 2 HC and standardized PCA and RA with very long coenoclines yield (N+2)-power polynomials for some or all axes).

Secondary gradients

Two-dimensional patterns or coenoplanes were simulated with axes of 0·7 to 10 HC, varying the relative and absolute lengths of the axes. The coenoplanes had thirty simulated species and forty samples arranged in a regular 8 × 5 grid.

Figure 3 (bottom) shows the non-standardized PCA ordination for a 2·5 × 1·5 HC coenoplane in three dimensions. The original configuration becomes somewhat rounded in the first two ordination axes; in three dimensions the shape is a rectangular surface with two opposite sides upturned. The RA result is similar, though less distorted. In
ordinations of square coenoplanes the opposite corners, rather than the opposite sides, are turned upward. At higher beta diversities (4·5 × 4·5 HC) RA reproduces the coenoplane in the first two axes with only minor distortion, as shown in Fig. 5, whereas non-standardized PCA involutes the corners of the coenoplane (cf. Austin & Noy-Meir 1972). Figure 5 also shows results with standardized PCA, PO with percentage difference and Euclidean distance, and simple ordination (Orlóci 1966).

When one coenoplane axis is considerably shorter than the other, for example 4·5 × 1·5 HC, the eigenvalue of the quadratic distortion of the longer axis exceeds the eigenvalue of the shorter axis. Consequently the first three axes in RA and PCA contain respectively: (1) the longer coenoplane axis, (2) the quadratic of the longer coenoplane axis, and (3) the shorter coenoplane axis. The ordination in axes 1 and 2 then looks like Fig. 3 bottom middle panel, and the second axis is meaningless for ordination. Axes 4–10 are complicated mixtures of various power functions of the original coenoplane axes.

Polar ordination endpoints were chosen in the middle of opposite sides of the sampling rectangle, or at its corners. In either case coenoplane structure was well recovered for squares and rectangles of low beta diversity (1·5 and 2·5 HC). A coenoplane 4·5 HC square was reproduced well when opposite corners were used for endpoints (Fig. 5), but corners were drawn in and sides were curved when endpoints were at the middles of the sides. A thin rectangle of 4·5 × 1·5 HC was compressed in its shortest dimension at the

Fig. 5. Ordination of a 4·5 × 4·5 half-change coenoplane by six techniques: (a) reciprocal averaging; (b) non-standardized PCA; (c) standardized PCA; (d) polar ordination with percentage difference; (e) polar ordination with Euclidean distance; (f) simple ordination. The sampling pattern and the expected result is a square grid of points, eight rows in one direction and five in the other. Arrows are drawn to help show the configurations.
extremities of the longer dimension, because the contrast defined by the median endpoints was less sensitive toward the extremes.

Sample errors

Sample errors were added to coenoclines as random, normally distributed departures of the species scores from the 'true' values in the simulated samples (Gauch & Whittaker 1972b). The levels of error used (10% and 25%) imply percentage similarity among replicate samples of 90% and 75%, and resemble properties of field data with low and moderate sample errors. Deterioration of ordination results was assessed by (a) counting the number of sequence reversals between consecutive samples along the first ordination axis and (b) observing the extent of sample scatter into the second axis of RA and PCA.

Observed scatter from noise was greatest for PCA and least for RA; it was slightly greater for PO than for RA. Table 1 shows percentage of first-axis sequence reversals for four techniques using coenoclines with 25% error and a range of beta diversities. For RA and PO reversals from sample scatter increase with decreasing diversity, because at low beta diversity the greater portion of the structure of the data is in the sample error

<table>
<thead>
<tr>
<th>Ordination technique</th>
<th>Beta diversity (half-changes)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reciprocal averaging</td>
<td>1    3    5    7    10</td>
</tr>
<tr>
<td>Polar with PD</td>
<td>41-3 25-0 15-2 6-5 4-3</td>
</tr>
<tr>
<td>Standardized PCA</td>
<td>39-1 33-7 23-9 22-8 16-3</td>
</tr>
<tr>
<td>Non-standardized PCA</td>
<td>40-2 28-3 20-7 31-5 30-4</td>
</tr>
</tbody>
</table>

rather than in the trends in sample composition. In non-standardized PCA with diversity above 3 HC, sequence reversals due to involution (see Fig. 2) mix with those due to scatter to obscure sample relationships. Among these techniques RA has increasing relative immunity to sample error toward higher beta diversities.

Sample clusters

Coenoplanes of $4.5 \times 1.5$ HC and $2.5 \times 1.5$ HC were used with twenty samples in a $5 \times 4$ grid. This sampling design was modified by adding one or two clumps of five samples duplicating a sample or samples already present.

Polar ordination places samples with respect to endpoint samples, and no other samples are involved in the calculation. Hence PO is unaffected by sample clusters. RA was affected very little by sample clusters. Axis direction was rotated slightly to align maximal variance along the first axis, but the configuration was fairly rigid. Non-standardized PCA showed slight to extensive deterioration with sample clusters (cf. Kessel & Whittaker 1976). One sample cluster near the centre of the $2.5 \times 1.5$ HC coenoplane changed the axis 1 and 2 configurations drastically, from one resembling Fig. 3 bottom left panel,
to one resembling Fig. 3 bottom middle panel. The same test with the 4·5 × 1·5 HC coenoplane showed little effect.

Clusters thus tend to attract the axes of eigenanalysis ordinations. PCA is more vulnerable than RA to modification of ordination results by this effect. Data sets in which different directions of sample variation (or polynomial axes thereof) have nearly equal eigenvalues are most vulnerable to alteration of ordinations by sample clusters. Rotations produced by sample clusters can in some cases change profoundly the appearance of the ordination as projected on to the first few axes, and consequently the interpretations of those axes.

Outliers

Field data sets often include deviant samples or 'outliers'—samples of unusual composition when compared to all other samples. Outliers were simulated by adding 1, 3 and 5 extra samples defined by two methods: (a) random selection, for each species, of one of its scores from among those in samples already present, and (b) random selection of one species to be strongly dominant, with about half the others of random but modest importance and about half zeros. We felt that the first method might approximate moderately deviant samples from atypical habitats, and the second strongly deviant samples from disturbed sites. Simulated outliers were added to coenoclines, a coenocline with 25% sample error, coenoplanes, and field data.

For polar ordination, all outliers not chosen as endpoints ordinate near or at the midpoint of the ordination axes without affecting positions of other samples. As endpoint samples, outliers are particularly poor choices because of their low relative similarities to all other samples. (Unfortunately the original technique of Bray & Curtis (1957) and the simple ordination of Orłóci (1966) both choose outliers in sample sets including these.)

RA was robust against effects of type 'a' outliers; they tended to ordinate around the centre of the ordination field but caused negligible displacement of the other samples. Type 'b' outliers, in contrast, ordinate around the periphery of the ordination field and strongly affect positions of the other samples. One such outlier from a coenocline ordnates at one end of the first axis and compresses the other samples into a tight cluster at the other end; the coenocline then emerges in the second axis. With 3 or 5 type 'b' outliers in a coenocline, the outliers are well scattered and other samples clustered. For a 2·5 × 1·5 HC coenoclone, one type 'b' outlier causes the first axis to have the outlier at one end and the remaining samples in a cluster at the other end; the 2·5 HC coenoplane axis then emerges in the second RA axis, and the 1·5 HC coenoclone axis emerges in the third RA axis. Three or five such outliers severely compress the original coenoclone samples, although their arrangement is still discernible. Outliers thus have somewhat unpredictable but potentially severe effects on RA.

PCA ordnates type 'a' outliers centrally to the other samples. One such outlier has relatively little effect, but a few cause some displacement of sample positions in both coenoclines and coenoplanes. Given type 'b' outliers, each determines the direction of an axis, causing rotations and strong compression of the other samples into a small region of the ordination field. Coenocline and coenoplane axes may then appear, together with distortions of these, in higher axes.

Disjunction

When groups of samples have no species in common, the resulting species-by-samples
data matrix is fully disjunct. Partial disjunction, in which groups of samples sharing many of their species are connected by few species to other groups, is more common in field data and is also more problematic for ordination. Even complete disjunction may not be obvious in an original data matrix, but it becomes apparent after arrangement of rows and columns by the first-axis RA scores. Since unrelated subsets are involved, the simplest course is to separate these to avoid effects of the higher intrinsic dimensionality that complicate ordination results. PO endpoints will be non-discriminating for samples not belonging to their subsets. Eigenvector ordinations, given a data set with N disjunct subsets, will first use N - 1 axes to separate subsets. The following eigenvectors will differentiate within only one subset each, and in order of decreasing variance accounted for will switch from subset to subset as in a story with pages interleaved from several sources.

Partial disjunction was tested using a 10 HC coenocline of evenly spaced Gaussian curves and samples. Two sections of 1, 2 or 3 HC were removed, thereby leaving three subsets related at three different levels of partial disjunction. PO ordinations were unaltered except for deletion of the missing samples. With different degrees of partial disjunction eigenvector ordinations (RA, non-standardized PCA, and standardized PCA) produce various types of axes: (1) differentiating between two or more subsets, (2) differentiating within one subset (with or without outlier effects of certain samples in other subsets), (3) differentiating within two or more subsets (the possibility for handling more than one subset being due to the polynomial nature of higher axes, as in Fig. 4), (4) polynomial distortions of one or more lower axes and (5) mixtures of these types. RA seemed to give a somewhat higher proportion of interpretable axes than standardized or non-standardized PCA. Noy-Meir (1973a) and Noy-Meir & Whittaker (1976) discuss disjunct sample sets and the application of non-centred PCA and classification to them.

Species amplitude and sample equitability

Gaussian distributions of various widths within a single data set were used to study effects of species distributions. In RA ‘characteristic’ species of narrow distributions are ordinated more distally (above the arch in the first two axes), whereas ‘companion’ species of wide distribution are ordinated more centrally. PCA showed similar effects, as does factor analysis (Dagnelie 1960, 1973). Species whose modes lie beyond the extremes of a coenocline have monotonic but truncated distributions in the sample set. These artificially narrowed species tend to be involuted toward central positions by non-standardized PCA, but RA and standardized PCA do not so involute. Analogous to the effects of species width or amplitude are those of sample equitability—relative similarity of adjacent values in the importance-value sequence (Lloyd & Ghelardi 1964; Whittaker 1972)—or its inverse, relative concentration of dominance. Equitable samples are ordinated more centrally, those of strong dominance more distally.

These effects can confound types of information. A sample (or species) may have a more central location for four different reasons: (a) it is an outlier of type ‘a’ (or a species of irregular occurrence), (b) it is an equitable sample (or a companion species of wide and regular occurrence), (c) it is (in non-standardized PCA) an involuted, extreme sample (or species), or (d) the central location correctly represents its position on axes expressing environmental gradients.
PCA variants

Several PCA variants were tested with coenoclines of lengths from 1 to 10 HC. Among these variants, non-centring appeared disadvantaged for ordination (although it may be advantageous for classification, see Noy-Meir 1973a; Noy-Meir & Whittaker 1976). Sample standardization gave little or no improvement in our tests (but may do so if samples are of different sizes). Wisconsin double standardization improved ordinations substantially in some cases (cf. Austin & Noy-Meir 1972) with results intermediate to RA and non-standardized PCA. Logarithm, square root, and cube root transformations gave some improvement, but there was no clear basis of preference among them. Presence/absence transformation gave various but usually poorer results. The effects of these variations on PCA are dependent on sample set properties. PCA ordinations may be improved, however, by data treatments that reduce the effects of dominant species on the ordination, whether by species standardization or by logarithmic or other transformations. These treatments extend the range of beta diversities that can be ordinated without severe distortion. Cassie (1969), Noy-Meir et al. (1975) and Chardy et al. (1976) further discuss transformations in PCA.

PO variants

Comparisons of PO and PCA (Gauch & Whittaker 1972b; Kessell & Whittaker 1976) have applied these to the same primary matrix without Wisconsin double standardization. Although double standardization can much improve the performance of PCA, it gave modest or no improvement in PO in our tests. (Double standardization or coefficient of community may have greater advantage for field data combining high alpha and beta diversity and sample error.) Corrections in PO for the curvilinearity of sample similarity values (Gauch 1973b) and non-orthogonality of axes (Orlóci 1966, 1974; Bannister 1968) gave little or no improvement in ordination of simulated data with sample error. Use of Euclidean distance rather than percentage similarity for PO (Orlóci 1966, 1974; Bannister 1968) usually increases sample displacement along the axis (Gauch & Whittaker 1972b; Kessell & Whittaker 1976) and can produce involution of the extremes, whereas percentage difference and complemented coefficient of community do not so involute (Fig. 5).

Orlóci (1966) suggested 'simple ordination' as a Euclidean variant of PO. The technique uses Euclidean distance, and the first axis goes through the maximally distant sample pair. Single endpoint samples define second (and higher) axes orthogonal to the first axis (or lower axes). Applied to a coenocline simple ordination creates a spurious second axis of relative distance from one sample that is highest on the arch off the first axis. Applied to coenoplanes exceeding a few HC simple ordination produces severely distorted configurations (e.g. Fig. 5).

Secondary reciprocal averaging

Index iteration (Goff & Cottam 1967) or secondary reciprocal averaging (SRA) was applied to matrices of percentage similarity values, by samples and by species, for coenoclines of 1 to 10 HC and a coenoplane of 2.5 × 1.5 HC. Results of SRA of samples were much like those of RA for the coenoplane and the 1 to 5 HC coenoclines, but the
10 HC coenocline was distorted less (about as much as a 5 HC coenocline with regular RA). Results of SRA of species (by percentage similarities of species distributions) were, in contrast, less satisfactory than RA species ordination because of problems caused by rare species. SRA may be useful for sample ordinations with high beta diversity and may also be useful for analysing data in papers where only the secondary matrix was published, for SRA can be applied to any matrix of similarity or distance values. Its performance in that use has not been compared with principal coordinates analysis (Gower 1966). For

![Diagrams](image)

**Fig. 6.** Ordinations of ten composite samples from a topographic moisture gradient at 1830–2140 m in the Santa Catalina Mountains, Arizona (Whittaker & Niering 1965; Gauch et al. 1974), in the first two dimensions of three kinds of ordination: (a) reciprocal averaging (RA), (b) centred and species-standardized principal components analysis and (d) centred, non-standardized PCA. The samples are indicated by circles numbered from 1 (most mesic) to 10 (most xeric); ordinated positions of the species are indicated by Xs and initials. In (c) positions are indicated along the first axis of RA, with numbers above the species initials being weights used for direct weighted-averages ordination on a moisture gradient by Whittaker & Niering (1964, 1965). The arrangement is considered realistic from field experience. The tree and arborescent shrub species are: *Pseudotsuga menziesii*, *Pinus ponderosa*, *Quercus rugosa*, *Arbutus arizonica*, *Quercus hypoleucoides*, *Pinus chihuahuana*, *Quercus arizonica*, *Arctostaphylos pinglei*, *Garrya wrightii*, *Pinus cembroides* and *Quercus emoryi* (nomenclature follows Kearney & Peebles 1960). The second axis is scaled by the square root of its eigenvalue relative to the square root of the first axis eigenvalue, and species and sample ordinations are scaled arbitrarily to the same range.

most uses SRA should have no advantage over RA with its effective, simultaneous ordinations of samples and species.

**Tests with field data**

RA, PO and PCA ordinations were applied to the six sample sets described earlier. Detailed studies of these combining direct gradient analysis, weighted averages, and
Gaussian ordination (Gauch, Chase & Whittaker 1974) provide understanding of relationships of communities and environments by which other ordinations may be judged.

Closely similar ordinations resulted in most cases from RA, PO, weighted averages, and Gaussian ordination. These four, but not PCA, seemed clearly better than ordination based directly on topographic position. With data set 4, a PO judged satisfactory was obtained only after division of the gradient into halves, whereas the RA ordination of the full set was judged satisfactory. With other sample sets, RA gave not an arched but an angled figure in the first two axes: the few most mesic samples (from ravines) were scattered along an ascending slope, while all the remaining samples formed a longer, descending slope. RA ordination was improved by removing the ravine samples from the sets. RA was judged somewhat better than PO in these tests; Gaussian ordination was judged to give results equivalent to (or marginally better than) those of RA.

PCA ordinations (non-standardized) were judged inferior in all cases. In some of these the sample distribution in the first two PCA axes was almost uninterpretable; in sample set 4 field information permitted interpretation of the PCA ordination as forming a spiral in the first two axes (Whittaker & Gauch 1973, Fig. 3; Westman 1975). Figure 6 illustrates the relation of RA and standardized and non-standardized PCA ordinations for the ten-step transect of data-set 2. The RA ordination is arched but clearly interpretable; the sample and species positions on the first axis, in lower left panel, are judged an effective and realistic ordination. In this, as in the other tests with field data, the second RA axis does not appear to offer useful information. The PCA ordinations in Fig. 6 are severely distorted by involution.

**DISCUSSION**

Ecological ordination refers to the arrangement of samples (or species) in relation to environmental gradients, or axes that may correspond to environmental gradients; a major purpose of such arrangement is the recognition of joint variation in community composition and environmental factors (Whittaker 1967, 1973; Austin 1976). The axes produced by indirect ordination are expected to differ in scaling and orientation from environmental gradients as usually recognized (Greig-Smith 1971); but the purpose of ordination is defeated if the axes are ecologically meaningless, or the ordained positions of samples and species are uninterpretable. The performances of ordination techniques are profoundly affected by the curvilinearity intrinsic to community data: the bell-shaped form of species distributions along environmental gradients, and the non-linear decrease of sample similarity with increasing sample separation (Whittaker 1967, Gauch 1973b). Problems of indirect ordination are understood in terms of these curvilinear relationships, and performance of ordination techniques is judged by relative success in producing, despite them, arrangements that are ecologically significant—realistic as abstract representations of relationships of species and communities to environmental gradients.

Beyond the general effects of curvilinearity, ordinations are subject to effects of various sample set characteristics. These characteristics—sample and total species number, alpha and beta diversity, trends in these and other community properties, number and relative importance of directions of community variation, level and character of sample errors, sample distribution in the range of variation sampled and presence of sample
A comparison of ordination techniques

clusters and gaps, and presence of outlier samples or disjunctions and of species with atypical distributions—define a hyperspace of data-set properties that seems beyond full exploration with the wide range of ordination techniques suggested (Whittaker & Gauch 1973; Dale 1975). We have sought only to test some major effects of such variables on three ordination techniques: polar ordination (PO), principal components analysis (PCA), and reciprocal averaging (RA). The tests show both that some of these properties have major effects on ordination performance, and that the effects differ from one ordination technique to another.

From the tests a summary evaluation of the three techniques is suggested.

Principal components analysis in its most familiar form (centred, non-standardized or sample-standardized) is relatively unreliable for ordination. Non-standardized PCA is subject to involution and severe distortion of sample positions at moderate beta diversities (three half-changes and above). Even without involution some of its higher axes may express only ecologically meaningless curvature of lower axes, and it is more vulnerable than the other techniques to rotation and distortion by sample clusters and outliers, and to effects of sample errors. We have not identified sample set properties for which PCA gives better ordination than RA. Despite its limitations, non-standardized PCA gives satisfactory ordination of some sample sets of moderate beta diversity and sample error (Austin 1968; Jeglum et al. 1971). With species standardization or double standardization PCA can ordinate sample sets of higher beta diversity without involution, and its vulnerability to other sources of distortion is reduced (cf. Noy-Meir et al. 1975). PCA may be appropriate for research on monotonic variables such as community structural characteristics (e.g. James 1971), and non-centred PCA is appropriate as a technique for numerical classification or grouping of samples and species (Noy-Meir 1973a, 1973b; Noy-Meir & Whittaker 1976).

Reciprocal averaging or correspondence analysis employs a simultaneous double standardization and is resistant to involution even at high beta diversities. RA can, however, involute when offered data with species distributions departing from Gaussian form (Austin 1976). RA has major advantages over non-standardized PCA and at least marginal advantages over standardized PCA in its lower vulnerability to distortion by sample clusters, sample error, and outliers. (Outlier samples, however, reduce ordination effectiveness and should generally be removed from a sample set.) RA produces simultaneous sample and species ordinations on axes that may be treated as co-ordinate (Fig. 6); and its species ordinations are superior to those of PO and PCA (Hill 1973). RA is a technique of choice for indirect ordination to reveal a first, major direction of sample variation in response to environment. RA will in some cases reveal a second direction of sample variation in its second axis; in other cases this direction is obscured by distortion in the second axis, and deferral of secondary gradients of sample variation into higher axes. Given the curvilinearity and other characteristics of community data, RA can no more than PCA be trusted to produce several independent axes as ecologically significant, potentially interpretable directions of community and environmental variation.

Polar ordination is a simple and in some respects robust technique, generally free from involution and little vulnerable to distortion by clusters and outliers (provided the last do not become endpoint samples). The technique’s major limitation is its requirement for endpoint choice and the vulnerability of the ordination to effects of different endpoint choices. PO has characteristics that limit distortions from non-linearity. First, the fact
that the axes are anchored by endpoint samples prevents involution of the extremes of these axes. (Involution can occur, however, with deviant samples or use of Euclidean distance.) Secondly, because sample positions on different axes are separately calculated so that the arch displacement of samples off a given axis has no effect on sample positions on other axes, PO is not subject to the coenocline curvature into higher axes characteristic of PCA and RA. Thirdly, the Pythagorean projection of sample distance from two endpoints reduces the effect of the curvilinear relationship of sample similarity to sample distance (Gauch 1973a). The effectiveness of the technique for ordination of non-linear data should not be overlooked because of its simplicity (Beals 1973). Modifications of PO to make it more like PCA can produce either moderate increase in sample displacement (with substitution of Euclidean distance for percentage similarity) or major increase in distortion (with the simple ordination of Orloci 1966). PO has continued usefulness for direct ordination, for trial ordination that may indicate some properties of a data set also to be subjected to other techniques, and for comparison with and aid in interpreting other ordinations.

A further finding of this study is the implication of interrelationships among sample-set characteristics for ordination. Field data sets differ by varying combinations of beta diversity, sample error, and other characteristics that will influence ordination but may be difficult to recognize before ordination. Effects of different combinations of these characteristics are relatively unpredictable. Sample error, in particular, tends to obscure distortions consequent on other sample set characteristics. Given moderate scatter in sample positions because of sample error, curvilinear distortions in the second axis (Fig. 2, Fig. 3 lower middle) and higher axes may be difficult to recognize. When effects of curvilinear distortion and sample error are combined with possible effects of clusters, deviants and sample equitability, interpretation of axes may be less than confident. In general, use of eigenvector techniques for multidimensional ordination should include careful consideration of sample-set properties, and use of other information (knowledge of environmental relations that may be represented in direct or polar ordination) to determine which axes are significant and which spurious.

This need for other information bears on two concepts that have influenced discussions of ordination—objectivity and mathematical appropriateness. Objectivity of a technique refers to the degree to which its production of information is uninfluenced by the investigator’s choices in applying the technique. PO is subjective in its requirement for endpoint choices, and the eigenvector techniques are attractive because axes are objectively produced by calculations employing the full range of sample data. The contrast is not, however, one-sided. For PCA a range of variants with different combinations of transformations, standardizations, centring, and rotation give different results among which an investigator may choose. In the chosen ordination the significant axes must be recognized and interpreted by largely subjective means, primarily observed correlations and intuitively accepted relationships. Supplementary information is needed, and the ideal is not a simple objectivity but an effective interaction of information and investigator. The process is one of progressive approximation (Poore 1956); ordination itself might be thought a kind of reciprocal averaging of field information against ecologists' understanding toward an optimal correspondence of these.

Mathematical appropriateness is necessarily defined in part in relation to the curvilinearities of community data. Accuracy in representation of a Euclidean space defined by species scores in samples (Gower 1966; Gittins 1969; Orloci 1973, 1975) is not itself
an objective, but realistic representation of the curvilinear relations of species populations and sample composition to environmental gradients is an objective of ecological ordination (Whittaker 1967; Beals 1973; Austin 1976). Given the linear assumptions of PCA, its use for ordination should not be justified on mathematical grounds. The justification is practical: the programs are widely available and can, with suitable sample sets and appropriate data treatment, give useful ordinations. Despite their assumptions and limitations, RA and PO are in different ways relatively well adapted to the non-linearity of ecological data. Non-linear ordinations are discussed further by Austin (1976) and Noy-Meir & Whittaker (1976); non-linear techniques being tested include Gaussian ordination (Gauch et al. 1974; Wentworth 1976; Ihm & Groenewoud 1975), continuity analysis or parametric mapping (Shepard & Carroll 1966; Noy-Meir 1974), and multi-dimensional scaling (Kruskal 1964a, b; Fasham 1977). Results so far (Austin 1976; Noy-Meir & Whittaker 1976) suggest that these will share places in the field with PO, PCA and RA, but that none will solve all ordination problems or escape the need for careful and informed ordination of community data.

ACKNOWLEDGMENTS

This research was supported by a grant from the National Science Foundation. We thank M. P. Austin, S. P. Bratton, A. Češka, S. A. Levin, L. Orlóci, S. Nichols, I. Noy-Meir, R. K. Peet, Z. Szöcs and especially M. O. Hill for comments and contributions, and S. B. Conley and C. E. French Jr for preparation of the manuscript and assistance with computations.

REFERENCES


A comparison of ordination techniques


(Received 9 July 1976)