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Compositional dissimilarity as a robust measure of ecological distance

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Abstract

The robustness of quantitative measures of compositional dissimilarity between sites was evaluated using extensive computer simulations of species' abundance patterns over one and two dimensional configurations of sample sites in ecological space. Robustness was equated with the strength, over a range of models, of the linear and monotonic (rank-order) relationship between the compositional dissimilarities and the corresponding Euclidean distances between sites measured in the ecological space. The range of models reflected different assumptions about species' response curve shape, sampling pattern of sites, noise level of the data, species' interactions, trends in total site abundance, and beta diversity of gradients.

The Kulczynski, Bray-Curtis and Relativized Manhattan measures were found to have not only a robust monotonic relationship with ecological distance, but also a robust linear (proportional) relationship until ecological distances became large. Less robust measures included Chord distance, Kendall's coefficient, Chi-squared distance, Manhattan distance, and Euclidean distance.

A new ordination method, hybrid multidimensional scaling (HMDS), is introduced that combines metric and nonmetric criteria, and so takes advantage of the particular properties of robust dissimilarity measures such as the Kulczynski measure.

Introduction

Many multivariate methods applied to community data operate, either explicitly or implicitly, on a matrix of compositional dissimilarities between samples. The degree of success in recovering ecological patterns in the data will depend on the nature and strength of the relationship between values of the chosen dissimilarity measure and the corresponding Euclidean distances between samples in ecological space ('ecological distances'). Equally important is the appropriateness of the assump-

tions about the form of this relationship which are implied by the mathematical model underlying the multivariate method.

In this study, we have used simulated vegetation data to examine directly the relationships between various coefficients of compositional dissimilarity and ecological distances. Of particular interest has been the relative *robustness* of coefficients to variations in the model of community variation in ecological space (cf. Minchin, 1987a). Attention was focused here on coefficients applicable to quantitative (abundance) data; the binary (presence-absence) case will be examined in a subsequent paper.

Our findings regarding the nature of the relationship between robust dissimilarity measures and ecological distance have consequences for the de-

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sign of robust ordination methods. We propose a new method, hybrid multidimensional scaling (HMDS), that is based upon those aspects of compositional dissimilarity which are found to be robust predictors of ecological distance.

Background

While the importance of the choice of a dissimilarity measure in ecological ordination has been emphasized in previous work (Austin & Noy-Meir, 1971; Gauch, 1973; Austin, 1976; Fasham, 1977; Lamont & Grant, 1979; Prentice, 1977, 1980; Clymo, 1980; Beals, 1984), individual recommendations differ. Gauch (1973), Gauch & Whittaker (1972), and Beals (1973, 1984) argued that the Bray-Curtis measure (Bray & Curtis, 1957) is robust to non-linearities in species' response. The Relativized Manhattan measure (Renkonen, see Whittaker, 1952; Orlóci, 1974) is listed as an appropriate measure for non-linear data by Orlóci (1978). Austin & Greig-Smith (1968) found that a successive double standardization (species adjusted to equal maxima, then samples standardized to equal totals) is preferable to the use of the Bray-Curtis measure on unstandardized data. Orlóci (1974, 1978) has presented theoretical arguments in favour of Chord distance (sensu Orlóci, 1967), and Fasham (1977) found that a related measure, 'cosine theta' (Gower, 1967), out-performed several other measures in limited simulation trials with Gaussian models.

Swan (1970), Gauch (1973) and Ihm & Van Groenewoud (1975) used explicit models of community variation in ecological space and examined the relationship between compositional dissimilarity and ecological distance directly. However, their models assumed that species' responses are unimodal and symmetric (Gaussian). Evidence suggests that other types of responses (e.g. skewed, multimodal) are common (Austin, 1976, 1980, 1987; Minchin, 1987b), hence the generality of results from Gaussian models is questionable. Some other theoretical and simulation-based studies have used even more restrictive models. For example, the approach of Hajdu (1981) implies linear response curves.

Because species' response patterns in ecological space are unlikely to conform with any specific model (Greig-Smith, 1983; Austin 1976, 1985; Minchin, 1987b), the choice of a measure of compositional dissimilarity for ordination must consider the *robustness* of the measure's relationship with ecological distance over a range of species' response models. It follows that the development and evaluation of dissimilarity-based ordination methods must be guided by only those aspects of the relationship between dissimilarity and distance which are robust.

Ordination methods which have an in-built measure of compositional dissimilarity are prone to the problem of limited applicability arising from a restricted underlying model. The weaknesses of principal components analysis (PCA) can be interpreted in terms of the restrictive linear model implied by Euclidean distance (Noy-Meir & Austin, 1970). Correspondence Analysis (CA) can be formulated as a weighted principal co-ordinates analysis (PCoA: Gower, 1966), based upon Chi-squared distance (Chardy *et al.*, 1976). CA's behaviour will therefore depend on the relationship between Chi-squared distance and ecological distance. Surprisingly, Gauch *et al.* (1981) consider that the freedom to choose an appropriate dissimilarity measure for use in ordination is a *disadvantage*.

Ordination methods which permit a choice of dissimilarity measure may allow the combination of a scaling method that assumes a particular form of relationship between compositional dissimilarity and ecological distance, and a measure of dissimilarity that provides this relationship robustly. PCoA and so-called 'classical' multidimensional scaling (Torgerson, 1952) assume that the dissimilarity measure has a linear relationship with ecological distance. In contrast, nonmetric multidimensional scaling (NMDS, Shepard, 1962a, b; Kruskal, 1964a, b) assumes only *monotonicity*: a configuration is derived in which the distances between sample pairs are in *rank order* with their dissimilarities. Prentice (1977, 1980) argues that the weaker assumption of monotonicity should be preferred in view of our lack of knowledge about models of species response. Limitations of nonmetric methods have also been raised. The assumption of monotonicity may be so general that uninformative degeneracies in the solution are permitted (for a discussion, see Shepard, 1974). A balance must be reached between assuming too little, with a loss of useful information which can constrain the solution, and assuming too much, with a loss in the method's robustness. There do not appear to have been any tests of the robustness, over a wide range of response models, of the metric (linear) and non-metric (monotonic) relationships of different dissimilarity measures to ecological distance. Such a study is a necessary first step in the solution to 'the

dissimilarity problem in ordination': what dissimilarity measure has a robust, informative, relationship with ecological distance; and what ordination method can take advantage of this relationship in its assumptions?

Methods

Dissimilarity coefficients evaluated

The dissimilarity measures evaluated in this study are listed in Table 1. Examination of two basic measures, Manhattan distance (MAN) and the complement of Kendall's coefficient (KEN), illustrate a problem which prompted consideration of many of the alternative measures in Table 1. MAN is defined by the sum of the absolute differences in abundance over all species. Such an index might be expected to reflect ecological distance, but a problem arises for larger ecological distances. When

two sites are sufficiently far apart in ecological space that they share no species, MAN yields a value that depends only on the total site abundances. Values of MAN can therefore suggest that one ecological distance is larger than another when the reverse is true. KEN initially appears to avoid spurious variation due simply to site totals, in that it reaches a constant maximum value when two sites share no species. However, for small ecological distances, when sites will tend to share many species, the actual value of KEN does reflect variation in site totals. Variation in site totals thus obscures predictive information about ecological distance for both simple measures.

A desirable measure would take a value of zero when ecological distance was zero, and some constant maximum value when ecological distance had increased to the point that shared abundance was zero (Beals, 1984). This theoretical argument has led us to focus on a number of measures that all have some form of standardization, such that the above properties are satisfied. These measures (Table 1) are the Kulczynski (QSK), Bray-Curtis (B-C), Chord distance (CHD), Canberra metric (CAN) and Relativized Manhattan (MAN:SAT) measures.

While the measures listed above are well constrained for large

Table 1. Basic measures with reference, abbreviation, standardizations used, and formula for dissimilarity between two objects, j and k , based upon attributes, $i = 1$ to N . Z is the number of attributes that are 0 for j and k . MAX_i is the maximum value of attribute i over all sites; MIN_i is the corresponding minimum. SPM is species adjusted to equal maximum abundance. SAT is sites standardized to equal totals. DBL is SPM followed by SAT. Equivalences of measure-standardization combinations reduced the total number of combinations to 29. For further explanation see text.

Name and reference	Abbreviation	Standardizations	Formula
Kendall (1970)	KEN	SPM	$\sum_i [MAX_i - \text{minimum}(X_{ij}, X_{ik})]$
Manhattan (Sokal & Michener, 1957)	MAN	SAT, SPM, DBL	$\sum_i X_{ij} - X_{ik} $
Gower metric (Gower, 1971)	GOW	SAT	$\sum_i [X_{ij} - X_{ik} / (MAX_i - MIN_i)]$
Euclidean (Sokal & Sneath, 1963)	EUC	SPS, SPM, SAT, DBL	$[\sum_i (X_{ij} - X_{ik})^2]^{1/2}$
Intermediate (Faith, 1984)	INT	SPM	$(1/2) \{ \sum_i X_{ij} - X_{ik} + MAX_i - \text{minimum}(X_{ij}, X_{ik}) \}$
Quantitative symmetric (Kulczynski) – See for instance, Hajdu (1981)	QSK	SPM	$1 - (1/2) \{ [\sum_i \text{minimum}(X_{ij}, X_{ik}) / \sum_i (X_{ij})] + [\sum_i \text{minimum}(X_{ij}, X_{ik}) / \sum_i (X_{ik})] \}$
Bray-Curtis (Bray & Curtis, 1957)	B-C	SPM	$(\sum_i X_{ij} - X_{ik}) / [\sum_i (X_{ij} + X_{ik})]$
Chord (sensu Orlóci, 1967)	CHD	SPM	$[2 (1 - \{ (\sum_i X_{ij} X_{ik}) / [(\sum_i X_{ij}^2) (\sum_i X_{ik}^2)]^{1/2} \})]^{1/2}$
Canberra metric, Adkins form (Lance & Williams, 1967)	CAN	SPM, SAT, DBL	$[1/(N-Z)] \sum_i X_{ij} - X_{ik} / (X_{ij} + X_{ik})$
Chi-squared (Chardy <i>et al.</i> , 1976)	CSQ	SPM, SAT, DBL	$\{ \sum_i (1/\sum_i X_{ij}) [X_{ij}] [\sum_i X_{ij}] - X_{ik} / (\sum_i X_{ik}) \}^{1/2}$

and small ecological distances, they may differ in their predictivity of distance between these two extremes. The simulation study therefore included all these measures and, for comparison, KEN, MAN, EUC, the Gower metric (GOW) and two other measures INT and CSQ (Table 1). INT has been recommended as useful in ordination because of its intermediate properties relative to KEN and MAN (Faith, 1984). CSQ represents the implicit dissimilarity measure in the widely-used ordination method, correspondence analysis (CA).

Data standardizations

Because many dissimilarity coefficients have in-built standardizations, it is difficult to compare dissimilarity coefficients without also considering the effects of prior data standardizations. Consequently, we chose to study the ten coefficients listed above both on unstandardized data and in combination with each of three standardizations:

1. Species adjusted to equal maximum abundances (SPM).
2. Samples (sites) standardized to equal totals (SAT).
3. Bray-Curtis successive double standardizations: 1 followed by 2 (DBL).

An additional standardization, of species to equal standard deviations (SPS), was only investigated in combination with Euclidean distance (EUC). This is the dissimilarity coefficient implied in an *R*-mode principal components analysis of a matrix of correlations among species. Subsequently, we refer to the combinations of standardizations and dissimilarity coefficients using the abbreviations given in Table 1.

Some of the dissimilarity measures are mathematically equivalent after certain data standardizations. For example, after the SAT standardization the coefficients MAN, KEN, INT, B-C and QSK are indistinguishable. In addition, the in-built standardization of certain measures make them unaffected by some data standardizations. Thus GOW:SPM is equivalent to GOW and CHD:SAT is equivalent to CHD. Consideration of these equivalences resulted in a total of 29 unique combinations of standardization and dissimilarity coefficient (Table 1).

Models

We used a simulation approach similar to that of Minchin (1987a). The comprehensive simulation program, COENOS, is described in detail by Minchin (1987b). The model properties which were varied (Table 2) include length (beta diversity) of gradient, response curve shape, sampling pattern of the sites in ecological space, trends in sample totals, and degree of noise in the data. Limited computing resources prevented the examination of these properties in all factorial combinations and also restricted the amount of replication within each combination of properties. The resulting design was therefore not fully balanced. Table 3 shows the structure of the simulation experiment for two-dimensional models: the unidimensional experi-

Table 2. Model properties varied in the simulation study of quantitative dissimilarity measures. For a complete description of the simulation approach, see Minchin (1987b).

Properties varied in the generation of species sets

Beta diversity (R units of Minchin, 1987b)

1D models, 3 levels: 0.5, 1.0, 2.0

2D models, 6 levels: 0.5 × 0.25, 0.5 × 0.5, 1.0 × 0.5, 1.0 × 1.0, 2.0 × 1.0, 2.0 × 2.0

Ecological response shape. 3 levels:

1. Unimodal, symmetric. $\alpha = \gamma = 4.0$ on each gradient
2. Unimodal, skewed. Both α and γ uniformly distributed between 0.5 and 4.0
3. Interaction between species with unimodal, skewed responses, leading to some shouldered, bimodal and multimodal ecological responses

Interaction parameters (see Minchin, 1987b, for explanation):

Modal abundance similarity interval = 0.75

Mode proximity interval = 0.2

1 to 3 interactors per species

Interaction coefficients all equal to 0.15

No negative interaction.

Properties varied in the generation of data matrices from species sets

Trend in sample totals. 4 levels:

1. No adjustments made to sample totals
2. Constant sample total over the ecological space
3. 3-fold linear trend across the ecological space
4. 3-fold unimodal trend, with maximum in the centre of the ecological space

Sampling pattern. 2 levels:

1. Regular grid in ecological space
2. Uniform random distribution over the ecological space

Quantitative noise. 3 levels:

1. No added noise
 2. Normal errors with SD proportional to square root of original abundance. Constants of proportionality uniformly distributed between 0.25 and 0.75
 3. Normal errors with SD proportional to square root of original abundance. Constants of proportionality uniformly distributed between 1.0 and 3.0
-

ment was similar. The model properties 'beta diversity' (6 levels) and 'response shape' (3 levels) were varied in all factorial combinations and three replicate species sets were produced in each of the 18 cells. The other model properties were varied during the generation of data matrices from these species sets, but not in all possible combinations. For example, all data matrices generated from the species sets with either 'symmetrical' or 'skewed' response shapes had 'regular' sampling patterns and 'no control' of sample totals. In total, the study was based on 255 data matrices with a single underlying gradient and 306 data matrices for which the ecological space had two dimensions.

Table 3. The design of the simulation experiment for two-dimensional models. Details of the model properties varied are given in Table 2.

Generation of species sets

Beta diversity (6 levels) \times Response shape (3 levels) = 18 combinations

3 replicates per combination = 54 species sets

Generation of data matrices

1. Species sets with 'symmetric' or 'skewed' response shapes:

Trend in sample total held at level 1 (no adjustment)

Sampling pattern held at level 1 (regular grid)

36 species sets

\times Quantitative noise (3 levels)

= 108 data matrices

2. Species sets with 'interaction' response shapes:

18 species sets

\times Trend in sample totals (3 levels: 2, 3 and 4)

\times Sampling pattern (2 levels, but level 2 only applied to the first replicate species set in each Beta diversity class and only with Quantitative noise at levels 1 and 3)

\times Quantitative noise (3 levels)

= 198 data matrices

Analysis of robustness

For each data matrix, a matrix of ecological distances was computed as the Euclidean distances between samples in the simulated ecological space. In addition, compositional dissimilarity matrices were calculated from the simulated abundance data, using each of the 29 combinations of data standardization and dissimilarity coefficient listed in Table 1. Scatter plots of dissimilarity *versus* ecological distance were prepared and the strength of the linear and monotonic relationships between dissimilarity and ecological distance were assessed using Pearson product-moment correlation and Spearman rank correlation respectively. Most of the computations were performed using the Numerical Taxonomy Package (NTP; Belbin *et al.*, 1984).

The simulation results were analyzed in several ways:

1. Mean linear and rank correlations were computed for each measure, over all data matrices and within each level of each model property, then arranged in descending order.
2. Tables were produced showing the number of data matrices for which each measure achieved a difference in correlation compared with each other measure which was greater than a chosen threshold.
3. Multiway analyses of variance (ANOVA) were performed on either the correlation values for a chosen measure or the *difference* in correlation between a chosen pair of measures. Separate analyses were carried out within subsets of the simulation experiment for which the combinations of model properties were sufficiently balanced, in order to examine the effects of model properties and their interactions.

The first two approaches did not take account of the unbalanced design and the possible interactions between model properties, but they did serve to distinguish the consistently poor measures from the remainder. The relative performance of the better measures was then examined in more detail using ANOVA.

Results and discussion

Results are presented only for two-dimensional models: the results for the unidimensional models were similar. Fig. 1 shows an example of the relationships between dissimilarity and ecological distance for the coefficients MAN (Fig. 1a), KEN (Fig. 1b) and QSK (Fig. 1c). The data are from a two-dimensional model, with a beta diversity of $1 \times 1R$, skewed response surfaces, random sampling pattern and no noise. The general forms of the relationships are typical for these three measures. They clearly illustrate the contrast between QSK, with its in-built standardization by sample totals, and measures without any such standardization. QSK shows a roughly linear relationship with ecological distance from the minimum dissimilarity value of zero to the point where the dissimilarity reaches a maximum.

Table 4a shows the 29 dissimilarity measures listed in order of mean rank correlation over all 306 two-dimensional models. In Table 4b, they are ordered by mean linear correlation over only those 102 models for which the beta diversity of each gradient was no greater than $0.5R$. At this level of beta diversity there are generally no sample pairs sufficiently far apart that they share no species.

In terms of *mean* rank correlation (Table 4a), the least successful measures were EUC, CSQ, INT and GOW, irrespective of prior data standardization, together with MAN and MAN:SPM. The measures with the highest mean rank correlations all included some form of standardization by species, either explicitly (SPM or DBL), or implicitly (variants of CAN). Excluding CAN, the best of the measures computed without prior data standardization were QSK and B-C. MAN:SAT performed similarly to these two measures and collectively QSK, B-C and MAN:SAT were more successful than CHD.

The measures with the lowest mean *linear* corre-

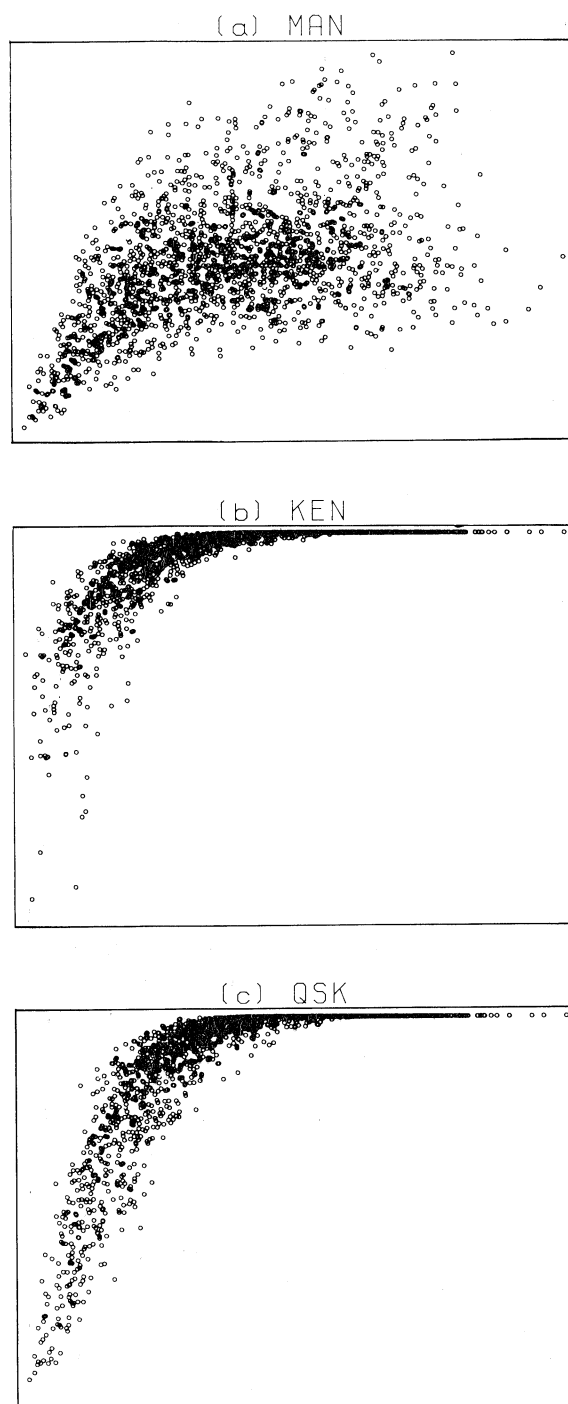


Fig. 1. Relationship between compositional dissimilarity value (vertical axis) and 'target' ecological distance (horizontal axis) for three measures: (a) MAN; (b) KEN; and (c) QSK. Scales of axes are arbitrary. Each circle represents the dissimilarity value - distance value combination for a single pair of sites, for one simulated model. For further explanation see text.

Table 4. Dissimilarity measures ranked in order of (a) mean rank correlation with ecological distance over all 306 two-dimensional models and (b) mean linear correlation with ecological distance over the 102 two-dimensional models in which the beta diversity of the longest gradient did not exceed 0.5R. The abbreviations for the dissimilarity measures are explained in Table 1.

(a) Mean rank correlation	(b) Mean linear correlation
1 QSK:SPM 0.8925	1 QSK:SPM 0.8722
2 B-C:SPM 0.8924	2 MAN:DBL 0.8684
3 MAN:DBL 0.8923	3 B-C:SPM 0.8682
4 CHD:SPM 0.8861	4 GOW:DBL 0.8491
5 CAN:SAT 0.8812	5 QSK 0.8325
6 CAN:DBL 0.8794	6 MAN:SAT 0.8321
7 CAN 0.8791	7 INT:SPM 0.8308
8 KEN:SPM 0.8637	8 CAN:SAT 0.8304
9 MAN:SAT 0.8551	9 CHD:SPM 0.8272
10 QSK 0.8550	10 CAN 0.8265
11 B-C 0.8548	11 CAN:DBL 0.8262
12 CHD 0.8158	12 B-C 0.8243
13 KEN 0.8157	13 GOW:SAT 0.8025
14 GOW:DBL 0.7487	14 KEN:SPM 0.7890
15 INT:SPM 0.7313	15 INT 0.7709
16 GOW:SAT 0.6917	16 EUC:DBL 0.7695
17 GOW 0.6523	17 CHD 0.7611
18 MAN:SPM 0.6522	18 GOW 0.7565
19 INT 0.6423	19 MAN:SPM 0.7564
20 CSQ:SAT 0.6325	20 CSQ:SAT 0.7539
21 EUC:SPM 0.6136	21 EUC:SAT 0.7442
22 CSQ 0.6087	22 KEN 0.7207
23 EUC:DBL 0.6046	23 EUC:SPM 0.7194
24 EUC:SAT 0.6022	24 CSQ 0.7099
25 CSQ:DBL 0.5926	25 MAN 0.6874
26 MAN 0.5617	26 CSQ:SPM 0.6636
27 CSQ:SPM 0.5605	27 CSQ:DBL 0.6625
28 EUC:SPS 0.5471	28 EUC:SPS 0.6424
29 EUC 0.4657	29 EUC 0.6079

lations (Table 4b) included all forms of EUC and CSQ, together with MAN, MAN:SPM, KEN, GOW, CHD and INT. Once again, the best measures included some type of standardization by species. Of the measures without species standardization, QSK and MAN:SAT had the highest mean linear correlations. Next best was B-C.

The relative performance of those measures which had the highest mean rank and linear correlations was examined in more detail using ANOVA. As an example, a summary of the analysis of the *difference* in rank correlation between QSK and CHD for models with symmetric and skewed response shapes is given in Table 5. In this case, the analysis indicates an interaction between beta

Table 5. Summary of the analysis of variance of the difference in rank correlation between QSK and CHD over the 108 two-dimensional models with 'symmetric' and 'skewed' response shapes.

Source of variation	DF	Mean square	Variance ratio	P
Between species sets				
Beta diversity (BD)	5	0.0108523	7.9	<0.001
Response shape (SH)	1	0.0013875	1.0	ns
BD.SH	5	0.0047089	3.4	0.01 – 0.05
Residual	24	0.0013760		
Total	35	0.0032062		
Within species sets				
Quantitative noise (NO)	2	0.0002449	1.9	ns
BD.NO	10	0.0001436	1.1	ns
SH.NO	2	0.0000371	0.3	ns
BD.SH.NO	10	0.0001039	0.8	ns
Residual	48	0.0001256		
Total	72	0.0001260		
Grand total	107	0.0011335		
Grand mean		0.0451		
Total number of observations		108		

diversity and response shape. Examination of the relevant mean values (Table 6) shows that:

1. QSK consistently achieved higher rank correlations than CHD (the difference is positive in all cells).
2. The difference in performance was most marked at the lowest levels of beta diversity, particularly for skewed response shapes.

The results and conclusions presented below are

Table 6. Means for beta diversity \times response shape.

Beta diversity	Response shape	
	Symmetric	Skewed
0.5 \times 0.25R	0.0592	0.1167
0.5 \times 0.5R	0.0747	0.0425
1.0 \times 0.5R	0.0288	0.0416
1.0 \times 1.0R	0.0129	0.0393
2.0 \times 1.0R	0.0241	0.0208
2.0 \times 2.0R	0.0493	0.0311

Standard error of difference of means = 0.0175.

Least significant difference (0.05 level) = 0.0360.

based on similar analyses, although limited space does not permit the inclusion of the ANOVA summaries.

These analyses confirmed that QSK, MAN:SAT, and B-C were similar in both rank and linear correlations. However, for low beta diversity (0.5R or less) together with a unimodal trend in sample totals, we find greater linear and rank correlations for QSK and MAN:SAT compared with B-C. This result may indicate a greater robustness of these measures compared with B-C when site totals vary over short ecological distances.

The results clearly indicate the importance of standardizations, both implicit and explicit. Previous work on data standardization (e.g. Austin & Greig-Smith, 1968; Austin & Noy-Meir, 1971; Noy-Meir *et al.*, 1975; Orłóci, 1978) has been mainly concerned with the implications of standardization in the Euclidean 'species space' assumed by PCA and other techniques based on EUC. In contrast, we emphasize the effects of standardization on the relationship between compositional dissimilarity and ecological distance. For example, MAN:SAT

was one of the most robust and effective measures, whilst MAN and MAN:SPM were among the least successful. The most effective measures all included some form of standardization by sample total, which decreases their sensitivity to variations in sample total and causes such measures to take a constant maximal value for all sample pairs with no species in common.

In this study, standardization of species to equal maxima (SPM) also consistently improved both linear and rank correlations. This standardization tends to equalize the contributions of all species in the calculation of dissimilarities. Without the standardization, the dissimilarities reflect mainly those few species which have high modal abundances. However, we can not unequivocally recommend the use of SPM on field data. There is a danger that it may cause a deterioration in the predictive value of dissimilarities, by increasing the effective weight of sporadic or noisy species which never attain high abundances.

Conclusions

1. The three most effective and robust measures, in terms of both rank and linear correlation, are QSK, MAN:SAT and B-C. MAN:SAT and QSK are indistinguishable over our models, with slight improvement in performance for both over B-C. Because MAN:SAT is equivalent to QSK with the SAT standardization, we can recommend QSK as a basic robust measure, with the possible use of SAT and/or SPM standardizations. Further work with real and artificial data sets may distinguish among these options.
2. CHD is clearly less successful than QSK, MAN:SAT and B-C, in both rank and linear correlation. The use of the B-C measure in ordination has been criticized (Orlóci, 1974, 1978) and the CHD distance recommended as an alternative (Orlóci, 1978). The greater robustness of B-C demonstrated here suggests that there has been undue emphasis upon CHD's metric properties and its absence of a changing scale of measure over different pairs of sites. The rela-

tively weak rank correlation for CHD also implies that the cosine theta (Gower, 1967) and the Geodesic measure (Orlóci, 1978) will also have a poor rank correlation, as they are monotonic with CHD.

3. CAN, with its in-built standardization by species, achieved higher rank correlations than QSK, MAN:SAT and B-C when the latter were applied without prior species' standardization. However, QSK:SPM, MAN:DBL and B-C:SPM consistently gave higher rank correlations than CAN. Furthermore, QSK and MAN:SAT had higher linear correlations than CAN at low beta diversities.
4. Of the measures compared, the least successful, in terms of both rank and linear correlation, were all forms of EUC, KEN, GOW and CSQ, together with MAN (when applied without the SAT standardization).

Implications for ordination

Ordination techniques such as principal components analysis (PCA), principal co-ordinates analysis (PCoA) and correspondence analysis (CA) produce configurations in which the distances between sample pairs are *proportional* to their compositional dissimilarities. Consequently, they would only be expected to recover the configuration of samples in ecological space if values of the dissimilarity coefficient were proportional to ecological distances. In PCA, the implied dissimilarity measure is some form of EUC (or possibly CHD), while CA is based on the CSQ measure. The relatively low linear correlations of EUC and CSQ with ecological distance, observed in this study, explain the poor performance of these techniques in simulation studies (e.g. Gauch & Whittaker, 1972; Gauch *et al.*, 1977; Fasham, 1977; Minchin, 1987a), especially at higher beta diversities.

None of the dissimilarity measures examined in this study has a linear relationship with ecological distance when beta diversity is sufficiently high that some samples have no species in common. However, QSK and MAN:SAT have reasonable linear correlations with ecological distance when beta

diversity is low (0.5R or less). These results imply that, when beta diversity is low, better recovery of ecological space can be achieved by applying a linear ordination technique (e.g. PCoA, metric multidimensional scaling) to QSK or MAN:SAT, rather than using PCA or CA.

The overall *rank* correlation between dissimilarity and ecological distance, as assessed in this study, should provide a basis upon which to predict the relative performance of dissimilarity measures in nonmetric multidimensional scaling (NMDS). The results suggest that QSK, MAN:SAT and B-C should give the most robust and effective ordinations, particularly for 'global' NMDS (Kruskal, 1964a, b; Fasham, 1977), which assumes a single monotone relationship over all sample pairs. Another variant, 'local' NMDS, fits a separate monotone regression for each row of the dissimilarity matrix (Sibson, 1972; Prentice, 1980; Minchin, 1987a). This study did not examine the local or row-wise rank correlations between dissimilarity and ecological distance, hence no firm evidence is available upon which to recommend the most appropriate measures for local NMDS.

We have commented separately on the implications of the linear and rank correlation results for ordination methods. On the one hand, QSK has a robust linear relationship with small ecological distance. On the other hand, QSK shows a robust overall monotonic relationship with distance. We now present a method that takes advantage of both of these aspects of QSK's relationship with ecological distance. This provides a solution to the 'dissimilarity problem' in ordination: the search for a combination of a method that assumes a particular relationship between dissimilarity and distance, and a measure that provides this relationship robustly.

We propose the following procedure, called hybrid multidimensional scaling (HMDS):

1. Compute a matrix of robust dissimilarities, using QSK (or perhaps MAN:SAT or B-C).
2. Make two copies of this matrix. In the first, set all dissimilarities as missing that are above a threshold value. Dissimilarities below this value are taken to have a linear relationship with distance. In the second matrix, keep all values.

3. Use these matrices as input to a multidimensional scaling program such as KYST (Kruskal *et al.*, unpubl. rep.). The first matrix, with missing values, is treated with the metric option (a *linear* regression of distance on dissimilarity) and the second with the non-metric option (a *monotonic* regression). These options can be used in either the 'global' or 'local' forms. The stress, or 'badness-of-fit' of any trial configuration is a combination of the stress contributions from the two matrices.

In practice, a starting configuration may be found using an initial run of NMDS. As another practical consideration, the choice of a fixed threshold may be replaced by a gradual down-weighting of the linear constraint with increasing dissimilarity. We currently use a fixed threshold with HMDS, equal to a value of 0.8 with the measure QSK.

A combination of metric and nonmetric models in multidimensional scaling has previously been suggested by psychometricians as a strategy to avoid degeneracies found in NMDS solutions (see Shepard, 1974). The metric criterion is usually a polynomial fit and the nonmetric criterion of monotonicity is used as a constraint on the form of the polynomial. Similar uses of constraints with NMDS are described in Shepard (1974), and Borg & Lingoes (1980). HMDS differs from these approaches in using a prescribed dissimilarity measure that has a robust metric (linear) relationship with distance only over a certain range. The monotonic regression serves as the only direct constraint on the larger dissimilarities. Critical to the concept of HMDS is that a nonmetric analysis is combined with a metric analysis, but with the values above the threshold value in this latter matrix viewed as misleading and therefore set as missing.

An example of HMDS is illustrated in Fig. 2, for the same complex two dimensional model used for Fig. 1. A plot of the target ecological distances (horizontal axis) versus the ordination distances (vertical axis) shows a close linear relationship (Fig. 2a). Fig. 2b shows the plot of input QSK dissimilarities (vertical axis) against the distances in the ordination (horizontal axis). This may be compared with Fig. 1c, which plots the QSK dissimilarity

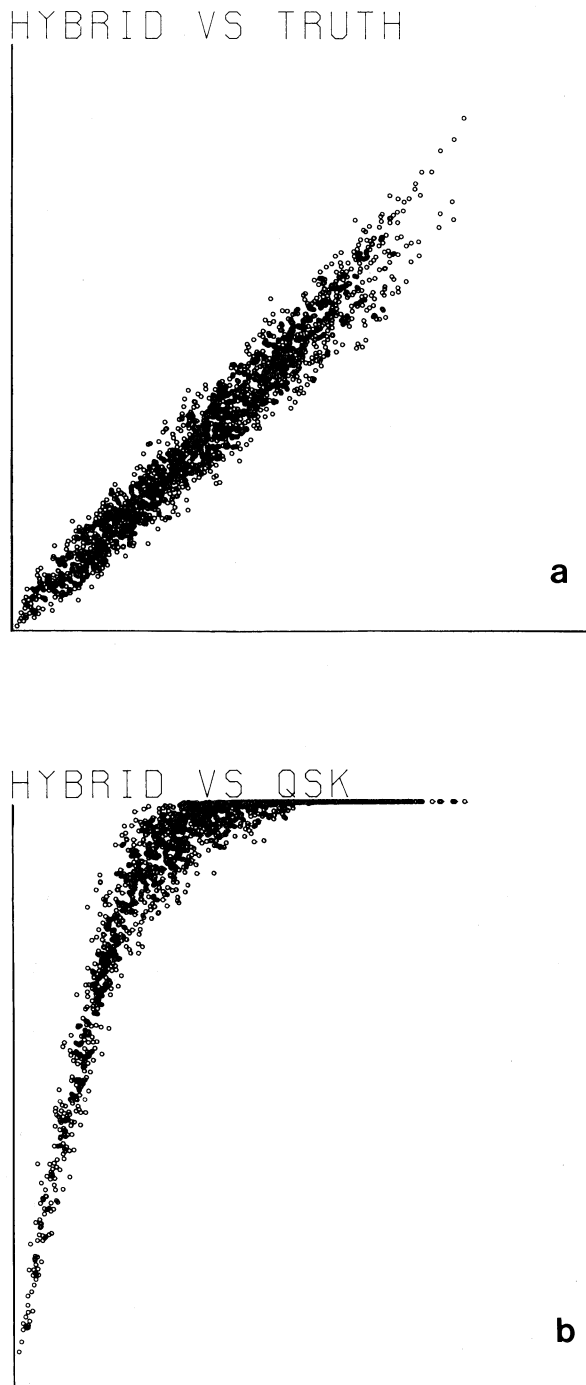


Fig. 2. (a) Plot of Euclidean distances between sites derived from HMDS configuration (vertical axis) versus ecological distances (horizontal axis); (b) Relationship between QSK dissimilarities used as input to HMDS (vertical axis) and the Euclidean distances from the HMDS configuration (horizontal axis). Simulated model used is that of Fig. 1.

ties against the target ecological distances. The metric constraint was enforced up to a threshold QSK dissimilarity value of 0.8, and the configuration distances have a strong linear fit to the dissimilarities up to this threshold. Above this threshold a monotonic relationship between dissimilarity and distance (Fig. 2b) is recovered similar to that for the target (Fig. 1c).

Careful comparisons based on computer simulations are needed to compare the robustness of HMDS with alternative methods. It is clear that meaningful comparisons can only be achieved if appropriate dissimilarity measures are used. In an extensive simulation study to be reported elsewhere (Minchin, Faith & Belbin, unpubl.), we demonstrate the relative robustness of HMDS compared with NMDS (both local and global), metric MDS, and network re-estimation (Williamson, 1978; Beals, 1984), even when all methods use the QSK measure. We hope in a later study to compare HMDS with another method, Parsimony Analysis (Faith *et al.*, 1985) which is in theory highly robust to variations in the model of species' response.

In conclusion, we note that the robust dissimilarity measures identified by this study should be useful in connection with other multivariate methods, (e.g. cluster analysis and network methods) when applied to compositional data with the aim of recovering patterns in ecological space.

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