

Ecology, 68(3), 1987, pp. 750-753
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NONLINEAR ORDINATION USING FLEXIBLE SHORTEST PATH ADJUSTMENT OF ECOLOGICAL DISTANCES¹

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An intriguing method for computing ecological distances between stands with no species in common was described by Williamson (1978) for use with presence-absence data. His example clearly demonstrated the ability of the so-called "step-across" method to recover successfully a gradient of high species turnover in an ordination space defined by principal co-ordinates analysis (PCoA). Despite the promise that this method of distance adjustment seemed to hold for the ordination of data showing high beta diversity, few applications have appeared in the ecological literature. Clymo (1980) outlined a quantitative variant of the distance adjustment, which he termed shortest path, in keeping with the conceptual basis of the method in graph theory (Floyd 1962, Minieka 1978). More recently, Williamson (1983) described a quantitative "step-along" algorithm that incorporates Kendall's (1971) similarity measure. Although these applications of shortest path adjustment improved ordination interpretability, results were inconclusive because they were based on subjective assessments of ordinations arising from single data sets.

We here examine the performance of shortest path adjustment using both real and simulated vegetation data, paying greater attention to an option of the technique alluded to by Williamson (1978:914) and cursorily tested by Clymo (1980). This option permits user flexibility in determining the conditions under which shortest path distances are calculated between stands.

Methods

Flexible shortest path adjustment. Application of shortest path adjustment to ecological data typically involves the replacement of certain values in a distance matrix prior to multivariate analysis. These replacements, termed shortest paths (SP), are recalculated distances between pairs of stands with little or no overlap in species composition. Specifically, each new distance is defined as a sum of distances representing the shortest pathway linking stands with a common floristic component.

The Williamson (1978) algorithm implicitly calcu-

lates shortest paths only between stands showing no overlap in species composition. We denote this as the SP-0 level. Flexibility can be achieved by relaxing this requirement; for example, shortest path distances can be calculated between stands with one or no species in common (SP-1), two species or fewer (SP-2), and so forth. Increasing the level of overlap permitted (SP-1, SP-2, . . .) represents a process in which pairs of stands must share more than a specified number of species in order to avoid having the distance between them calculated as a shortest path. In practice, a level is eventually reached at which the constraints are too stringent, with the result that shortest paths for some stand pairs are not defined. These are termed disjunctions and may indicate regions for partitioning the collection of stands into more homogeneous groups. An efficient FORTRAN routine for performing flexible shortest path adjustment, written by Ki-Sun Kim after Minieka (1978), was used to perform the necessary calculations.

Test data sets. The effectiveness of flexible shortest path adjustment in recovering known data structure was assessed by applying the method to the four sets of quantitative simulated coenoplane data characterized in Table 1. Each consisted of a 6 × 6 systematic grid of stands onto which 36 species (Gaussian responses) were placed in a stratified random manner (see Kenkel and Orlóci 1986 for details). The method was also tested using quantitative (percent cover) data obtained from 26 contiguous 1 × 1 m quadrats placed along an elevational transect through an historical oxbow of the Assiniboine River near Delta, Manitoba. The transect spanned an elevation range of ≈ 2 m, from a cattail marsh (*Typha glauca*) to the edge of a mature gallery forest of bur oak (*Quercus macrocarpa*) and green ash (*Fraxinus pennsylvanica*).

Nonmetric multidimensional scaling. Shortest path adjustment of Euclidean distances implies a loss of metric properties, since the triangle inequality property will be violated. While Gower (1967) and Williamson (1978) have defended the use of nonmetric resemblance measures with PCoA, problems arise in

TABLE 1. Characterization of the four simulated coenoplane data sets used in the study. Species richness and Shannon-Wiener alpha diversity (H') values are means of 36 stands.

Coenoplane dimensions (HC-units)*	Species richness	H'	Percent zeros
2 × 2	18.1	2.96	50.0
3 × 3	13.3	2.61	63.0
4 × 4	10.6	2.12	71.0
5 × 5	8.7	1.91	76.0

* Half-changes (HC) indicate rates of species turnover along two independent gradients of the coenoplane.

theory and practice (Dale 1975, Seber 1984). We therefore used nonmetric multidimensional scaling (NMDS; Kruskal 1964a, b) to ordinate the data. Since this method attempts to preserve only the rank order relationships of the resemblance matrix in a reduced ordination space, nonmetric coefficients can be accommodated without violating statistical assumptions (Kenkel and Orlóci 1986). Ordinations were performed using program ALSCAL (Young et al. 1980) based on a Euclidean distance matrix before and following various levels of shortest path adjustment. In each case adjustment levels were raised until a disjunction was encountered; in total, 37 ordinations were performed. Evaluations of the coenoplane ordinations were based on Kruskal's (1964b) stress index, and on Procrustes error sum of squares values (Schönemann and Carroll 1970) obtained by comparing each ordination scattergram to the systematic grid of stands. Success of the oxbow

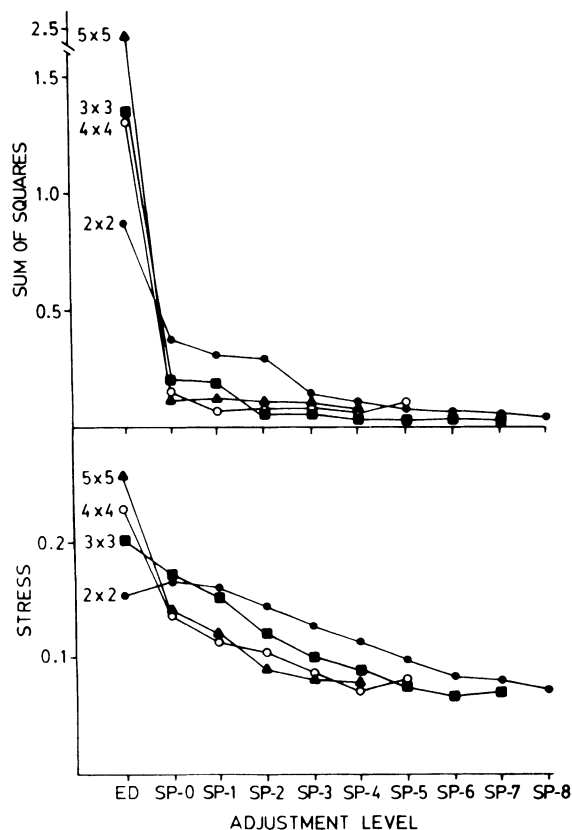


FIG. 1. Effects of increasing shortest path (SP) adjustment levels in nonmetric multidimensional scaling (NMDS) ordinations of four simulated coenoplanses, whose dimensions are in half-change units. The upper graph shows changing error sum of squares values from Procrustes analysis comparing ordinated coenoplanses with a target grid. The lower graph shows changing stress values in the NMDS ordinations.

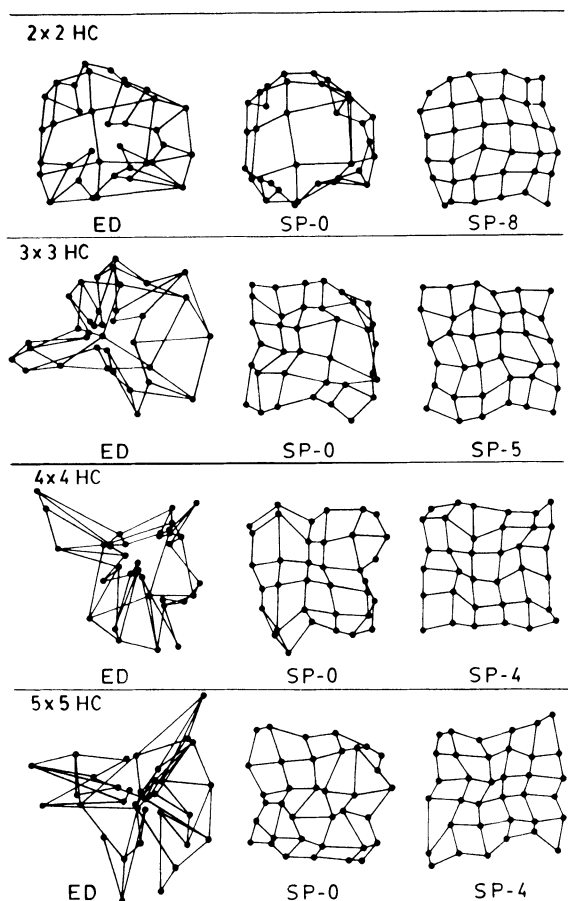


FIG. 2. Selected NMDS ordinations of simulated coenoplane data (Table 1) illustrating improvements attributable to higher levels of shortest path (SP) adjustment.

transect ordinations in recovering the elevational gradient was assessed visually. In addition, Kruskal stress values were computed and Shepard diagrams (Kruskal and Wish 1978) plotted to examine the relationship between calculated and spatially derived distances.

Results

Simulated coenoplanses. Procrustes sum of squares and Kruskal stress values for the NMDS ordinations are presented graphically in Fig. 1. In general, the replacement of Euclidean distances by shortest path values for stands with no species in common (SP-0) led to the largest single-level reduction in these values. Moreover, the magnitude of this initial reduction increased with the amount of species turnover on the coenoplane. The only exception was a slight increase in the stress value for the 2 × 2 HC coenoplane, reflecting the increased compression of coenoplane margins in the initial stage of unfolding (Fig. 2). The other

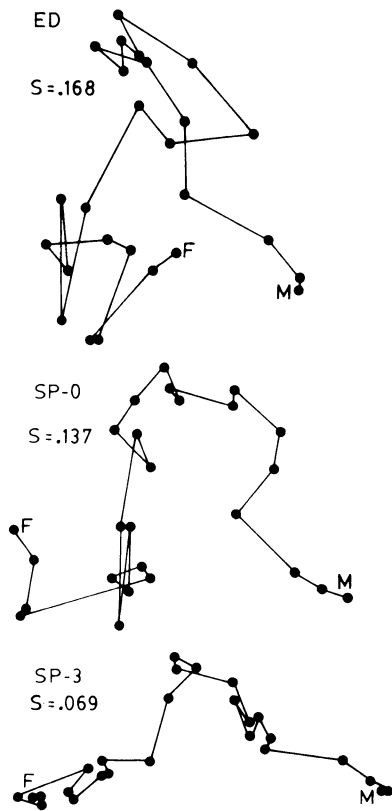


FIG. 3. NMDS ordinations of the oxbow transect, using a Euclidean distance matrix before (ED) and after two levels of shortest path adjustment (SP-0 and SP-3). Kruskal stress values (S) are also given. Gradient endpoints are indicated by M (*Typha* marsh) and F (gallery forest edge).

coenoplanes exhibited nearly complete unfolding at the SP-0 level owing to a greater number of shortest path replacements in their respective distance matrices. Further increases in the level of shortest path adjustment produced modest reductions in stress and sum of squares values for the 3×3 , 4×4 , and 5×5 coenoplanes, except that slight increases in these values were observed in some cases at the highest adjustment levels. In contrast, notable stress reduction in the 2×2 coenoplane did not occur until the SP-3 adjustment level, but continued to the SP-8 level. As expected, disjunctions were encountered at lower adjustment levels as the degree of species turnover on the coenoplanes increased. The selected ordination scattergrams shown in Fig. 2 summarize the effectiveness of flexible shortest path adjustment in recovering known relational structures of the data.

Oxbow transect. The oxbow transect ordinations at selected levels of shortest path adjustment are presented in Fig. 3. The use of unadjusted Euclidean dis-

tance (ED) led to severe distortion and infolding of the elevation gradient. Standard shortest path adjustment (SP-0) partially corrected for the gradient infolding, though substantial distortion remained. Further improvements were gained by increasing the level of shortest path adjustment, and at the highest level (SP-3) the elevation gradient was recovered well. The corresponding Shepard diagrams (Fig. 4) indicate that as adjustment levels are raised, the distances portrayed in ordination space are more linearly related to those on which the calculations are based.

Discussion

Our results suggest that the use of flexible shortest path adjustment with NMDS ordination has great promise as a general strategy for the analysis of ecological data sets showing moderate to high levels of species turnover. Such an approach appears to be capable of recovering nonlinear data structures as well as any of the conventional ordination methods, many of which involve abstract data standardizations and manipulations (Kenkel and Orlóci 1986). With flexible shortest path adjustment of Euclidean distances, the user retains a clear conceptual understanding of the distance calculations and may therefore be confident that the resultant ordination reflects the underlying data structure (Williamson 1983). Although we have illustrated the method using Euclidean distance, in practice any distance function could be used.

Increasing the level of shortest path adjustment has been shown to lead to an improved ordination config-

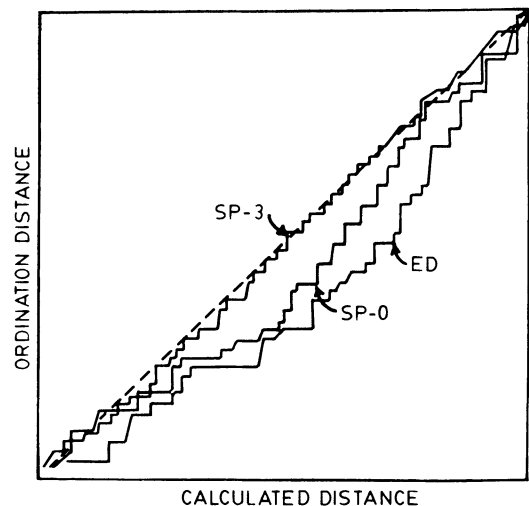


FIG. 4. Shepard diagrams associated with the ordinations shown in FIG. 3. Diagrams for the SP-1 and SP-2 levels (not shown) lie between those for SP-0 and SP-3. Dashed line signifies a perfect linear relationship between calculated and ordination distances.

uration. Users must therefore select an adjustment level suitable to their data. Our results indicate that at high levels of species turnover (5×5 HC) there is little to be gained by increasing the adjustment level above SP-0. At more moderate turnover levels (2×2 HC), the highest possible adjustment level appears to give the best results. With real data, numerical indices such as Kruskal's stress may provide guidelines for selecting among alternative NMDS configurations, although the final decision necessarily remains subjective. For the oxbow transect data, two noteworthy features have emerged from raising the adjustment level: (a) stress tends to decline, though not monotonically (the stress value rose slightly from the SP-0 to the SP-1 level, then dropped at SP-2), and (b) relationships between original distance values and ordination distances become more linear. As a result, the highest adjustment level (SP-3) led to a configuration most consistent with hypothesized ecological relationships.

Acknowledgments: Both authors received financial support from the Natural Sciences and Engineering Research Council of Canada. We thank J. Podani and three anonymous reviewers for their helpful comments and criticisms. Contribution Number 149 from the University of Manitoba Field Station (Delta Marsh).

Literature Cited

- Clymo, R. S. 1980. Preliminary survey of the peat-bog Hummell Knowe Moss using various numerical methods. *Vegetatio* **42**:129–148.
- Dale, M. B. 1975. On objectives of methods of ordination. *Vegetatio* **30**:15–32.
- Floyd, R. W. 1962. Algorithm 97: shortest path. *Communications of the Association for Computing Machinery* **5**:345.
- Gower, J. C. 1967. Multivariate analysis and multidimensional geometry. *The Statistician* **17**:13–28.
- Kendall, D. G. 1971. Seriation from abundance matrices. Pages 215–252 in F. R. Hodson, D. G. Kendall, and P. Tautu, editors. *Mathematics in the archeological and historical sciences*. Edinburgh University Press, Edinburgh, Scotland.
- Kenkel, N. C., and L. Orlóci. 1986. Applying metric and nonmetric multidimensional scaling to ecological studies: some new results. *Ecology* **67**:919–928.
- Kruskal, J. B. 1964a. Multidimensional scaling by optimizing goodness of fit to a nonmetric hypothesis. *Psychometrika* **29**:1–27.
- . 1964b. Nonmetric multidimensional scaling: a numerical method. *Psychometrika* **29**:115–129.
- Kruskal, J. B., and M. Wish. 1978. *Multidimensional scaling*. Sage, Beverly Hills, California, USA.
- Minieka, E. 1978. *Optimization algorithms for networks and graphs*. M. Dekker, New York, New York, USA.
- Schönemann, P. H., and R. M. Carroll. 1970. Fitting one matrix to another under choice of a central dilation and a rigid motion. *Psychometrika* **35**:245–255.
- Seber, G. A. F. 1984. *Multivariate observations*. J. Wiley, New York, New York, USA.
- Williamson, M. H. 1978. The ordination of incidence data. *Journal of Ecology* **66**:911–920.
- . 1983. The land-bird community of Skokholm: ordination and turnover. *Oikos* **41**:378–384.
- Young, F. W., Y. Takane, and R. Lewyckyj. 1980. ALSCAL: a multidimensional scaling package with several individual differences options. *American Statistician* **34**:117–118.

¹ Manuscript received 16 June 1986; revised 12 October 1986; accepted 20 October 1986.

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