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Differences in performance of four ordination methods on a complex vegetation dataset

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Ordination is a widely used method in describing main relationships of multidimensional data. Properties of different ordination techniques have mostly been tested with simulated data. Although simulations provide valuable information about the behaviour of different methods, they are likely to be too simplistic to be able to completely predict the outcome with real data. We used post-fire vegetation succession data to compare four commonly used ordination techniques: CA (correspondence analysis), DCA (detrended correspondence analysis), PCoA (principal coordinates analysis), and NMDS (non-metric multidimensional scaling). Fire intensity was used as a method-independent criterion for comparing the performance of the different methods. Solutions produced by these methods were compared using Procrustean analysis. According to our results, the compared ordination techniques presented different aspects of the multidimensional species space. In general, metric scaling methods, particularly CA and DCA, were far better in reflecting the main gradient in numerical terms, as compared with NMDS. In contrast, non-metric scaling out-performed metric scaling in graphical terms. We conclude that none of the compared methods is perfect in reflecting a complex vegetation gradient. Also, the difference in their abilities makes it difficult to point out the most suitable method for our data.

Key words: comparison, forest succession, indirect gradient analysis, ordination, Procrustean analysis

Introduction

Ecologists often want to display main relationships of their multidimensional data in few dimensions in order to be able to examine the ordering of, and relationships between, different samples and species. Hence, ordination in reduced space is widely used in ecological studies. The aim of ordination analysis is to find the main compositional gradients and to identify the main underlying environmental factors (e.g. Økland 1996), or to study changes in species composition along previously identified gradients. However, it is not always clear which of the available methods fits best the collected data.

The two most frequently used techniques to evaluate the relative merits of ordination methods are: comparison by means of simulated data (e.g. Kenkel & Orloci 1986, Minchin 1987), and by means of real data (e.g. Prentice 1977, Oksanen 1983), respectively. Simulated datasets may provide a good basis for evaluation of ordination methods. However, the problem (and at the same time the advantage) is that simulation tests require *a priori* specification of dataset properties. This makes the comparison of different methods easy, but at the same time they may lack realism (Økland 1990). All currently available ordination methods assume all species having the same response curve (Rydgren *et al*. 2003), which makes simulated data ideal for testing the theoretical properties of different methods. However, this assumption can never be satisfied with real data.

A reliable comparison of methods relies on an evaluation criterion independent of the methods themselves. As the true structure of real data is unknown (Oksanen 1983, Minchin 1987), a reliable comparison of ordination methods cannot be achieved in the same way as in simulated tests. When there is no pre-known gradient structure, which a successful ordination is expected to recover, an alternative, independent criterion is needed (e.g. Prentice 1977). When performed objectively, analyses on the behaviour of ordination methods on real data provide a necessary supplement to a comprehensive evaluation and comparison of ordination techniques.

In this paper we compared the performance of four different ordination methods (CA = correspondence analysis, DCA = detrended correspondence analysis, PCoA = principal coordinates analysis, and NMDS = non-metric multidimensional scaling) on a complex vegetation data. The data comprehend ten years of succession after wildfire of different intensities and unaffected control areas (> 80 years old) in a middle boreal *Vaccinium–Empetrum* type (Cajander 1921) *Pinus sylvestris*-dominated heath forest. The ordination solutions were visually compared using Procrustean analysis (e.g. Økland 1990).

Materials and methods

Data description

We used a quantitative vegetation dataset, collected during a 10-year period after a wildfire in Kitsi (North Karelia, Finland), in order to compare the performance of different methods of reduced space ordination on vegetation composition along a succession gradient. The data comprise the initial succession (ten years) and the climax community (> 80 years) as the control. The study area was distributed on two adjacent semi-dry heath stands; Jäkäläkangas (Jk) and Pöytäkangas (Pk). After the fire in 1993, 22 permanent sampling plots (100 m^2 each) were established in the burned areas and adjacent unburned stands (controls CJ and CP on Jäkäläkangas and Pöytäkangas, respectively) (Table 1). Within each plot, at each sampling event, percent coverage of all plant species was estimated. The collected data was used to construct a sites by species matrix, with 70 rows (sites) and 81 columns (species).

The sampling plots represent, in addition to unburned control, four apparently different fire intensities (based on visual evaluation of the vegetation development and inspection of responses of individual species): Ground fire after clear

Table 1. Details considering the sampling design. Letters refer to different sites within the study area, being differently affected by the fire.

Area	Number of plots	Sampling events (years after fire)	*n*	Notions
A	4	1, 3, 5, 10	16	
B	4	2, 3, 5, 10	16	Plots established in 1994
C	4	1, 3, 5, 10	16	
D	4	5, 10	8	Plots established in 1997
CJ	2	3, 5, 10	6	Plots established in 1995, only two plots due to lack of available space
CP	4	5, 10	8	Plots established in 1997

cutting (on Jk) (A), ground and canopy fire (on Jk) (B), ground fire on Jk (C), and ground fire on Pk (D). Relative fire intensity at ground level was: A > B > C > D.

Data analysis and description of the applied methods

There is evidence for fire intensity influencing post-fire vegetation recovery (e.g. Schimmel 1993) and according to Økland (2000) it is likely to be one of the most important determinants of postfire species composition. Against this background we tested how well the first two axes of the considered methods reflected the fire intensity gradient in our data. This was done using dummy-variable regression. A variable with five states of fire intensity (A–D and control) was coded to four binary variables (Legendre & Legendre 1998). Statistical significance was tested with 9999 permutations. According to the regression analyses, fire intensity explained on average 73% of the variation on the first axis and 38% on the second axis of the selected ordination methods (Table 2). Moreover, the importance of fire intensity was also assessed on individual species. These analyses resulted in an average 24% (p = 0.098, n = 81) explained variation for all species and 33% (p = 0.02, n = 50) for species with a significant relationship with fire intensity. As a considerable amount of variation in different ordination axes and species abundances could be accounted to fire intensity, it could be utilized in comparing ordination performance. The Permute! 3.4a9 software was used in the analysis (available at http://www.bio.umontreal.ca/legendre).

We applied the following ordination methods to the data: CA (Hill 1974), DCA (Hill & Gauch 1980), PCoA (Gower 1966), and NMDS (Kruskal 1964). CA is a metric scaling method that optimizes the dispersion of sample optima in relation to species scores in a data table (Økland 1990, Legendre & Legendre 1998). The species scores are estimates for species optima. Thus it assumes a unimodal model. As an inherent property of the method, it preserves a χ^2 distance between samples (or species, depending on scaling type). Two main problems associated with CA are the *arc effect* (the appearance of ordination axes that are polynomial functions of one or more axes of lower rank) and the *edge effect* (a tendency for samples and species near gradient end-points to be strongly compressed). DCA is an *ad hoc* modification of CA (Økland 1990) that aims to remove both the *arch* (detrending) and *edge effect* (rescaling). This method assumes species having symmetrical, unimodal distributions, with equal standard deviation (Legendre & Legendre 1998). PCoA is a metric scaling method that projects the distances in the original multidimensional space to lesser dimensions (Legendre & Legendre 1998). It maximises a linear correlation (Pearson) between the original distances and those in the reduced space. Any distance measure can be used to define the original space. PCoA is also known to produce curved structures (e.g. Minchin 1987, Legendre & Legendre 1998). NMDS is a non-metric scaling method. As PCoA, it uses a given resemblance matrix, but it constructs a configuration of points in a specified number of dimensions, in a way that maximises the rank order agreement between inter-point distances and the resemblance values (Minchin 1987). The 'best' configuration is found through an iterative process by optimising a stress function.

In the analyses, PCoA and NMDS were based on a Bray & Curtis dissimilarity matrix. This coefficient is designed for quantitative data and it is frequently used in ecological studies (Legendre & Legendre 1998). NMDS was run with the following options: maximum number of iterations = 500, tolerance = 0.000 000 01. Stable minimum stress solution was sought with Procrustean rotation. Final solution was rotated to its principal components, in order to maximize

Table 2. Coefficients of determination (R^2) for dummy variable regressions between fire intensity (independent) and the first and the second axis (dependent) of the considered ordination methods. p = 0.0001 for all analyses.

Method	Axis 1	Axis 2
CA	0.87	0.50
DCA	0.88	0.29
NMDS	0.45	0.46
PCoA	0.73	0.28

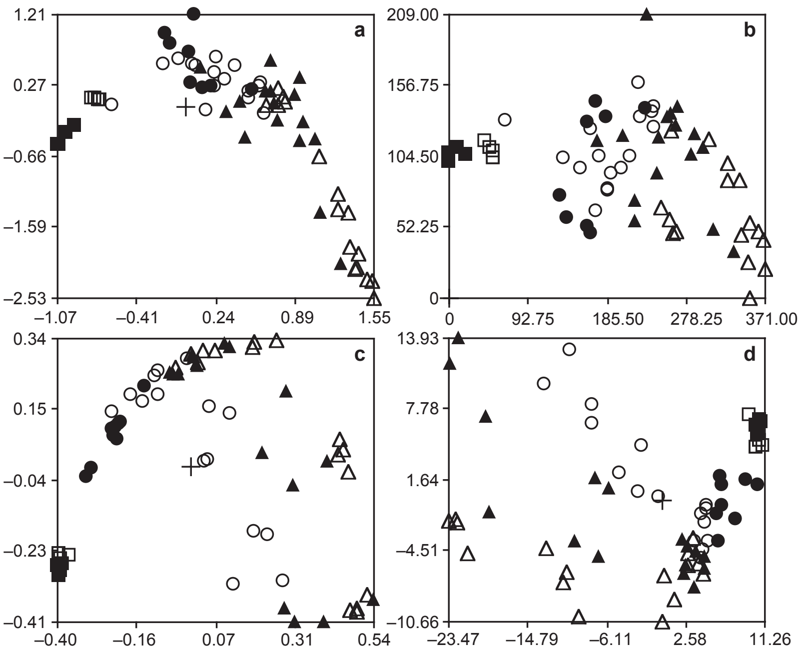

Fig. 1. Four different ordinations representing four methods: — **a**: CA, — **b**: DCA, — **c**: PCoA (Bray & Curtis distance), and — **d**: NMDS (Bray & Curtis distance). The axes are the first and the second ordination axis for each method. Labels: White triangle = site A, black triangle = site B, white circle = site C, black circle = site D, white square = CJ, black square = CP (controls).

the variation accounted for the selected axes. In DCA, detrending was performed with segments and the resulting axes were rescaled using non-linear rescaling. Rare species were not down-weighted. The analysis was run with standard options, as recommended by Økland (1990). Both a two and a three dimensional solution was calculated for all methods.

The ordinations (two dimensional) were made visually comparable with Procrustean rotation (Minchin 1987, Økland 1990). This technique fits one configuration to another, minimizing the sum of squared distances between each point in the fitted configuration and its corresponding point in the target configuration. Hence, it rotates a solution in a way that maximizes its similarity with another solution. Procrustean analysis also provided a correlation coefficient between configurations (significance was tested with 999 permutations). Both the ordination and Procrustean analyses were run with the R software.

Results

CA arranged the data in a clear and compact arch, suggesting a strong dominant gradient (apparently a temporal one) in the data (Fig. 1a). DCA did somewhat flatten the arch producing a tongue effect (Fig. 1b). The detrending procedure did also stretch out the points in the mid-portion of the diagram, separating the different sites (A–D) more clearly. Like CA, PCoA also expressed strong curvature of the main gradient. Moderate curvature was also observed in the NMDS solution. However, only minor distortion was observed.

Apparently, PCoA and NMDS perform far better than CA and DCA in displaying differences between the sites during the first three years of succession. In contrast, CA and particularly DCA seemed to express greater differences between sites in later succession. All methods separated the control plots from the burned plots.

According to the Procrustean analyses, PCoA and NMDS solutions were the most similar of all pairs (Tables 3 and 4). Also CA and DCA seemed to resemble each other more than they did PCoA or NMDS. These results could be expected to some extent from the properties of the methods (same resemblance measures). Moreover, NMDS differed the most in comparison to the other methods.

Visual comparison of the pairwise rotation of the two dimensional ordinations revealed great differences in the relative ability of different methods to uncover differences between the sites A–D (Fig. 2). NMDS was the only ordination technique that found clear differences between all the different sites, as compared with the other methods. However, the metric techniques were able to separate A from D and C, and B from D, but the separation between B and C, and A and B were not that pronounced or nonexistent.

Discussion

The ability of an ordination technique to express differences between sites that were differently affected by wildfire was used to compare the performance of four ordination methods. According to our results NMDS ordination performed visually best on the basis of the selected comparison criterion. However, it seemed possible for the metric scaling methods to also achieve the selected goal, if a sufficient number of dimensions would have been examined. Nonetheless, NMDS needed only two dimensions whereas the other methods would have required three or more. Moreover, higher axes are often difficult to interpret in ecological terms (Økland 1990), which makes a low dimensional solution desirable. As the selected comparison criterion was independent of the methods, these observations should be relatively reliable.

However, the NMDS solution was the worst in reflecting the underlying fire intensity gradient in numerical terms. The metric scaling methods, especially DCA, were far better in recovering this gradient in the first two dimensions. Not knowing the quantitative difference in fire intensity, the ability to separate differently affected sites can be used only as a crude measure of performance. Nevertheless, as the data structure was non-linear (as shown by all the methods), a linear fit cannot completely describe the relationship between the fire intensity gradient and the ordination space.

All methods, especially CA and PCoA, displayed distortion of the main gradient. The nature of curvilinear structures has been debated extensively. They have been characterised both as mathematical artefacts (e.g. Gauch *et al*. 1977, Hill & Gauch 1980) and as true properties of the data (e.g. Dale 1975, Van Der Maarel 1980, Wartenberg *et al*. 1987). The present view seems to be that the distortions are a result of a mismatch between the ordination model and species response curves. According to Økland (1990), the variation in response curve shapes is an inevitable cause of distortions in ordinations that cannot be amended within the concept of ordinations based upon one statistical model. In this case, the least curvature observed in the NMDS solution might have been due to NMDS being less sensitive to the variation in species response curves.

This curvature (although minor) in the NMDS solution may be the reason for high similarity between NMDS and PCoA. Although curvilinear distortions are not generally considered to burden NMDS, they may well appear although they have been described only a few times with ecological data (e.g. Økland & Eilertsen 1993). Typically, polynomial axes appear in NMDS if a too high dimensionality is chosen for the solution. In this case a two dimensional solution was considered. As there was also a clear temporal gradient in the data, two dimensions could not be considered excessive.

Our results with real data coincide with results obtained using simulated data, regarding NMDS, PCoA and CA (e.g. Kenkel & Orlóci

Table 3. Correlations between different ordination methods in symmetric Procrustes rotations. Significance in all correlations: $p < 0.001$. Based on 999 permutations. *r* is the correlation coefficient.

	r
PCoA × NMDS	0.84
CA × NMDS	0.60
DCA × NMDS	0.65
CA × PCoA	0.66
DCA × PCoA	0.69
CA × DCA	0.77

Table 4. Procrustes sum of squares of pair-vice rotations of the ordination solutions. Read left to right.

	CA	DCA	NMDS	PCoA
CA		40.7	2595	5.661
DCA	107.2		2359	5.31
NMDS	167.4	57.77		2.893
PCoA	146.7	52.25	1162	

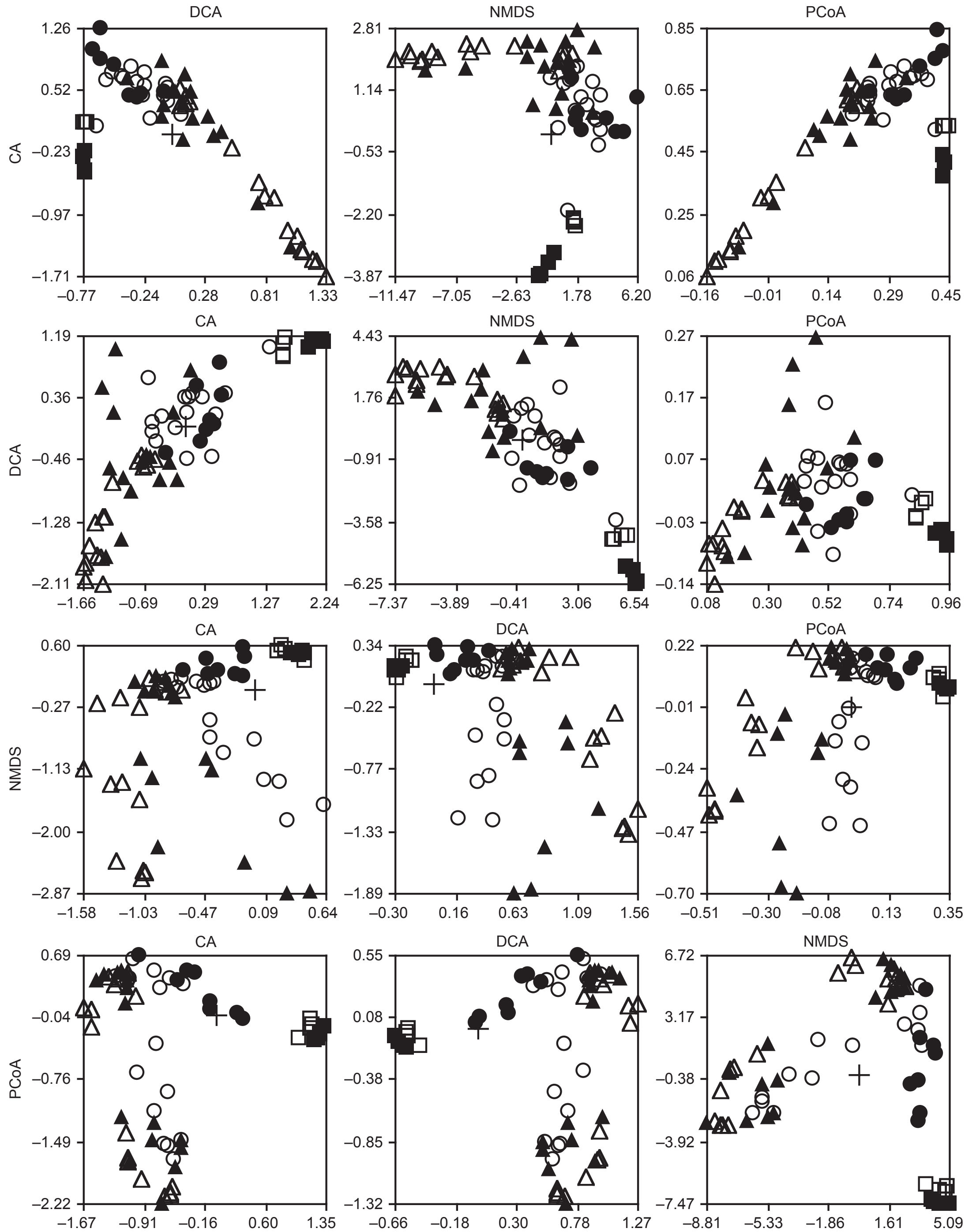

Fig. 2. Configurations obtained from pairwise Procrustean rotation between four 2D ordination solutions. Read left to right. The axes are the first and the second ordination axis for each method. For label description *see* Fig. 1.

1986, Minchin 1987), but not regarding DCA. According to e.g. Kenkel and Orlóci (1986), DCA should perform almost as well as NMDS. However, this was not the case with our data. The solutions obtained with DCA and NMDS differed remarkably, both visually and in their ability to reflect the fire intensity gradient. One possible explanation is that detrending by segments is sensitive to error variation (Oksanen 1988) that is inevitably present in a field dataset.

Conclusions

It is clear that the underlying model and assumptions, particularly in DCA, of ordination methods perform better the more homogeneous the species response curves are. However, when species are heterogeneous in their distributions (which often is the case), metric scaling methods seem particularly defective.

So far, there is no basis for picking out the best method. Further, the arch of NMDS, the tongue of DCA and the strong arches of CA and PCoA interestingly show that no method is perfect. Also the differences in their ability to reflect the underlying fire intensity gradient shows that it is not a straightforward procedure to point out the most suitable method.

Our results, although they provide only one aspect, show that simulated tests are not always successful in predicting the outcome with real data. Therefore, methodological comparison with real data is also needed for a thorough assessment of the characteristics of different methods.

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