Revisions for the Bray and Curtis ordination

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Received November 22, 1973

Orlóci, L. 1974. Revisions for the Bray and Curtis ordination. Can. J. Bot. **52**: 1773–1776.

The revisions suggested remove from the Bray and Curtis method certain unwanted inconsistencies while retaining the use of freely chosen ordination poles. The revised method performs metric scaling on oblique axes.

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L'auteur suggère des modifications à la méthode d'ordination de Bray et Curtis. Ces modifications éliminent certaines inconsistances indésirables, tout en conservant le libre choix des pôles d'ordination. La méthode revisée effectue une graduation métrique sur des axes obliques.
[Traduit par le journal]

Introduction

It seems to me that those who have used the Bray and Curtis (1957) method have done so because they wanted to take advantage of an ordination in which they can freely select axes with no mandatory constraints to satisfy certain optimality criteria. They might have found also attractive the simplicity of the arithmetic in the face of more complicated methods of multidimensional scaling. Among the many ecologist users, however, few apparently may have realized that this method is burdened by the following serious inconsistencies:

(1) the distance function can change its scale of measure from one pair of stands to the next;
(2) the distance function is not always capable of forming ordinary Euclidean triangles, and yet the method requires manipulations of such triangles to determine ordination coordinates for the stands;
(3) the method of scatter diagram construction assumes perpendicular coordinate axes, when in fact the axes are normally oblique.

These inconsistencies in the procedure present a dilemma to the user in deciding whether to accept the ordination and apply it as originally proposed or instead to seek improvements in the method before subjecting it to further applications. In the present paper I propose revisions that remove the unwanted inconsistencies while still retaining the original method's free selection of ordination poles. In the first part of the paper the distance function is examined. Problems related to the construction of scatter diagrams are treated in the second part.

The Distance Function

In their description of the method, Bray and Curtis suggest $1 - 2w/(a + b)$ as the distance formula to define stand relationships in a sample. In this formula w = SUM MIN (X_{ij}, X_{ik}), a = SUM(X_{ij}), and b = SUM(X_{ik}), where MIN indicates minimum value, SUM means summation over all species from $i = 1$ to p, X_{ij} signifies the value of species i in stand j, and X_{ik} indicates the value of the same species in stand k. We can see from the relations in $b(j, k) = 1 - 2w/(a + b) = 1 - 2$ SUM MIN $(X_{ij}, X_{ik})/Q_{jk}$ = SUM ABS$(X_{ij} - X_{ik})/Q_{jk}$, where ABS indicates absolute value and $Q_{jk} = a + b$, that actually $b(j, k)$ is a scrambled absolute value function. Such a function has two definitely undesired properties:

(1) a new scale of measure for measuring distance with each new value of Q_{jk};
(2) possible failure of distance on the triangle inequality condition ($d(j, k) \leq d(j, m) + d(k, m)$ for any three stands j, k, m whose distances are $d(j, k)$, $d(j, m)$, $d(k, m)$).

Property 1 makes the scale of measure dependent on the stands which happened to be compared. Property 2 means that the distance is not suited to construction of triangles on the manipulation of which the entire ordination procedure is founded. These are a direct consequence of the division of the sum of absolute differences by a variable quantity, Q_{jk}.

The relation $Y_{ij} = b(j, k) \cos \alpha_{jm} = [b^2(j, k) +$

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$b^2(k, m) - b^2(j, m)]/2b(k, m)$ formalizes the algebraic operation in the Bray and Curtis procedure. Here Y_{ij} is the coordinate of stand j on axis i through stands k, m as ordination poles. It can be seen that this formula incorporates a cosine relation. This relation necessarily implies that $Y_{ij}/b(j, k)$ itself must qualify as a cosine function. However, if $b(j, k)$ fails on the triangle inequality condition, the value of $Y_{ij}/b(j, k)$ may exceed 1 or it may be less than -1.

The point in the preceding paragraph is demonstrated in an example based on my data in Table 1. In this table the entries represent species abundance values in three quadrats for five different species. The $b(j, k)$ values of the quadrats are given by

$b(1, 1) = 0,$ $b(2, 3) = 0,$ $b(3, 3) = 0$
$b(1, 2) = 0.0588235,$ $b(2, 3) = 0.5333333$
$b(1, 3) = 0.6000000$

These indicate an inequality

$$b(1, 3) > b(1, 2) + b(2, 3) = 0.5921568$$

in direct contrast with the inequality expected from Euclidean triangles. Because of this, the quantity $Y_2/b(1, 2)$ turns out to be equal to 1.1193910. But the cosine of an angle should not exceed unity. Any value in excess of 1 indicates that $b(j, k)$ is not a metric. We conclude then that $b(j, k)$ in this case failed to form a suitable triangle and that if it were used as a measure of distance it could considerably distort the ordination.

To overcome this problem the Bray and Curtis ordination should be based on a distance function other than $b(j, k)$. Such a function should measure consistently on the same scale and should not fail on the triangle inequality axiom. There are many functions that have these properties, such as the following.

(1) $e(j, k)$ = SQRT[SUM$(X_{ij} - X_{ik})^2$]. This is an Euclidean distance. While its scale does not change, and it always satisfies the triangle inequality condition, it does not have a fixed upper bound, and it is influenced by differences in absolute species quantity between the stands;

TABLE 1

Sample data. Entries represent species abundance values

Species	Quadrat 1	2	3
X_1	2	3	9
X_2	5	5	1
X_3	2	2	1
X_4	5	4	1
X_5	3	3	1
Total	17	17	13

(2) $c(j, k)$ = SQRT[2(1 − cos α_{jk})] = SQRT [SUM$(X_{ij}/S_j - X_{ik}/S_k)^2$]. This represents an Euclidean distance measuring a chord length (Orlóci 1967) between points placed on the surface of a unit radius sphere. The $c(j, k)$ are relative measures with minimum at 0, when the quadrats have identical species in the same proportions, and maximum at SQRT(2), when there are no species in common. S_j and S_k are defined respectively by SQRT(SUM(X_{ij}^2)) and SQRT (SUM(X_{ik}^2));

(3) $a(j, k)$ = SUM ABS$(X_{ij} - X_{ik})$. This is another distance measure, known as the absolute value function. This has no fixed upper bound, and similarly to $e(j, k)$, it reflects differences in absolute species quantity between the stands;

(4) $w(j, k)$ = SUM ABS$(X_{ij}/Q_j - X_{ik}/Q_k)$. This relativizes the absolute value function (Whittaker 1952). Its maximum is 2, when the quadrats have no species in common, and minimum 0, when the quadrats contain identical species, and the quantities of species are proportional. Here Q_j = SUM(X_{ij}) and Q_k = SUM (X_{ik}).

Functions $c(j, k)$ or $w(j, k)$ are preferred in the kind of manipulations to which a distance function is subjected by the Bray and Curtis ordination. The fact of the matter is that these functions do everything which $1 - 2w/(a + b)$ was intended to do, and they do it in a manner completely consistent with the ordination algebra. Functions $c(j, k)$ and $w(j, k)$ are both relativized, retain the same scale of measure in all comparisons, and never fail to form suitable triangles. It may be that in spite of these properties the user would still prefer to base ordination on $1 - 2w/(a + b)$; but if he does, he should choose some ordination technique other than the one suggested by Bray and Curtis.

Construction of Scatter Diagrams

When it comes to constructing scatter diagrams based on the Bray and Curtis axes, the user faces two specific problems: (1) the axes (X, Y) may not intersect as lines in higher space; (2) the axes do not have any predictable directional relationship. Stands of vegetation may be ordered on such axes individually, but problems arise when the user wishes to show the joint distribution of the axes.

A revision that can remedy this problem is suggested in the present paper. The revised method requires no assumptions about the orientation of *X* and *Y* (whether perpendicular or oblique). *X* and *Y* are projected perpendicularly onto a common plane *M*. This plane is so selected that it incorporates *Y* and it is parallel to *X*. Furthermore, plane *M* is the locus of a scatter diagram which shows the joint distribution of *X* and *Y*. The solution is outlined below in connection with Fig. 1.

The sample distances of the ordination poles (*ABCD*) and of a stand *j* are given in Table 2. A scatter diagram can be constructed according to the following steps.

1. Draw triangles *ABC* and *ABD* (Fig. 1).
2. Draw line *M′* through point *D* parallel to

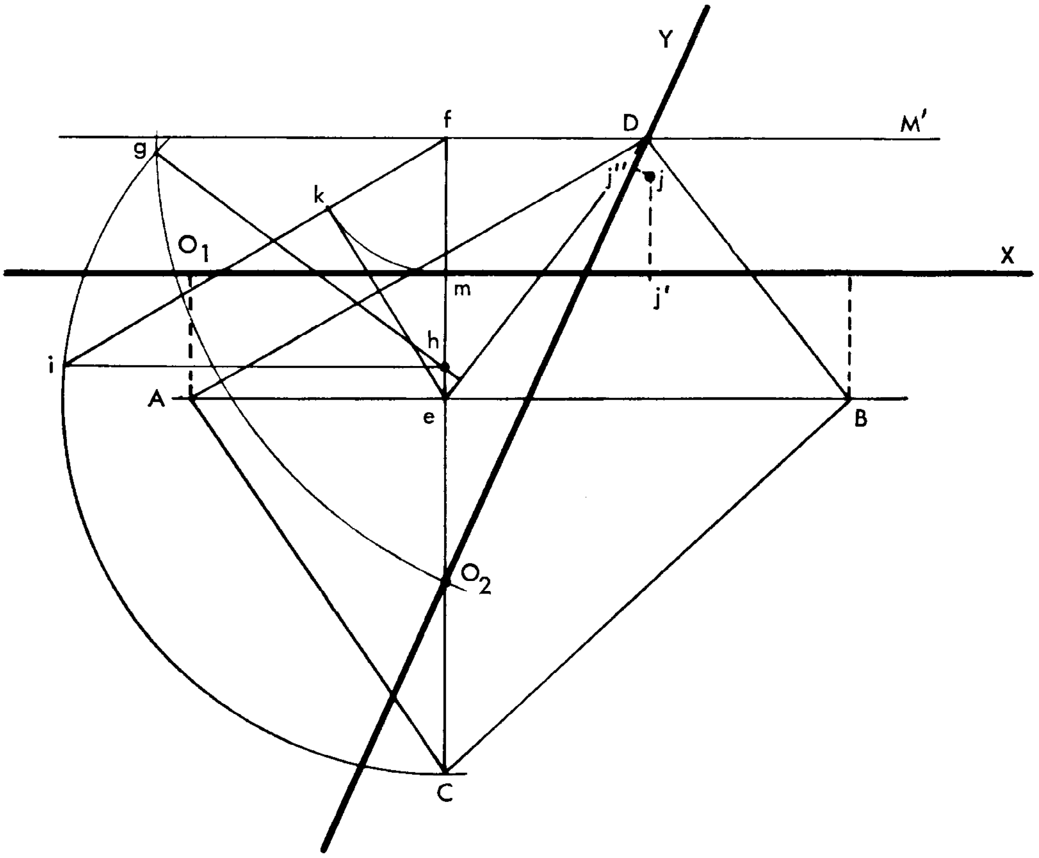

FIG. 1. Graphical solution for oblique axes (X, Y) in a modified Bray and Curtis ordination. See description of method in the main text.

TABLE 2

Sample distances for ordination poles *ABCD*, and stand *j*. *A*, *B* are poles for axis *X*, and *C*, *D* for axis *Y*

$$\begin{bmatrix} c(A,A) & c(A,B) & c(A,C) & c(A,D) & c(A,j) \\ & c(B,B) & c(B,C) & c(B,D) & c(B,j) \\ & & c(C,C) & c(C,D) & c(C,j) \\ & & & c(D,D) & c(D,j) \\ & & & & c(j,j) \end{bmatrix} = \begin{bmatrix} 0 & 1.20 & 0.84 & 0.96 & 0.93 \\ & 0 & 1.02 & 0.63 & 0.54 \\ & & 0 & 0.90 & 0.84 \\ & & & 0 & 0.12 \\ & & & & 0 \end{bmatrix}$$

line AB. (M' is the trace of M on plane ABD.)

3. Draw line through C perpendicular to M' to meet AB in e and M' in f.
4. Draw arc with center in D and radius $c(C, D)$ (taken from Table 2) to meet Cf in O_2. The line Y through D and O_2 is the projection image of Y on plane M. Line Y is the Y axis of the scatter diagram. Its origin is in O_2.

At this point the user may draw a line through O_2 parallel to AB, regard this as the X axis with origin in O_2 and proceed directly to step 10. However, the user may wish to determine the exact projection of X on M, in which case he should continue with step 5.

5. Draw arc through C with center in e to meet arc O_2g in g.
6. Draw a line through g perpendicular to eD to meet Cf in h.
7. Draw line through h parallel to AB to meet arc Cg in i (hi is the height of point C above plane ABD).
8. Draw line through e perpendicular to fi to meet fi in k, and draw arc through k with center in f to meet Cf in m. (Point m is the projection of e of AB on M.)
9. Draw X through m parallel to AB. Line X is the X axis of the ordination with origin in O_1.
10. Transfer lines X and Y onto a clear sheet of paper. The X and Y lines now represent the oblique ordination axes with origins O_1 and O_2. If so desired, each axis may be moved parallel to itself until O_1 and O_2 coincide as the common origin. (This step has not been done in Fig. 1).

The coordinates (stand values) on the ordination axes can be determined graphically, by actually drawing triangles, as in the original Bray and Curtis method, or on the basis of the Beals (1960) formula,

$$X_j = [c^2(A,j) + c^2(A, B) - c^2(B,j)]/2c(A, B).$$

For stand j (Table 2) this quantity becomes $X_j = (0.93^2 + 1.2^2 - 0.54^2)/(2 \times 1.2) = 0.839$. It is important to remember that coordinates on the Y axis must be determined according to a similar formula,

$$Y_j = [c^2(C,j) + c^2(C, D) - c^2(D,j)]/2c(C, D)$$

(The formula recommended by Beals for the Y axis should not be used when the axes are oblique.) The Y coordinate of stand j (Table 2) thus is $Y_j = (0.84^2 + 0.9^2 - 0.12^2)/(2 \times 0.9) = 0.834$. The coordinates are plotted according to the following instructions.

1. Measure distance X_j from O_1 on X and mark the point as j'.
2. Measure distance Y_j from O_2 on Y and mark the point j''.
3. Draw line through j' perpendicular to X and another line through j'' perpendicular to Y. These lines meet in point j, the projection of stand j in the XY scatter diagram.

The projections of other stands can be similarly determined.

Discussion

The revisions described in this paper produce an ordination that differs from the Bray and Curtis method in two important respects: (1) the original distance measure is discarded and a consistently metric function is put in its place; (2) the scatter diagram is constructed based on oblique ordination axes. The revised method is not more tedious for computation than the original method, except that the construction of the scatter diagram may be more complicated. Although the present paper outlines only a graphical solution, an analytical solution for computer processing has been derived.

Acknowledgment

The results reported in this paper represent part of a broader research project supported by a National Research Council of Canada grant.

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