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NOTES AND COMMENTS

THREE NOTES ON ALSCAL

FORREST W. YOUNG
YOSHIO TAKANE
AND
ROSTYSLAW LEWYCKYJ

UNIVERSITY OF NORTH CAROLINA

It is reported that (1) a new coordinate estimation routine is superior to that originally proposed for ALSCAL; (2) an oversight in the interval measurement level case has been found and corrected; and (3) a new initial configuration routine is superior to the original.

Key words: multidimensional scaling, optimal scaling, data quantification, data analysis, euclidian, nonmetric.

1. Coordinate Estimation

Takane, Young and de Leeuw [1977], in Section 5 of their paper, discuss a theoretical difficulty with the coordinate estimation routine in their *a*lternating *l*east *s*quares *scal*ing (ALSCAL) algorithm for Nonmetric Individual Differences Multidimensional Scaling. They also proposed a revised routine which avoided the difficulty, although they stated (a) that the difficulty appeared to have no practical effects, and (b) the revised routine was of unknown efficiency. We have now fully evaluated the revised routine and it appears to be at least as efficient as the original routine in terms of computation speed, and is considerably simpler to program. Thus, the revised routine has been incorporated in ALSCAL.

2. Interval Measurement Level

In their discussion of the optimal scaling procedure appropriate to interval level data, Takane, Young and de Leeuw [1977] discuss the additive constant problem [their equations (25) through (32)]. Unfortunately, their procedure can generate negative disparities. We have modified their procedure to obtain the least squares estimate of the additive constant under the constraint that there be no negative disparities. Specifically, in their equation (25), which states that $d^*_{ijk} = a(o_{ijk}) + b$, we restrict a and b so that all $d^*_{ijk} \geq 0$. Whenever the minimum d^*_{ijk} obtained by their unconstrained procedure is negative, then in

$$d^*_{ijk} = a(o_{ijk} + \tilde{b}), \tag{1}$$

where $\tilde{b} = b/a$, we set $\tilde{b} = -\text{MIN}(o_{ijk})$. We then define

$$\tilde{o}_{ijk} = o_{ijk} - \text{MIN}(o_{ijk}), \tag{2}$$

and estimate the squared distances as

$$\hat{d}^2_{ijk} \doteq d^{*2}_{ijk} = a^2\tilde{o}^2_{ijk}. \tag{3}$$

This reduces to the ratio scale case.

3. Initial Configuration

Takane, Young and de Leeuw [1977] state that ALSCAL uses an initial configuration procedure based on SUMSCAL (*su*bjective *m*etrics *scal*ing) procedure proposed by de Leeuw and Pruzansky [Note 1], which in turn is based on the algebraic solution proposed by Schönemann [1972] for error free data. In the terminology of Takane, Young and de Leeuw, we suppose that there are N scalar product matrices P_i (for each of N subjects i) of order n (there are n stimuli) which in the error free case would satisfy

$$P_i = XW_iX' \tag{4}$$

Dr. Takane is currently at McGill University, Department of Psychology.
Requests for reprints should be sent to Forrest Young, Psychometric Laboratory, Davie Hall 013-A, University of North Carolina, Chapel Hill, North Carolina 27514.

where X is an $n \times r$ matrix of common stimulus coordinates on r dimensions, and W_i is a diagonal $r \times r$ matrix of positive weights for subject i. It follows immediately from (4) that

$$W_i = (X'X)^{-1}X'P_iX(X'X)^{-1}. \tag{5}$$

However, with an arbitrarily oriented configuration Y such that $X = YK$ where K rotates Y into the desired orientation X, we have

$$\begin{aligned} W_i &= K'(Y'Y)^{-1}Y'P_iY(Y'Y)^{-1}K \\ &= K'C_iK \end{aligned} \tag{6}$$

where

$$\begin{aligned} C_i &= (Y'Y)^{-1}Y'P_iY(Y'Y)^{-1} \\ &= KW_iK'. \end{aligned}$$

Schönemann's algebraic solution finds the rotation K which simultaneously diagonalizes the C_i ($i = 1, \cdots, N$) by obtaining the spectral decomposition of C_i for any i. However, this only applies when there is no error in the data. The SUMSCAL procedure [de Leeuw & Pruzansky, Note 1] finds the K which minimizes the sum of the squared off-diagonal elements of W_i ($i = 1, \cdots, N$) in the presence of error, giving essentially the same solution as Carroll and Chang's [1970] INDSCAL (*In*dividual *D*ifferences *Scal*ing), but in much less time. While working on SUMSCAL, de Leeuw suggested [Note 2] that it would be desirable to find the K which diagonalizes a linear combination of the C_i matrices, where the linear combination is such that the resulting matrix, when diagonalized, has diagonal elements which have maximum variance. He based this suggestion on the observation that K is not uniquely defined when the W_i have constant diagonals. Thus, at least in some sense, K is most uniquely defined when the diagonals have maximum variance.

To achieve this goal let us define the linear combination of the matrices C_i as

$$l(C_i) = \sum_{i=1}^{N} e_iC_i. \tag{7}$$

Let $l(C_i) = K\Delta K'$, where K is a matrix of eigenvectors, and Δ a diagonal matrix of eigenvalues (K diagonalizes $l(C_i)$, and Δ has diagonalized elements on its diagonal). The variance of the diagonal entries (eigenvalues) can be written,

$$\rho = \operatorname{tr}(\Delta^2) - \frac{\operatorname{tr}^2(\Delta)}{r} = \operatorname{tr}[l^2(C_i)] - \frac{\operatorname{tr}^2[l(C_i)]}{r} \tag{8}$$

where r is the order of $l(C_i)$. We maximize ρ with respect to $e' = (e_1, \cdots, e_N)$ under the restriction that $e'e = 1$. Let

$$\rho^* = \rho - \lambda(e'e - 1) = \sum_{i,j} e_ie_j \operatorname{tr}(C_iC_j) - \frac{\left[\sum_i e_i\operatorname{tr}(C_i)\right]^2}{r} - \lambda(e'e - 1), \tag{9}$$

then

$$\frac{1}{2}\frac{\partial\rho^*}{\partial e_k} = \sum_i e_i\operatorname{tr}(C_iC_k) - \frac{\operatorname{tr}(C_k)\sum_i e_i\operatorname{tr}(C_i)}{r} - \lambda e_k = 0. \tag{10}$$

Thus

$$\lambda e_k = \sum_i a_{ik}e_i \tag{11}$$

where

$$a_{ik} = \operatorname{tr}(C_iC_k) - \frac{\operatorname{tr}(C_k)\operatorname{tr}(C_i)}{r} \tag{12}$$

Equation (11) is an eigenequation for the matrix A whose elements are defined by (12), and $\mathbf{e}$ (with elements e_i) is the eigenvector of matrix A. It can be readily shown that $\mathbf{e}$ is the eigenvector corresponding to the dominant

eigenvalue of A. Once $\mathbf{e}$ is determined we define the linear combination $l(C_t)$ by (7) to find the rotation K and the desired initial configuration X.

While this procedure is not as elegant as the SUMSCAL procedure (since it does not minimize the off-diagonal weights) it provides an initial configuration which is essentially the same as that provided by SUMSCAL, is as efficient as SUMSCAL in speed, and is a much simpler program. Thus, we have decided to use the procedure defined by (5) through (12) to initiate the ALSCAL computations.

Note that maximum variance among eigenvalues does *not* necessarily imply that each eigenvalue is maximally distinct from the others. Maximum distinctness may be construed as equal intervals between adjacent eigenvalues when they are ordered according to their magnitude, given that the difference between the largest and the smallest eigenvalues is constant (which, in turn, should be as large as possible). Thus, maximum distinctness among eigenvalues may not be exactly realized by the maximum variance criterion in certain situations (as one of the referees suggested), but from the practical point of view of obtaining an initial configuration, the above procedure works very well.

REFERENCE NOTES

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