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Unfolding a Symmetric Matrix

John C. Gower*
and
Michael Greenacre†

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* Department of Statistics, Open University, Milton Keynes, U.K.

† Department of Economics, Universitat Pompeu Fabra, Balmes 132, 08008 Barcelona, Spain.



Abstract

Graphical displays which show inter-sample distances are important for the interpretation and presentation of multivariate data. Except when the displays are two-dimensional, however, they are often difficult to visualize as a whole. A device, based on multidimensional unfolding, is described for presenting some intrinsically high-dimensional displays in fewer, usually two, dimensions. This goal is achieved by representing each sample by a pair of points, say R_i and r_i , so that a theoretical distance between the i -th and j -th samples is represented twice, once by the distance between R_i and r_j and once by the distance between R_j and r_i . Self-distances between R_i and r_i need not be zero. The mathematical conditions for unfolding to exhibit symmetry are established. Algorithms for finding approximate fits, not constrained to be symmetric, are discussed and some examples are given.

1. Introduction

Many multivariate techniques are concerned with displaying data as points in a Euclidean space. Ideally, approximations to the data in two or three dimensions are sought, but such approximations may be poor. We shall be concerned mainly with p -dimensional representations of n samples and show, in a certain quite simple sense, how some sets of n points in $n - 1$ dimensions can be exactly represented in p dimensions, where p is a small integer, ideally two or three. In practice, we are also concerned with using these representations for approximations in a specified number of dimensions p . Conventional representations are a special case of our general class of representations and so our approximations must be at least as good as, and will usually be better than the former.

The basic idea can be illustrated by considering a regular simplex of n vertices with common intervertex distance d , which is known to occupy $n - 1$ dimensions. For conventional Euclidean representations each *self-distance*, that is the distance between a point and itself, is zero. But if we are prepared to relax this condition we may consider a representation in which each vertex i is displayed as 2 points, (R_i, r_i) , $i = 1 \dots n$. Suppose that all the points labeled R_i are coincident at a point R and that all the points labeled r_i are coincident at a point r , where R and r are distance d apart. Then the distance between a point R_i and a point r_j is equal to d for all i, j including $i = j$. Thus by representing each vertex by two points and sacrificing the representation of the zero self-distances, we have represented the $(n - 1)$ -dimensional simplex exactly using only one dimension.

In the following we explore representations of this type for irregular simplices. Thus a set of samples will be represented in a Euclidean space where each original sample has two positions, possibly coincident, and the representation of zero self-distances is forfeited. Throughout we use uppercase letters to denote the points in one set and corresponding lowercase letters in the other set. Notice that the

representation need not be unique, for the regular simplex could also be represented in one dimension by a central point R , as before representing all the points of one set, and two points r_1, r_2 at a distance d either side of R , to which the points of the other set are allocated arbitrarily. It will be shown that this arbitrariness can be conveniently resolved to give a unique representation.

By doubling the number of points per sample we do not wish to replace the curse of dimensionality by the "curse of profusion". Our results show that this danger is avoided because the two sets of points usually have some simple geometric relationship. Furthermore, the fundamental Euclidean property of closeness survives in our representations. This result can be seen by considering two identical samples represented by point-pairs (A, a) and (B, b) for which the distances Ab and aB must both be zero, so that A coincides with b and a with B . Any third sample (C, c) must be equidistant from the first two, so that $aC = bC = Ac = Bc$ and if C is identical to the first two samples, then a, b, c, A, B, C must all coincide. If in the above "identical" is replaced by "similar", then "coincident" is replaced by "close", showing that groups will appear as groups in our representations.

The methodology that we use is a variant of that of multidimensional unfolding (Coombs 1964; see Muller 1988 for an introduction and origin of the name). Multidimensional unfolding is concerned with fitting the following model, including the residual term:

$$d_{ij}^2 = \sum_{k=1}^p (x_{ik} - y_{jk})^2 + e_{ij} \quad i = 1 \dots n, \quad j = 1 \dots m \quad (1)$$

where d_{ij} is the (i, j) -th element of a given $n \times m$ matrix D , whose elements are considered as approximate squared distances in p -dimensional Euclidean space, and e_{ij} is the residual term. Thus R_i , with coordinates $x_{i1} \dots x_{ip}$, and r_j , with coordinates $y_{j1} \dots y_{jp}$, may be considered as points representing the i -th row and j -th column of D . This model, and variants of it, have been studied extensively by psychometricians, especially as a method for analyzing preference data (e.g.,

see Carroll 1980), but it has general interest as a technique for data analysis.

If we define the following notation:

- ▣ $\mathbf{D} = \{d_{ij}^2\}$, the $n \times m$ matrix of squared distances;
- ▣ $\mathbf{X} = \{x_{ik}\}$, the $n \times p$ matrix of coordinates of the rows;
- ▣ $\mathbf{Y} = \{y_{jk}\}$, the $m \times p$ matrix of coordinates of the columns;
- ▣ $\mathbf{1} = \{1\}$, a column-vector of ones, whose length will be apparent from the context;
- ▣ $\mathbf{U} = \mathbf{1}\mathbf{1}^\top$, the $n \times m$ matrix of ones;
- ▣ $\mathbf{E} = \text{diag}(\mathbf{X}\mathbf{X}^\top)$, $\mathbf{F} = \text{diag}(\mathbf{Y}\mathbf{Y}^\top)$;
- ▣ $\mathbf{R} = \{e_{ij}\}$, the $n \times m$ matrix of residuals;

then (1) may be written in matrix notation as:

$$\mathbf{D} = \mathbf{E}\mathbf{U} + \mathbf{U}\mathbf{F} - 2\mathbf{X}\mathbf{Y}^\top + \mathbf{R}. \quad (2)$$

Henceforth the special case of a square symmetric matrix \mathbf{D} is considered, that is where $n = m$ and $\mathbf{D} = \mathbf{D}^\top$. Now the rows and columns may represent different modes of the same row and column classifications. We call the unfolding of the non-diagonal values of this matrix *symmetric unfolding*. One of the main theoretical issues of interest is whether solutions of a symmetric unfolding are themselves geometrically symmetric, that is whether the best unfolding fit to a symmetric matrix \mathbf{D} is necessarily itself symmetric. In Section 2 we consider admissible configurations of n pairs of points in multidimensional space which exactly yield symmetric matrices of squared distances. However, in our examples we have allowed the possibility that solutions be geometrically asymmetric, i.e., the fitted distance between points R_i and r_j is not constrained to be equal to the fitted distance between R_j and r_i , although in our experience solutions are generally close to symmetric. The existence of asymmetric solutions, which is counter-intuitive, is demonstrated in an example and discussed in the Appendix. In Section 3,

algorithms for unfolding a symmetric matrix are discussed. Section 4 presents some applications of the method and Section 5 gives a concluding discussion.

2. Symmetric Configurations

2.1 Introduction.

This section considers what forms of symmetric representation are admissible. Thus we are considering squared distances generated by the row and column coordinates X, Y , which give the non-diagonal values of the symmetric $n \times n$ matrix D . Writing Δ for the unknown and irrelevant diagonal values, with the previous notation, symmetry requires that

$$D + \Delta = EU + UF - 2XY^T = UE + FU - 2YX^T. \quad (3)$$

Double-centering $D + \Delta$ by pre- and post-multiplying (3) by $(I - N)$, where $N = \frac{1}{n}U$, and multiplying the result by $-\frac{1}{2}$ gives the matrix of "quasi-scalar products" (Schönemann 1970) :

$$B \equiv -\frac{1}{2}(I - N)(D + \Delta)(I - N) = (I - N)XY^T(I - N). \quad (4)$$

B is symmetric, and if it is positive semi-definite, it has real decompositions of the form $B = ZZ^T$ where Z is $n \times p$ and $p = \text{rank}(B)$. The solutions $Z = (I - N)X = (I - N)Y$, which are equivalent up to an arbitrary orthogonal transformation of Z , would suffice for classical scaling where $X = Y$. But they are too restrictive in the context of unfolding, where indeterminacy is expressed by an arbitrary non-singular $p \times p$ matrix K , say, and $n \times q$ matrices L and M where $LM^T = 0$, to give:

$$B = [ZK \ L][Z(K^T)^{-1} \ M]^T$$

where $[ZK \ L]$ is an augmented matrix of order $n \times (p + q)$.

The positive semi-definite condition is automatically satisfied if D is Euclidean. The effect of Δ , which has non-negative elements, is to extend the class of matrices

for which \mathbf{B} is positive semi-definite. Without loss of generality it may be assumed that one set of coordinates is centered at the origin so that $\mathbf{N}\mathbf{X} = \mathbf{0}$, giving the following general decomposition of \mathbf{B} :

$$\mathbf{X} = [\mathbf{Z}\mathbf{K} \ \mathbf{L}] \quad \text{and} \quad (\mathbf{I} - \mathbf{N})\mathbf{Y} = [\mathbf{Z}(\mathbf{K}^\top)^{-1} \ \mathbf{M}].$$

Because $\mathbf{1}^\top \mathbf{Z} = \mathbf{0}$, it follows that $\mathbf{1}^\top \mathbf{L} = \mathbf{1}^\top \mathbf{M} = \mathbf{0}$.

This solution may be separated into its p - and q -dimensional components to give:

$$\begin{aligned} \mathbf{X}_p &= \mathbf{Z}\mathbf{K}, & \mathbf{Y}_p &= \mathbf{Z}(\mathbf{K}^\top)^{-1} + \mathbf{1}\bar{\mathbf{y}}_p^\top \\ \mathbf{X}_q &= \mathbf{L}, & \mathbf{Y}_q &= \mathbf{M} + \mathbf{1}\bar{\mathbf{y}}_q^\top \end{aligned} \quad (5)$$

where $\bar{\mathbf{y}}_p, \bar{\mathbf{y}}_q$ are the means of $[\mathbf{Y}_p \ \mathbf{Y}_q] = \mathbf{Y}$ in the two spaces, and where it will be shown in Section 2.3 that $q \leq 2$. For the p -dimensional part of the solution we have:

$$\mathbf{Y}_p = \mathbf{X}_p(\mathbf{K}^\top \mathbf{K})^{-1} + \mathbf{1}\bar{\mathbf{y}}_p^\top$$

showing that \mathbf{Y}_p and \mathbf{X}_p are necessarily related by the affine transformation

$$\mathbf{Y}_p = \mathbf{X}_p \mathbf{S} + \mathbf{1}\bar{\mathbf{y}}_p^\top \quad (6)$$

where \mathbf{S} is non-singular and symmetric.

Apart from the conditions $\mathbf{L}\mathbf{M}^\top = \mathbf{0}$, $\mathbf{1}^\top \mathbf{L} = \mathbf{0}$ and $\mathbf{1}^\top \mathbf{M} = \mathbf{0}$, the q -dimensional part of the solution is, so far, very general. In practice \mathbf{L} and \mathbf{M} may be chosen to have disjoint columns of zeros, i.e., the i -th column of \mathbf{M} is $\mathbf{0}$ if the i -th column of \mathbf{L} is not equal to $\mathbf{0}$ and vice versa.

Equation (6) is a necessary but not sufficient condition for admissible solutions. The above derivation of (6) has appealed only to the symmetry of \mathbf{B} and by imposing the stronger condition of the symmetry of \mathbf{D} in (3) the solution may be refined. This gives the vanishing skew-symmetric part of $\mathbf{D} + \Delta$ (3) as:

$$(\mathbf{E} - \mathbf{F})\mathbf{U} - \mathbf{U}(\mathbf{E} - \mathbf{F}) - 2(\mathbf{X}\mathbf{Y}^\top - \mathbf{Y}\mathbf{X}^\top) = \mathbf{0}. \quad (7)$$

Substituting for Y_p given by (6) gives:

$$(E - F)U = PU - (\bar{y}_p^T \bar{y}_p)U - 2X_p S \bar{y}_p \mathbf{1}^T$$

where $P \equiv \text{diag}\{X_p(I - S^2)X_p^T\}$ and $XY^T - YX^T = X_p \bar{y}_p \mathbf{1}^T - \mathbf{1} \bar{y}_p^T X_p^T$, so that (7) may be written as:

$$(PU - UP) - 2X_p(I + S)\bar{y}_p \mathbf{1}^T + 2\mathbf{1} \bar{y}_p^T(I + S)X_p^T = 0 \quad (8)$$

Similarly, substituting for X_q and Y_q into (3) gives:

$$(QU - UQ) - 2(L + M)\bar{y}_q \mathbf{1}^T + 2\mathbf{1} \bar{y}_q^T(L + M)^T = 0. \quad (9)$$

where $Q \equiv \text{diag}(LL^T - MM^T)$. The full condition for the symmetry of D is that the sum of the left sides of (8) and (9) is zero, but we first examine the two conditions separately.

2.2 The p -dimensional solution.

Post-multiplying (8) by $\mathbf{1}$ gives:

$$\{P - \frac{1}{n}(\mathbf{1}^T P \mathbf{1})I\}\mathbf{1} - 2X_p(I + S)\bar{y}_p = 0$$

showing that for any X_p which satisfies this equation, the points lie on the conic with quadratic form:

$$\mathbf{x}^T(I - S^2)\mathbf{x} - 2\mathbf{x}^T(I + S)\bar{y}_p - \frac{1}{n}(\mathbf{1}^T P \mathbf{1}) = 0. \quad (10)$$

Recalling that $\mathbf{1}^T P \mathbf{1}$ is a function of X_p shows that different X_p which satisfy (8) for some S and \bar{y}_p give conics with the same centres and orientation of axes, but of different sizes. The points \mathbf{y} in the rows of Y_p lie on conics whose axes' lengths are related to those of the points \mathbf{x} in the rows of X_p by the transformation $\mathbf{y} = S\mathbf{x} + \bar{y}_p$.

The implication of (10) is that, given any S and \bar{y}_p , then for X_p whose rows \mathbf{x} satisfy (10), a corresponding Y_p exists that preserves symmetry. Such X_p, Y_p pairs

will generate certain symmetric distance matrices \mathbf{D} . Although it is interesting to note the existence of distance matrices with such solutions, it is more fruitful to search for general solutions which will be valid for any \mathbf{X}_p . Such general solutions of (8) exist when:

$$(i) (\mathbf{I} + \mathbf{S})\bar{\mathbf{y}}_p = \mathbf{0} \quad \text{and} \quad (ii) \mathbf{S}^2 = \mathbf{I}. \quad (11)$$

Here (ii) ensures that \mathbf{P} is zero and shows that \mathbf{S} must be orthogonal. The conditions (i) and (ii) ensure that each term of (8) vanishes independently of \mathbf{X}_p .

Note that (6) and (11) define the mutual inverse transformations:

$$\mathbf{y} = \mathbf{S}\mathbf{x} + \bar{\mathbf{y}}_p$$

$$\text{and} \quad \mathbf{x} = \mathbf{S}\mathbf{y} + \bar{\mathbf{y}}_p$$

Since \mathbf{S} is a symmetric orthogonal matrix and $\mathbf{S}^2 = \mathbf{I}$, it has spectral form:

$$\mathbf{S} = \sum_{i=1}^r \mathbf{u}_i \mathbf{u}_i^T - \sum_{i=r+1}^p \mathbf{u}_i \mathbf{u}_i^T$$

where \mathbf{u}_i ($i = 1, 2, \dots, p$) are an orthogonal basis of unit vectors. Noting that $\mathbf{I} = \sum_{i=1}^p \mathbf{u}_i \mathbf{u}_i^T$, it follows that \mathbf{S} may be written as:

$$\mathbf{S} = \mathbf{I} - 2 \sum_{i=r+1}^p \mathbf{u}_i \mathbf{u}_i^T \quad (12)$$

showing that \mathbf{S} is a generalized form of the Householder transform $\mathbf{S} = \mathbf{I} - 2\mathbf{u}\mathbf{u}^T$. This transform represents a reflection in a plane, with normal \mathbf{u} , through the origin, and is of special interest in two-dimensional solutions where \mathbf{Y}_p is the reflection of \mathbf{X}_p in some line. The form (12) represents simultaneous reflections through planes with normals $\mathbf{u}_{r+1}, \mathbf{u}_{r+2}, \dots, \mathbf{u}_p$ and hence a reflection through their intersection.

There exist scalars μ_i , not all zero, such that $\bar{\mathbf{y}}_p = \sum_{i=1}^p \mu_i \mathbf{u}_i$, so the condition (i) becomes:

$$\begin{aligned} (\mathbf{I} + \mathbf{S})\bar{\mathbf{y}}_p &= 2 \sum_{i=1}^r (\mathbf{u}_i \mathbf{u}_i^T) \sum_{i=1}^p \mu_i \mathbf{u}_i \\ &= 2 \sum_{i=1}^r \mu_i \mathbf{u}_i = \mathbf{0}, \end{aligned}$$

showing that $\bar{\mathbf{y}}_p$ must be chosen to satisfy:

$$\bar{\mathbf{y}}_p = \sum_{i=r+1}^p \mu_i \mathbf{u}_i. \quad (13)$$

The conditions (12) and (13) give the more detailed form of the admissible affine transformation for a general solution of the p -dimensional part of unfolding the symmetric matrix \mathbf{D} .

The special case $r = p - 1$, $\bar{\mathbf{y}}_p = \mathbf{0}$ gives the simple Householder transform; the case $r = p$, $\bar{\mathbf{y}}_p = \mathbf{0}$ gives $\mathbf{S} = \mathbf{I}$. The case $r = 0$ gives $\mathbf{S} = -\mathbf{I}$ with arbitrary translation term $\bar{\mathbf{y}}_p$, which represents a reflection through a point $-\frac{1}{2}\bar{\mathbf{y}}_p$ expressed algebraically by $\mathbf{y} - \frac{1}{2}\bar{\mathbf{y}}_p = -(\mathbf{x} - \frac{1}{2}\bar{\mathbf{y}}_p)$. Similarly, the Householder transform with $\bar{\mathbf{y}}_p = \mu \mathbf{u}$ is a reflection in a plane through $-\frac{1}{2}\mu \mathbf{u}$ and orthogonal to \mathbf{u} , expressed algebraically by $(\mathbf{y} - \frac{1}{2}\mu \mathbf{u}) = \mathbf{S}(\mathbf{x} - \frac{1}{2}\mu \mathbf{u})$.

It is instructive to exhibit the fitted symmetric matrix implied by the conditions (i) and (ii). Some algebraic manipulation gives:

$$\Delta + \mathbf{D} = \mathbf{a}\mathbf{1}^T + \mathbf{1}\mathbf{a}^T - 2\mathbf{X}_p \mathbf{S} \mathbf{X}_p^T \quad (14)$$

where $\mathbf{a} \equiv \mathbf{E}\mathbf{1} - 2\mathbf{X}_p \bar{\mathbf{y}}_p + \frac{1}{2}\bar{\mathbf{y}}_p^T \bar{\mathbf{y}}_p \mathbf{1}$. Substituting (12) for \mathbf{S} gives, after further manipulation:

$$\Delta + \mathbf{D} = \mathbf{D}_X + \mathbf{v}\mathbf{v}^T + 4\mathbf{X}_p \sum_{i=r+1}^p \mu_i \mathbf{u}_i^T \mathbf{X}_p^T - 4 \frac{\mathbf{X}_p \bar{\mathbf{y}}_p \bar{\mathbf{y}}_p^T \mathbf{X}_p^T}{\bar{\mathbf{y}}_p^T \bar{\mathbf{y}}_p} \quad (15)$$

where $\mathbf{D}_X \equiv \mathbf{E}\mathbf{U} + \mathbf{U}\mathbf{E} - 2\mathbf{X}_p \mathbf{X}_p^T$ is the matrix of squared distances among the \mathbf{X} -set and $\mathbf{v} \equiv 2\mathbf{X}_p \bar{\mathbf{y}}_p / \sqrt{\bar{\mathbf{y}}_p^T \bar{\mathbf{y}}_p} - \sqrt{\bar{\mathbf{y}}_p^T \bar{\mathbf{y}}_p} \mathbf{1}$. When \mathbf{S} is a simple Householder transform, (15) becomes:

$$\Delta + \mathbf{D} = \mathbf{D}_X + \mathbf{v}\mathbf{v}^T \quad (16)$$

so that the elements of the vector \mathbf{v} are the self-distances for the n points. Thus $\Delta + \mathbf{D}$ deviates from a matrix of squared distances only by a rank one matrix; the special case $\mathbf{v} = \lambda \mathbf{1}$ relates to the well-known additive constant problem of

multidimensional scaling. Note, however, that \mathbf{D}_X is not itself a matrix that optimally approximates \mathbf{D} and that \mathbf{v} has a special form. One could find \mathbf{D}^* , say, by minimizing the criterion known as ‘‘SSTRESS’’, that is the sum of squared residuals of (1) (Takane, Young, and de Leeuw 1977, Browne 1987), and then find the $\mathbf{D}^* + \mathbf{v}\mathbf{v}^\top$ that gave the best fit to \mathbf{D} conditional on the given \mathbf{D}^* . This gives $\lambda^2 = \mathbf{1}^\top(\mathbf{D} - \mathbf{D}^*)\mathbf{1}/(n(n-1))$ but this solution does not have a convenient geometrical representation and could give a poorer fit than (16).

2.3 The q -dimensional solution.

Turning now to the q -dimensional solution given by (9), it is convenient to return to the basic form (3) that $(\mathbf{D} + \Delta)_q$, the q -dimensional component of $\mathbf{D} + \Delta$, is:

$$(\mathbf{D} + \Delta)_q = \text{diag}(\mathbf{L}\mathbf{L}^\top)\mathbf{U} + \mathbf{U} \text{diag}(\mathbf{M}\mathbf{M}^\top) - 2\mathbf{L}\bar{\mathbf{y}}_q\mathbf{1}^\top + 2\mathbf{1}\bar{\mathbf{y}}_q^\top\mathbf{M}^\top + \bar{\mathbf{y}}_q^\top\bar{\mathbf{y}}_q\mathbf{1}\mathbf{1}^\top$$

which may be written

$$(\mathbf{D} + \Delta)_q = \mathbf{a}\mathbf{1}^\top + \mathbf{1}\mathbf{b}^\top + \bar{\mathbf{y}}_q^\top\bar{\mathbf{y}}_q\mathbf{1}\mathbf{1}^\top$$

where $\mathbf{a} \equiv \text{diag}(\mathbf{L}\mathbf{L}^\top)\mathbf{1} - 2\mathbf{L}\bar{\mathbf{y}}_q$ and $\mathbf{b} \equiv \text{diag}(\mathbf{M}\mathbf{M}^\top)\mathbf{1} + 2\mathbf{M}\bar{\mathbf{y}}_q$. Thus $(\mathbf{D} + \Delta)_q$ is symmetric if and only if $\mathbf{b} = \mathbf{a} + \lambda\mathbf{1}$, for arbitrary λ , i.e., $\text{diag}(\mathbf{L}\mathbf{L}^\top - \mathbf{M}\mathbf{M}^\top)\mathbf{1} = 2(\mathbf{L} + \mathbf{M})\bar{\mathbf{y}}_q - \lambda\mathbf{1}$. Then

$$\begin{aligned} (\mathbf{D} + \Delta)_q &= \mathbf{a}\mathbf{1}^\top + \mathbf{1}\mathbf{a}^\top + (\lambda + \bar{\mathbf{y}}_q^\top\bar{\mathbf{y}}_q)\mathbf{1}\mathbf{1}^\top \\ &= (\mathbf{a} + \rho\mathbf{1})\mathbf{1}^\top + \mathbf{1}(\mathbf{a} + \rho\mathbf{1})^\top \end{aligned} \quad (17)$$

where $2\rho \equiv \lambda + \bar{\mathbf{y}}_q^\top\bar{\mathbf{y}}_q$, showing that the squared distance d_{ij}^2 , for $i \neq j$, is given by

$$d_{ij}^2 = a_i + a_j + 2\rho.$$

Equation (17) gives the fitted values for the q -space, which may be compared with (14), (15), and (16) which give the fitted values for the p -space. Geometrically (17) shows that only certain two-dimensional configurations can be represented and that therefore $q \leq 2$. When $\mathbf{a} = \mu\mathbf{1}$, for any scalar μ , then (17) has unit rank

and $q = 1$ with d_{ij} constant (cf. the regular simplex described in paragraph 2 of Section 1). The rank 2 solutions may be represented in several ways expressed by the following general form for the rows of \mathbf{X}_q and \mathbf{Y}_q : $x_{qi} = [(a_i + \rho + \alpha)^{1/2} \quad 0]$ and $y_{qi} = [0 \quad (a_i + \rho - \alpha)^{1/2}]$. The square roots allow arbitrary signs for x_{qi} and y_{qi} which give different configurations all generating the same distances, so nothing is lost by excluding negative roots. Generally the relationship between \mathbf{X}_q and \mathbf{Y}_q is not affine, but it is affine when

- (i) $\mathbf{a} = \mu \mathbf{1}$, and hence $q = 1$, and α is chosen to be $\mu + \rho$ which gives $\mathbf{Y}_q = \mathbf{X}_q - \sqrt{2(\rho + \mu)}\mathbf{1}$, a simple reflection in a point, and
- (ii) α is chosen to be zero so that $\mathbf{Y}_q = \mathbf{X}_q \mathbf{S}$, where $\mathbf{S} = \mathbf{I} - 2\mathbf{u}\mathbf{u}^\top$ with $\mathbf{u}^\top = [1/\sqrt{2} \quad -1/\sqrt{2}]$, representing a reflection in the 45° line.

So far no restriction has been put on the position of the origin of \mathbf{X}_q and \mathbf{Y}_q , and indeed there is no need to impose any such restriction. However, just as for the p -dimensional solution, the origin may be chosen to be at the mean of \mathbf{X}_q , without affecting distances. Translating to this new origin, \mathbf{X}_q and \mathbf{Y}_q become \mathbf{X}_q^* and \mathbf{Y}_q^* where:

$$\mathbf{X}_q^* = (\mathbf{I} - \mathbf{N})\mathbf{X}_q \quad \text{and} \quad \mathbf{Y}_q^* = (\mathbf{I} - \mathbf{N})\mathbf{Y}_q.$$

Thus $\mathbf{Y} = \mathbf{X}\mathbf{S}$ becomes

$$\begin{aligned} \mathbf{Y}_q^* &= \mathbf{X}_q^* \mathbf{S} + \mathbf{N}\mathbf{X}_q(\mathbf{S} - \mathbf{I}) \\ &= \mathbf{X}_q^* \mathbf{S} + \mathbf{1}\bar{\mathbf{y}}_q^{*\top} \end{aligned} \tag{18}$$

where $\bar{\mathbf{y}}_q^* \equiv \mathbf{1}^\top \mathbf{Y}_q^* / n$, the mean of \mathbf{Y}_q^* . With this parameterization, $\mathbf{L} = \mathbf{X}_q^*$ and $\mathbf{M} = \mathbf{X}_q^* \mathbf{S}$, thus complying with the condition $\mathbf{1}^\top \mathbf{L} = \mathbf{1}^\top \mathbf{M} = \mathbf{0}$ as well as with $\mathbf{L}\mathbf{M}^\top = \mathbf{0}$. Thus, among the many ways of presenting the q -dimensional solution is included the symmetric orthogonal affine transform (18) just as for the p -dimensional case, but of less generality because here $q = 2$ and \mathbf{S} is a fixed Householder transform. The different solutions all give the same distances and

are therefore equivalent; to resolve the arbitrariness, a single solution is needed and the affine solution is the obvious one to choose because of its similar form to the p -dimensional affine solution and because it gives the simplest representation. Because \mathbf{S} does not depend on \mathbf{X}_q , the affine solution is always a general, rather than particular, solution.

2.4 The combined solution.

The full set of solutions requires that the sum of the left sides of (8) and (9) vanish. Both equations are quadratic in the $(p + q)$ -dimensional vectors of \mathbf{X} , \mathbf{Y} , so that these will be particular conic solutions of rather more general form than was given by the p -dimensional solutions above. General solutions, however, are merely the combination of the separate general solutions already described in Sections 2.2 and 2.3 for the separate p -dimensional and q -dimensional cases, either one of which may be null.

Insert Figure 1 about here

2.5 Examples of representations.

Some examples of symmetric configurations are given in Figure 1. Figure 1a is a simple reflection in a line through the origin, expressed by $\mathbf{Y} = \mathbf{X}(\mathbf{I} - 2\mathbf{u}\mathbf{u}^T)$. In Figure 1b, $\mathbf{Y} = \lambda\mathbf{X}$, and this is a particular solution because it depends on the x -values lying on a circle; it is a simple case of the concentric conics discussed in Section 2.2. Figure 1c is a non-affine representation given by (i) a $p = 1$ -dimensional solution $\mathbf{Y}_p = \mathbf{X}_p$ and, in the notation of Section 2.3, (ii) a $q = 1$ -dimensional solution with $x_{qi} = 0$ and $y_{qi} = \pm\lambda$, where λ is the distance of the two outer parallel lines from the central line. As explained in Section 2.3, nothing is gained over the more simple affine solution $x_{qi} = 0$ and $y_{qi} = \lambda$, i.e., $\mathbf{Y} = \mathbf{X} + 1\bar{\mathbf{y}}^T$ where $\bar{\mathbf{y}}^T = [0 \ \lambda]$, which needs only two parallel lines. Furthermore the alternative affine representation with $q = 2$ described in Section 2.3 yields $x_{qi} = [\lambda/\sqrt{2} \ 0]$ and $y_{qi} = [0 \ \lambda/\sqrt{2}]$; together with the one-dimensional part, a total of three

dimensions is required. Figure 1d is again a non-affine transformation in which the two lines intersect at right angles. Here $p = 0$ and $q = 2$ and $x_{qi} = [a_i \ 0]$; $y_{qi} = [0 \ \pm a_i]$. The affine equivalent is $Y_q = X_q S$, where $x_{qi} = [a_i \ 0]$; $y_{qi} = [0 \ a_i]$. Finally in Figure 1e, the two sets of points are not seen to be related in any clear way. This figure was constructed by trial and error and presumably represents one of the particular solutions given by (8) and (9).

3. Algorithms

The ways in which X, Y pairs having the symmetry property arise were discussed in Section 2. Just as $Y = X$ leads to classical Young-Householder-Torgerson scaling, so could other forms of solution such as $Y = -X + 1m^T$ or $Y = X(I - 2uu^T) + 1m^T$ with $m = \mu u$, generate their own class of algorithms. Indeed, (6), (10), (11), (14) and (16) give the forms of matrix to fit to \mathbb{D} . We have not followed this line of development because we are now concerned with approximation, and for given \mathbb{D} and p there seems to be no *a priori* method for deciding which form of solution gives the best fit or indeed whether the best fit is necessarily given by a symmetric matrix (see Appendix). If one insisted on a symmetric solution then algorithms would have to be developed which handle the constraints implied by the solutions of Section 2. Most of these constraints are non-linear and are likely to lead to optimization problems whose solution requires further research. The exception is (6) when the symmetry of S implies a set of simple linear constraints ($s_{ij} = s_{ji}$) which could probably be handled algorithmically. Unfortunately (6) is only a necessary condition for symmetric solutions so these constraints do not necessarily lead to symmetric solutions. Accordingly, we have applied existing multidimensional unfolding algorithms to operate on square matrices, with appropriate modifications to exclude the fitting of the self-distances. The fitted values are not constrained to be symmetric but, in our limited experience, solutions generally turn out to be symmetric or incorporate a substantial

degree of symmetry.

One way to do multidimensional unfolding is to use standard nonmetric scaling techniques. The matrix \mathbf{D} may be regarded as the $n \times m$ corner of an $(n + m) \times (n + m)$ symmetric matrix with the two symmetric matrices of order $n \times n$ and $m \times m$ missing. Since nonmetric scaling readily copes with missing data, a solution is found giving the coordinates of $n + m$ points, n representing the rows and m the columns of \mathbf{D} . Similarly the diagonal values of \mathbf{D} can be treated as missing so that the nonmetric scaling may permit non-zero self-distances. In the case considered here, every element of the distance matrix is tied with its symmetric counterpart and the treatment of ties in the nonmetric algorithm becomes an important issue. If a configuration with symmetric distances is to be encouraged, the so-called "secondary" treatment of ties would be preferable (Kruskal 1964); that is, the algorithm would result in a matrix of distances fitted to a set of "disparities" which are themselves symmetric and monotonically related to the original distances. However, an example given in the Appendix shows that non-symmetric fits may sometimes be preferable, in which case the primary treatment of ties would be applicable.

Metric least-squares criteria for fitting model (1) for a rectangular matrix \mathbf{D} have been studied by Schönemann (1970), Gold (1973), Greenacre (1978), Heiser (1981) and Greenacre and Browne (1986). In the following, we discuss a variant of the unfolding problem where \mathbf{D} is a conventional matrix of squared distances and hence approximation of the diagonal terms is not required. Any of the existing unfolding algorithms can be adapted to solve this specific problem and the choice is not crucial for obtaining the kinds of representation that we seek. For the purposes of this study we have chosen to minimize the sum of squared residuals of (1), or SSTRESS. We call the scaling method associated with this optimization criterion "least-squares squared scaling" (LSSS). There are, admittedly, some problems with this particular criterion, mainly the fact that the fitting of large

distances dominates the fitting of small distances, so that local structure may be poorly represented in the display. On the other hand, there are algebraic and computational advantages in using this form.

The criterion to be minimized is thus $\text{trace}(\mathbf{R}\mathbf{R}^T)$, which leads to the normal equations:

$$\mathbf{R}\mathbf{Y} = \text{diag}(\mathbf{R}\mathbf{U}^T)\mathbf{X} \quad \text{and} \quad \mathbf{R}^T\mathbf{X} = \text{diag}(\mathbf{R}^T\mathbf{U})\mathbf{Y}. \quad (19)$$

This pair of equations may be used as the basis for an efficient least-squares algorithm which alternates between two equations. This algorithm was first described by Greenacre (1978) and is further discussed by Greenacre and Browne (1986). A further algebraic advantage is the ANOVA-like decomposition, obtained from (2) and (19):

$$\text{trace}(\mathbf{D}\mathbf{D}^T) = \text{trace}(\mathbf{R}\mathbf{R}^T) + \text{trace}[(\mathbf{D} - \mathbf{R})(\mathbf{D} - \mathbf{R})^T] \quad (20)$$

(Gower 1984). The fitted sum-of-squares, $\text{trace}[(\mathbf{D} - \mathbf{R})(\mathbf{D} - \mathbf{R})^T]$, may be further broken down into row and column components in the usual way, as for two-way tables.

There are two ways in which a metric unfolding algorithm may be adapted to ignore the diagonal of the symmetric distance matrix. First, weights w_{ij} may be assigned to each term of the objective function and a weighted fit optimized. In the present case the objective function would thus be:

$$\sum_{i=1}^n \sum_{j=1}^n w_{ij} e_{ij}^2.$$

Our specific problem would then be solved by setting $w_{ii} = 0$ for all $i = 1, \dots, n$, and $w_{ij} = 1$ for all $i \neq j$. In general, the introduction of differential weighting of the terms in the objective function would also allow compensation for the excessive emphasis on large distances; for example, if we set the off-diagonal weights to $w_{ij} = d_{ij}^{-4}$. The inclusion of weights, however, leads to an increase in computation

per iteration and it is then doubtful whether the alternating least-squares algorithm still holds a substantial advantage over more familiar gradient techniques of optimization.

In the simpler case of a zero-one weighting scheme, the algorithm for general unfolding based on SSTRESS (Greenacre 1978, Greenacre and Browne 1986) can be adapted as follows for the particular problem where the diagonal terms are excluded. At a particular stage of the iterative process, we replace the existing values of the diagonal squared distances d_{ii}^2 by the squared self-distances according to the solution at that stage. The contribution of the diagonal terms in the objective function is thus maintained at zero throughout the iterative process, and when the algorithm converges, the fitted self-distances themselves converge. This method can be thought of as unfolding the complete matrix of squared distances, including fitted diagonal values, as if these were known initially. While the weighted solution would be preferable, the present strategy entailed only a minor modification of our present algorithm and was thus much easier to implement. In the original testing of this adapted algorithm, it became clear that to replace the self-distances after each iteration sometimes led to numerical instability of the algorithm, because of instability in convergence of some of the fitted self-distances. This has led us to perform the iterations in a nested fashion, fixing the self-distances for a number of iterations until a convergent unfolding solution is obtained, and only then replacing the self-distances for a subsequent set of iterations. This strategy has definitely led to stabilization of the self-distances and to consequent convergence of the algorithm in most cases.

Because of the danger of local minima in unfolding solutions, it is advisable to try a number of different starting points. Our present algorithm uses a starting configuration based on the matrix \mathbf{B} given by (4). But before this initial solution can be computed, we have to select starting values for the self-distances Δ themselves. We have tried two ways of initializing these distances and we suggest

that both be tried and the ultimate solutions of the algorithm compared. The first method is to set these distances equal to zero, implying that the algorithm commences at the classical scaling solution. The second method initializes the diagonal squared distances d_{ii}^2 as the average of the non-diagonal squared distances $(\sum_{i \neq j} d_{ij}^2)/(n-1)$. Thus, the first method can be imagined as the row and column points initially close together and drifting apart to optimize the objective, and the second method as the row and column points initially fairly far apart and drifting either toward one other or even further apart to reach an optimum.

Insert Figures 2 and 3 about here

4. Examples

4.1 Galaxy data.

Nathanson (1971) gives the squared Mahalanobis distances between ten types of galaxies, which he uses in a discriminant analysis of the galaxies. Figure 2 shows the metric scaling of these distances in two dimensions, using the metric scaling algorithm of Browne (1987) which also minimizes residual sum-of-squares (RSS) and gives a minimum value of 45.78 (SSTRESS=0.041). Figure 3 shows the symmetric unfolding of the same data, using the algorithm described in Section 3. In this case the value of RSS is 9.71, with a corresponding SSTRESS of 0.009. Since the decomposition is based on fourth powers of original and fitted distances, these SSTRESS values are highly optimistic summaries of the errors incurred in the respective displays. Another way of summarizing the quality of fit is to examine the residuals in the respective analyses. In fact, the metric scaling results in a set of residuals whose absolute values have mean 0.58 and standard deviation 0.41, while the absolute residuals in the symmetric unfolding have mean 0.25 and standard deviation 0.21. This improvement can be judged against the fact that the original squared distances themselves have mean 3.15 and standard deviation 1.54.

The fitted distances given by Figure 3 are very nearly symmetric, although the representation is not one of the general types discussed in Section 2. However, a strong element of reflection is observable, albeit not reflections in a line or plane. In particular, galaxies H, I, and J have a different, curvilinear, axis of symmetry from the other galaxies. These three galaxies were also picked out in a three-dimensional nonmetric unfolding of these data (Gower and Digby 1981). It seems that the gain in accuracy of the two-dimensional metric unfolding compared with the two-dimensional scaling has been obtained by accommodating higher dimensional differences between H, I, J and the remaining galaxies.

Insert Figures 4 and 5 about here

4.2 Cultural distances between ethnic groups.

If the resultant display yields asymmetric fitted distances, one of the pair of distances will be fitted better than its counterpart. In this case we retain only half of the fitted values and call this a "reduced fit". Some theoretical examples where a reduced solution is better than the full symmetric unfolding solution are given in an Appendix.

We consider a case arising in the symmetric unfolding of a set of distances originally in a study by Funk et al. (1974), relating to cultural distances between 13 ethnic groups. These data are also discussed and analyzed in a description of a metric scaling program by Heiser and de Leeuw (1977).

In a two-dimensional LSSS of these data, reproduced in Figure 4, there are quite clearly three groups of points, indicated by the symbols A, B and C, which lie roughly at the vertices of a triangle. In a one-dimensional scaling, not given here, the three groups are still separated but the smallest group (group B) is forced to lie between the other two and is thus displayed with large errors. In a one-dimensional symmetric unfolding the display turns out to be highly asymmetric

(Figure 5). One set of points (the rows, say) is bunched up at the origin, although the separation of the three groups is still apparent. The displayed distances with the most asymmetry are those between the points in cluster B and the other points. It appears that the displayed distances from the row points of cluster B to the other column points are fairly accurate, while the transposed distances are fairly inaccurate. This result can be seen clearly in Table 1, which shows percentage contributions to the RSS of the solution – about 87% of the RSS is contained in the columns labelled 3 and 8, i.e., the members of group B. Hence the column points 3 and 8 are useful only in their representation of the distance between 3 and 8, otherwise they should not be interpreted.

Insert Table 1 about here

This example demonstrates the existence of reduced fits as well as the ability of symmetric unfolding to represent higher-dimensional structures in a low-dimensional space.

5. Discussion

In a scaling of an $n \times n$ symmetric matrix in p dimensions, the number of free parameters is $np - \frac{1}{2}p(p+1)$. Since we have not constrained the symmetric unfolding solution to be symmetric, its number of free parameters is theoretically $2np - \frac{1}{2}p(p+1)$, although the constraint of symmetry would considerably reduce this number. Referring to (6), (11), (12) and (13), we can deduce that the number of free parameters under this constraint would be $np - \frac{1}{2}p(p+1)$ plus the number of free parameters in S and \bar{y}_p which define the affine transformation between the two sets of coordinates. This number depends on r , where $p - r$ is the number of orthonormal vectors in the generalized Householder transform (12), and is equal to $p(p-r) - \frac{1}{2}(p-r)(p-r+1)$ in the case of S , and $(p-r)$ in the case of \bar{y}_p , the sum of which simplifies as $\frac{1}{2}p(p+1) - \frac{1}{2}r(r+1)$. Thus, the number of free

parameters under the symmetry constraint would be at most $np - \frac{1}{2}r(r + 1)$. For example, in a $p = 2$ -dimensional solution which is constrained to be a reflection in a line (cf. Figure 1a), i.e. the simple Householder transform with $r = 1$ and $\bar{\mathbf{y}}_p = \mathbf{0}$, the number of free parameters would be $np - \frac{1}{2}r(r + 1) - 1 = np - 2$, just one more than the scaling solution. The analysis of Section 2 has shown that most useful unfolding solutions giving symmetry are subsumed in the class of symmetric affine transformations, but it is not clear how such a constraint could be imposed in the unfolding algorithm. Indeed it is not clear that any such constraint is necessary, as many of the unconstrained solutions so far constructed have turned out to be symmetric.

Since symmetric unfolding offers more free parameters for representing a space of given intrinsic dimensionality but includes conventional scaling representations as special cases, it must lead to an approximation which fits the distance matrix at least as well as does conventional scaling, in a prescribed number of dimensions. Thus, symmetric unfolding extends the class of data that can be represented in a low-dimensional space, especially in two dimensions which are the most convenient for viewing distances. Apart from ignoring self-distances in the display, the interpretation of a symmetric unfolding is usually only slightly more difficult than the intuitively simple interpretation of a conventional multidimensional scaling display. For those already familiar with conventional unfolding, there is little to learn. The interpretation of the displayed self-distances themselves also needs further investigation, as these seem to be related to the dimensionality of different groups of points. For example, when symmetric unfolding in two dimensions leads to a display where two sets of points are the same, an intrinsic two-dimensional set of distances is indicated. Other types of symmetry would indicate higher intrinsic dimensionality. It is important to point out that the presence of patterns in the pairs of points in symmetric unfolding solutions effectively compensates for the expense of increasing the number of parameters in the model. If the two sets

of points were randomly related, the price paid for the extra parameters might be considered too high. However, the Euclidean concept of closeness survives in our representations and we have shown that often, but not necessarily always, the two sets of points may show some simple geometric relationship. When this happens, the extra complexity is much reduced, making the price affordable and interpretation easier.

Based on some initial results given in the Appendix, the occurrence of asymmetric solutions does not necessarily appear to be a disadvantage. The reduced fits described there can be very satisfactory, but the complexity of interpretation is admittedly increased. The few reduced fits which we have examined have been obtained from an inspection of full fits; a possibility for further work is to examine the possibility of obtaining reduced fits by direct methods.

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Appendix

We give a simple example intended to elucidate the existence of optimal asymmetric approximations when unfolding a symmetric matrix. With asymmetric solutions, one of the pair of approximations to each d_{ij} must be better than the other, thus leading to reduced symmetric unfolding solutions. We use the term “reduced fit” when a distance matrix is fitted by symmetric unfolding, followed by a selection of half the fitted values: for each fitted pair (d_{ij}, d_{ji}) the one is discarded which has the bigger residual. Thus, only one of each pair of fitted values is used for interpretation – one might say that the unfolding diagram is interpreted as a restricted directed graph (i.e., restricted to the better of each pair). Thus we could refer more specifically to a “conditional reduced fit”, the conditioning being with respect to a subset of the complete fit. A true reduced fit would attempt to fit the directed graph *ab initio*, which we have not done. In the following examples, however, it will be seen that many, often all, of the selected residuals are zero, so these conditional reduced fits cannot be improved and therefore must also be true reduced fits. Clearly, reduced fits must be better than full asymmetric solutions. In the following, the residuals from the fitted distances retained in a reduced fit are denoted by an asterisk, as are the associated fitted sums-of-squares.

Consider a simplex A, B, C, D which is regular (side unity) except that C and D coincide. Thus we have two equilateral triangles ABC and ABD where C and D are different labels for the same point; alternatively the point pair C, D may be regarded as a single point with weight two. The distance matrix is

$$\mathbf{D} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{pmatrix}.$$

The four points occupy a two-dimensional Euclidean space, but we shall investigate various forms of one-dimensional approximation. The best classical fit minimizing

SSTRESS (S_1 , say) is a line of length $2v$ with A and B at either end, and with C, D coincident at the centre. Here $v^2 = \frac{2}{5}$ and $S_1 = 3\frac{3}{5}$, corresponding to a reduced fit of $S_1^* = 1\frac{4}{5}$ when only the upper (lower) triangular fit is considered.

Now consider symmetric unfolding solutions. First take the classical solutions just described augmented by a second set of points a, b, c, d all coinciding with C , and hence also with D . The fitted matrix of squared distances is asymmetric with values:

$$\begin{array}{c} A \\ B \\ C \\ D \end{array} \begin{pmatrix} a & b & c & d \\ v & v & v & v \\ v & v & v & v \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

with $v = 1$ and residual sum-of-squares $S_2 = 4$, where diagonal contributions have been ignored. This solution is clearly worse than the classical solution so cannot be the best unfolding solution. However the off-diagonal residuals are:

$$\begin{array}{c} A \\ B \\ C \\ D \end{array} \begin{pmatrix} a & b & c & d \\ - & 0^* & 0^* & 0^* \\ 0 & - & 0^* & 0^* \\ 1 & 1 & - & 0^* \\ 1 & 1 & 0 & - \end{pmatrix}$$

and if fitted values are taken only for asterisked residuals, an exact one-dimensional reduced fit is found (i.e., now $S_2^* = 0$).

The best symmetric fit seems to be that described in the second paragraph of Section 1, where a regular simplex is represented by two points, distance v apart, with A, B, C, D coinciding at one point and a, b, c, d at the other. Because the matrix \mathbb{D} is not quite a regular simplex the best fit is not when $v = 1$ but turns out to be when $v^2 = \frac{5}{6}$. This situation gives a full fit with $S_3 = 1\frac{2}{3}$ which is better even than the reduced classical solution of $S_1^* = 1\frac{4}{5}$. However the best symmetric unfolding solution we have found, and which we believe to be globally optimal, is

not symmetric. This solution is given by consecutive points A, C, D, B on a line with inter-distances $v, 2u, v$ and where a, b, c, d coincide at the center, i.e., distance $u + v$ from A and B and distance u from C and D . The values of u and v which minimize SSTRESS are $u + v = 1$, $u^2 = \frac{2}{3}$ giving a full fit with $S_4 = 1\frac{1}{3}$. In this case the fitted squared distances and residuals are:

$$\begin{array}{c}
 \begin{array}{cccc}
 & a & b & c & d \\
 A & \left(\begin{array}{cccc} 1 & 1 & 1 & 1 \end{array} \right) \\
 B & \left(\begin{array}{cccc} 1 & 1 & 1 & 1 \end{array} \right) \\
 C & \left(\begin{array}{cccc} u^2 & u^2 & u^2 & u^2 \end{array} \right) \\
 D & \left(\begin{array}{cccc} u^2 & u^2 & u^2 & u^2 \end{array} \right)
 \end{array}
 &
 \begin{array}{c}
 \begin{array}{cccc}
 & a & b & c & d \\
 A & \left(\begin{array}{cccc} - & 0^* & 0^* & 0^* \end{array} \right) \\
 B & \left(\begin{array}{cccc} 0 & - & 0^* & 0^* \end{array} \right) \\
 C & \left(\begin{array}{cccc} 1 - u^2 & 1 - u^2 & - & -u^{2*} \end{array} \right) \\
 D & \left(\begin{array}{cccc} 1 - u^2 & 1 - u^2 & -u^2 & - \end{array} \right)
 \end{array}
 \end{array}
 \end{array}$$

By taking the reduced fit associated with the asterisked values, we obtain $S_4^* = \frac{4}{9}$ but this result is not so good as S_2^* . Thus S_2^* is the best reduced, S_3 the best symmetric fit, and S_4 the best (unconstrained) full fit found by one-dimensional symmetric unfolding, and all are substantial improvements on the classical solution.

FIGURE LEGENDS

Figure 1: Some two-dimensional solutions of symmetric unfolding. (a) Two sets of points, symmetric with respect to a straight line. (b) Two sets of points on concentric circles. (c) Two sets of points on three equidistant parallel lines, with one set exclusively on the central line. (d) Two sets of points on two perpendicular straight lines. (e) Two sets of points in no apparent pattern of symmetry.

Figure 2: Two-dimensional metric scaling of the galaxy data of Nathanson (1971), using least-squares squared scaling (LSSS).

Figure 3: Two-dimensional symmetric unfolding by LSSS of the galaxy data.

Figure 4: Two-dimensional LSSS scaling of the ethnic group data of Funk et al. (1978).

Figure 5: One-dimensional symmetric unfolding by LSSS of the ethnic group data.

TABLE LEGENDS

Table 1: Percentage contributions to sum of squared residuals (RSS) by each element of the distance matrix, showing row and column totals. A dot (.) represents a contribution of less than 0.1%. The contributions of the diagonal elements are zero by construction of the algorithm.

Figure 1 (a)

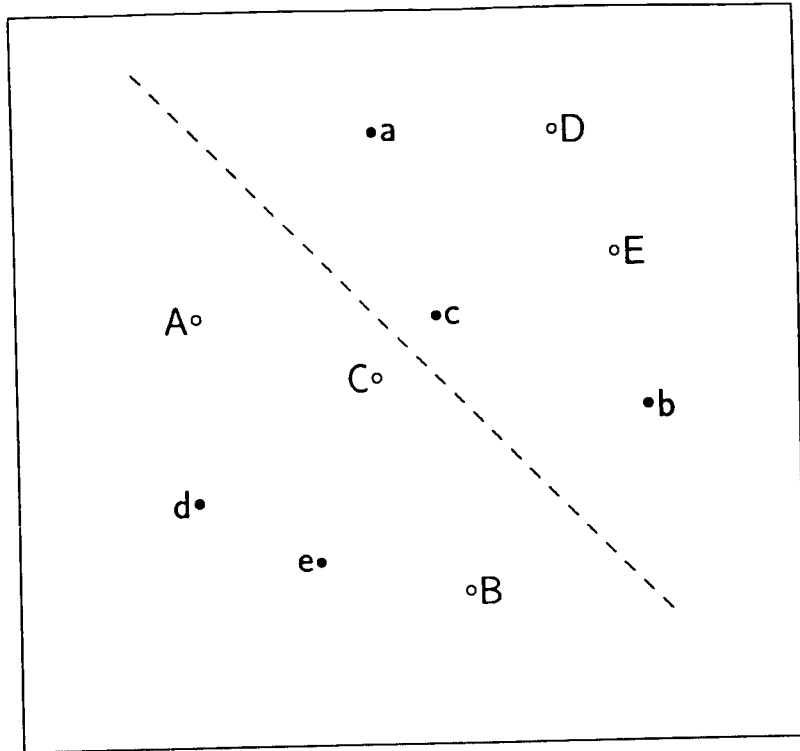


Figure 1 (b)

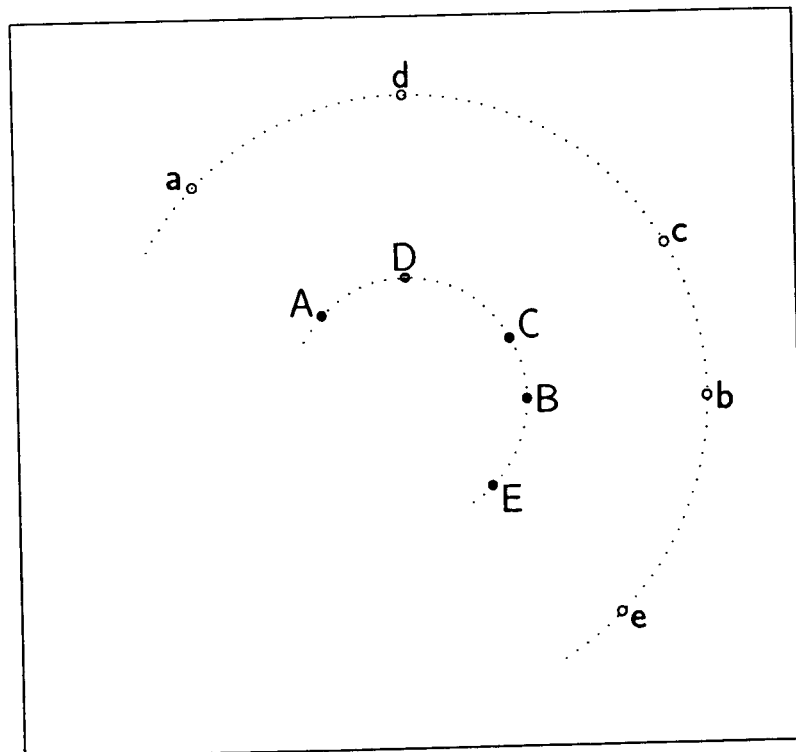


Figure 1 (c)

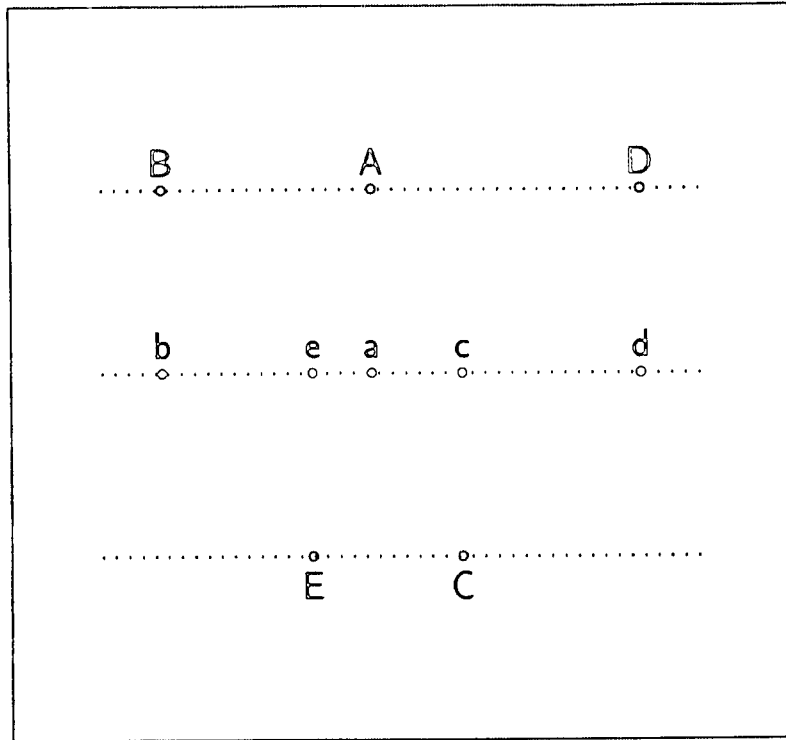


Figure 1 (d)

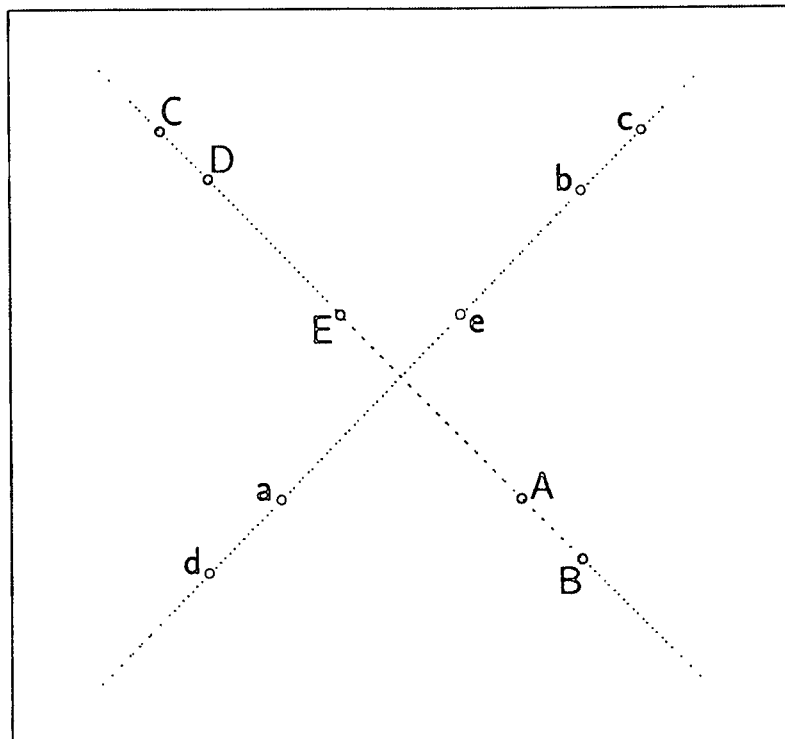


Figure 1 (e)

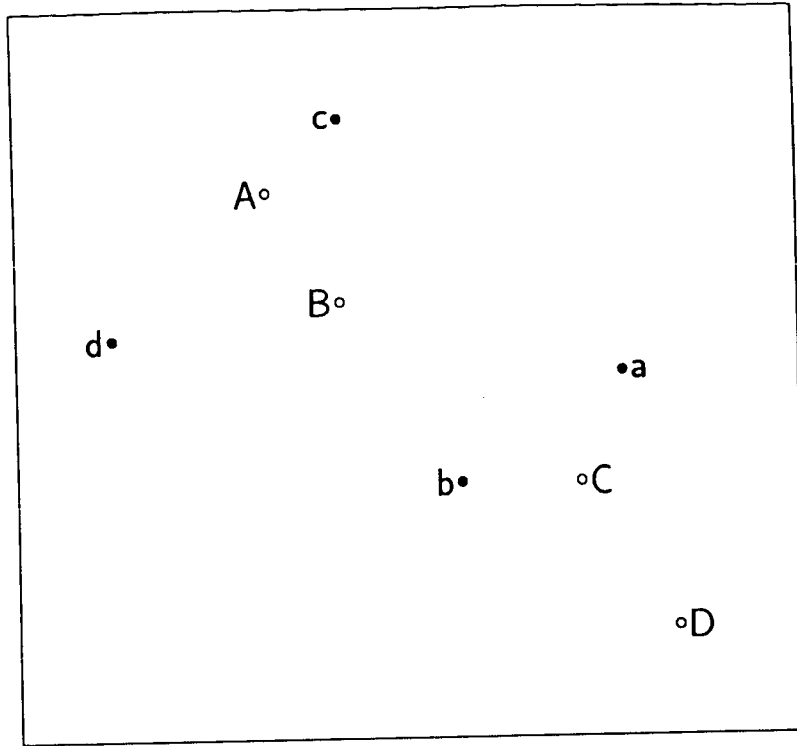


Figure 2

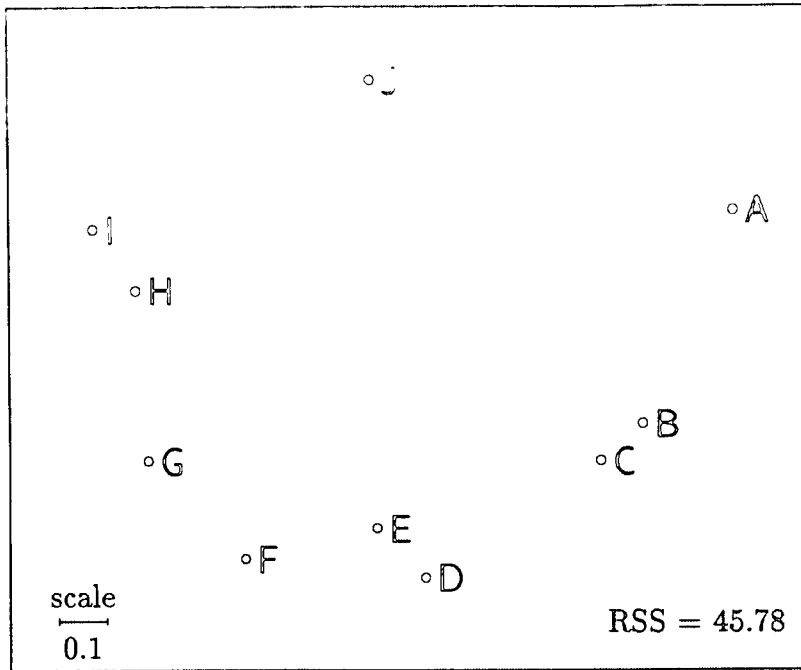


Figure 3

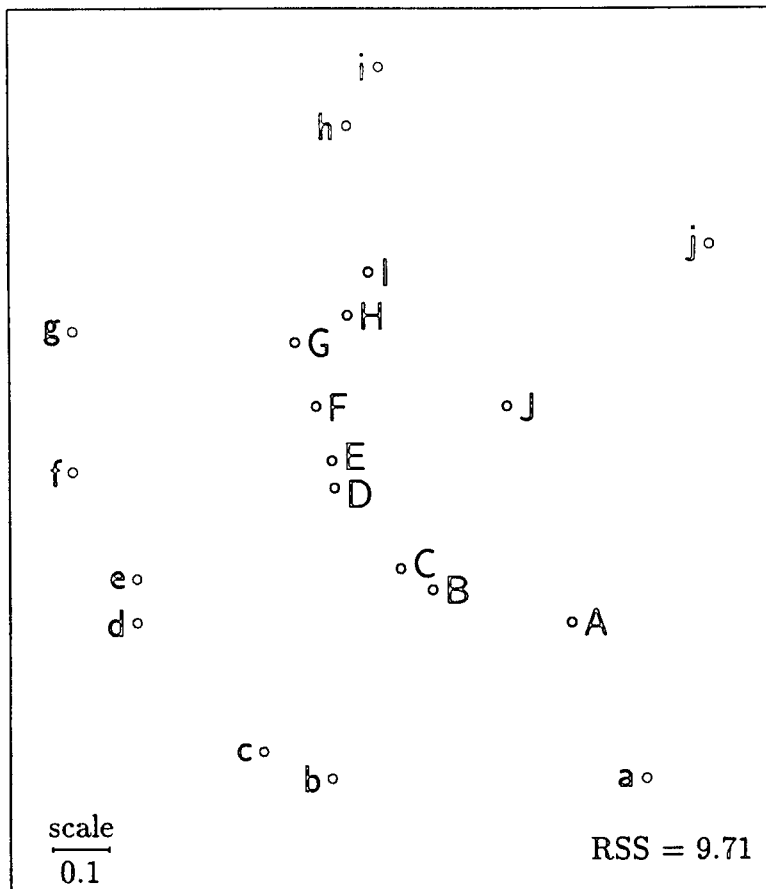


Figure 4

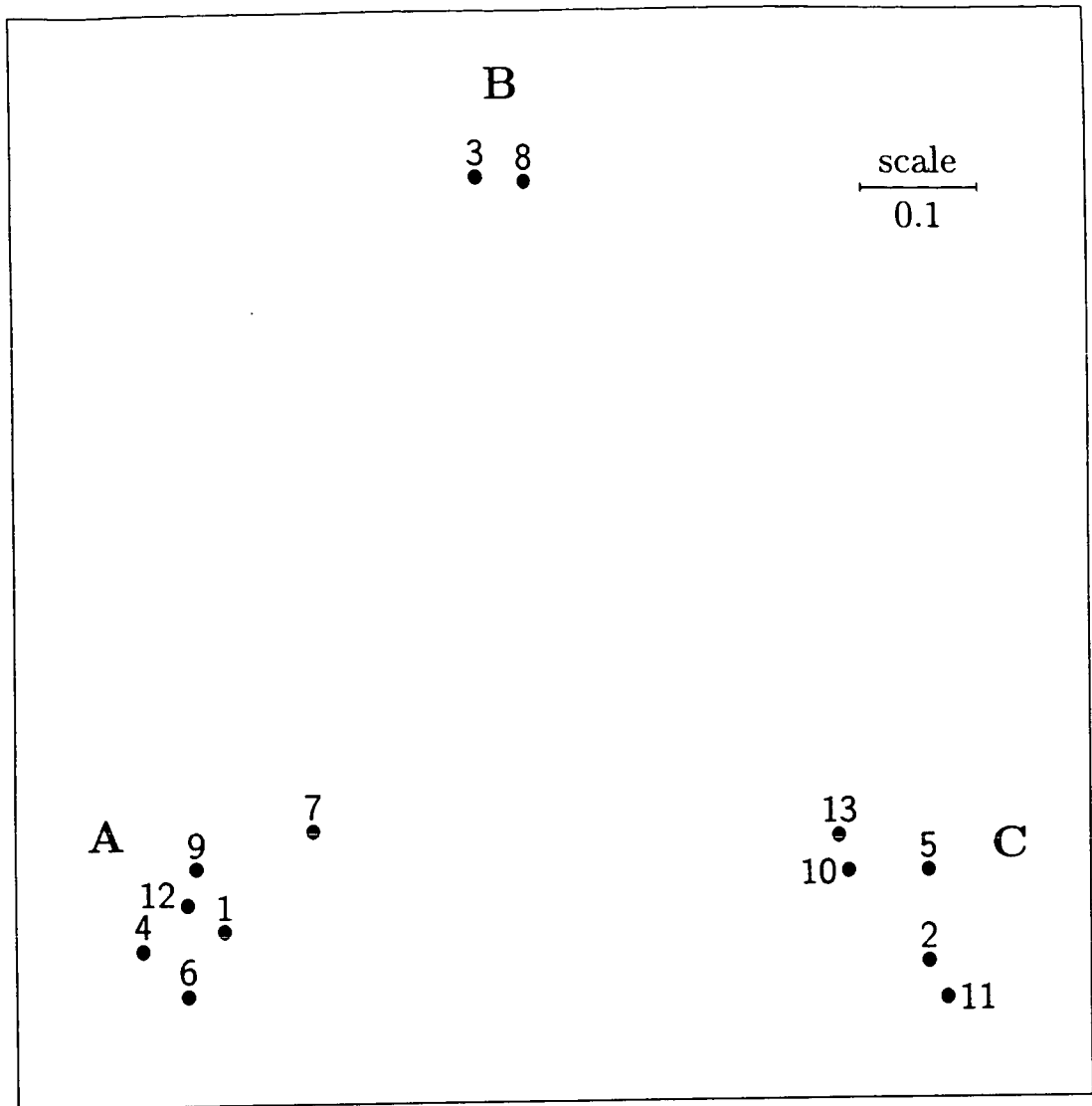


Figure 5

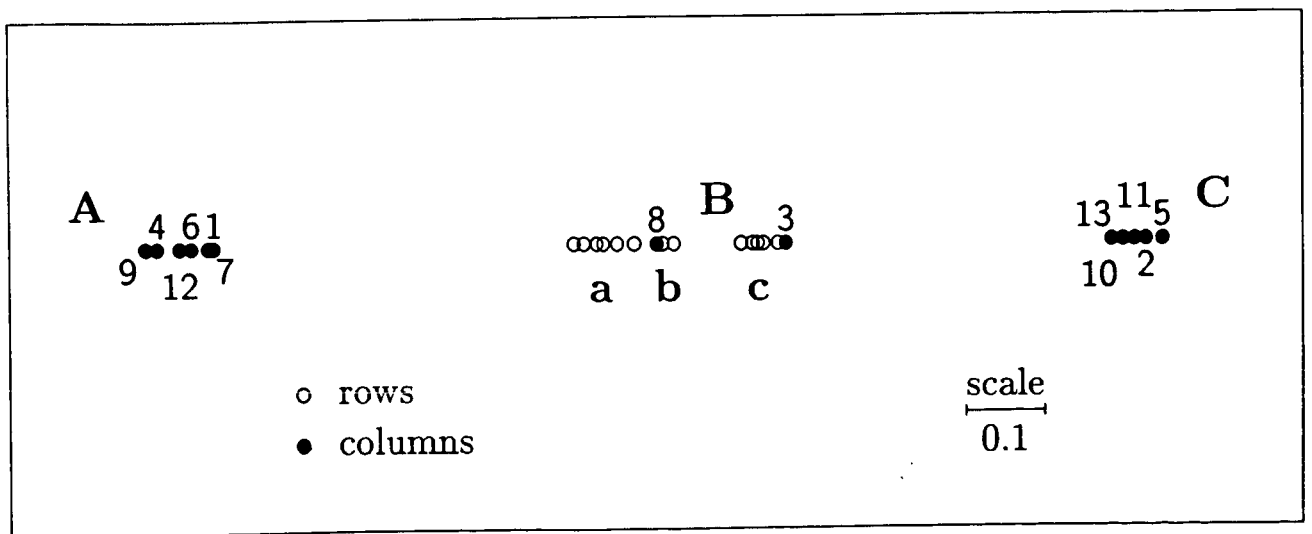


Table 1

| | | A | | | | | B | | C | | | | | | |
|---|----|------|------|------|------|------|------|-------|-------|------|------|------|------|------|--------|
| | | 1 | 4 | 6 | 7 | 9 | 12 | 3 | 8 | 2 | 5 | 10 | 11 | 13 | |
| a | 1 | 0 | . | 0.42 | . | . | . | 3.09 | 3.71 | . | 0.10 | . | 0.13 | . | 7.74 |
| | 4 | . | 0 | 0.10 | . | 0.15 | . | 3.72 | 3.64 | . | . | . | . | . | 7.85 |
| | 6 | 0.24 | 0.15 | 0 | 0.10 | . | . | 3.76 | 4.48 | . | . | . | . | . | 8.95 |
| | 7 | . | . | . | 0 | . | . | 2.62 | 3.50 | . | . | . | . | 0.24 | 6.53 |
| | 9 | . | 0.17 | 0.10 | . | 0 | . | 3.59 | 4.49 | . | . | . | . | . | 8.43 |
| | 12 | . | 0.13 | . | . | . | 0 | 3.45 | 4.23 | . | . | . | . | . | 8.03 |
| b | 3 | 0.18 | 0.24 | 0.23 | . | 0.10 | 0.15 | 0 | 0.18 | 0.29 | 0.19 | 0.29 | 0.15 | 0.24 | 2.69 |
| | 8 | 0.21 | 0.10 | 0.27 | 0.13 | 0.16 | 0.20 | 0.13 | 0 | 0.46 | 0.20 | 0.28 | 0.20 | 0.22 | 2.77 |
| c | 2 | . | . | . | . | . | . | 4.26 | 4.90 | 0 | . | 0.12 | . | . | 10.15 |
| | 5 | . | . | . | . | . | . | 4.47 | 4.50 | . | 0 | . | . | 0.14 | 9.31 |
| | 10 | . | . | . | 0.10 | . | . | 3.96 | 4.06 | . | . | 0 | . | 0.32 | 8.79 |
| | 11 | . | . | . | . | . | . | 5.08 | 4.59 | 0.78 | 0.19 | . | 0 | . | 10.71 |
| | 13 | . | . | . | 0.38 | . | . | 3.55 | 3.61 | . | . | 0.41 | . | 0 | 8.05 |
| | | 0.83 | 0.92 | 1.26 | 0.93 | 0.72 | 0.65 | 41.70 | 45.90 | 1.74 | 0.74 | 1.39 | 1.99 | 1.22 | 100.00 |

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