

Abstract: The "additive constant" problem proposed by W. S. Torgerson (1958) in Multidimensional Scaling methods is generalized in this paper: The Dissimilarity data $(d(i, j))$ is transformed to $((d(i, j) + \alpha)^\gamma)$, where α and γ are two parameters which are chosen so that the transformed data is 'nearly' Euclidean in a low dimensional space. The optimum solutions in the sense of maximum variance for α and γ are discussed and illustrated.

Key words: power transformation, order, variance

1. Introduction: Multidimensional Scaling

In the framework of analysis of ordinal data, multidimensional scaling may be considered as introduced by Shepard (1962) under the original name of "analysis of proximities". In fact, prior to Shepard's method, multidimensional scaling of numerical data has been proposed by Torgerson (1965). To distinguish the two variants, many workers use the adjectives nonmetric for the former one, and metric for the later one. We will drop these adjectives since the context always make it clear which variant is being considered.

Given a finite metric set whose metric is only known up to a monotonic transformation, we attempt to find in some Euclidean space a configuration of points whose distances are in the prescribed order. Intuitively, this is always possible when the Euclidean space is of dimension high enough; but if the dimension is specified, in general this can only be achieved in some approximate sense. To formalize this idea, Kruskal (1964) introduced a goodness-of-fit measure which he called stress; he also worked out a method to compute the configuration of points optimizing the stress. The Shepard-Kruskal method will be described briefly in a manner that it be easily viewed:

A dissimilarity function (D.F. for short) δ on a finite set I is a quasimetric $(\delta(i, i') = \delta(i', i) \geq 0$ and $\delta(i, i) = 0)$. Denote δ the set of all D.F.'s inducing the same order on $I \times I$, i.e., iff $(\delta'(i, j) > \delta'(k, l) \iff \delta(i, j) > \delta(k, l)$ or $\delta'(i, j) = \delta'(k, l) \iff \delta(i, j) = \delta(k, l))$, for all $i, j, k, l \in I$. Let \mathcal{D}_E^2 be the collection of all D.F. which are representable in the Euclidean plane. Define a function S on the cartesian product $\mathcal{D}_E^2 \times \mathcal{D}$ by $S(d, \delta') = [\sum_{i,j} (d(i, j) - \delta'(i, j))^2]^{1/2} / [\sum_{i,j} d^2(i, j)]$ for all $d \in \mathcal{D}_E^2$ and $\delta' \in \mathcal{D}$. The Shepard-Kruskal method is an iterative method which computes δ_d for each given $d \in \mathcal{D}_E^2$ so that $S(d, \delta_d) \leq S(d, \delta')$, for all $\delta' \in \mathcal{D}$ and then minimizes $S(d, \delta_d)$ for $d \in \mathcal{D}_E^2$. The procedure repeats with $\mathcal{D}_E^2, \mathcal{D}_E^2, \dots$ and ends for $S(d_0, \delta_{d_0})$ close enough to 0, e.g., $S(d_0, \delta_{d_0}) < 0.05$. This is in fact an isotonic regression of d on δ as rediscovered by Barlow et al., after a remark from Kendall. The solution d_0 needs not be unique. If the number of objects to be scaled is sufficiently larger than the dimension of the embedding space, e.g., 15 objects in 2 dimensions, Monte Carlo studies have shown that the solution is essentially unique. Although this method is used in as many fields as biological sciences, political sciences, marketing

research, psychology and archeology and so on, there remains several difficulties to overcome such as the cost of computation and some lack of mathematical analysis (Shepard, 1974) to cite but a few.

From the user point of view, the most serious problem may be the cost of computation entailed by the slowness of convergence due to: 1) the gradient method on which the algorithm is based, 2) an eventual structure in clusters on I induced by the D.F.

In case 2), complementary methods known as hierarchical clusterings are available to represent the set of objects I not by a configuration of points in Euclidean space but by a tree. (Cf. Benzecri (1973,b), Hartigan (1975), Jardin and Sibson (1971), Johnson (1967), Sokal and Sneath (1973).

Another alternative to multidimensional scaling

To avoid the problems caused by using the Shepard-Kruskal method as mentioned above, some authors (Benzecri, (1973,b)), Cooper (1972), Gower (1966)

) propose the analysis of the metric data instead of their ranking. If the data are not metric, methods have been proposed which transform them to be metric by special linear transformations (Torgerson (1965), Cooper (1972)). Although other monotone transformations such as exponential, logarithmic and power transformations are frequently used in biology, taxonomy (Stephenson, 1974), it seems that no theoretical investigation has been done.

2. Transformation of D.F.

According to some authors, including Williams and Dale (1965), Johnson (1968), Sokal and Sneath (1975), it is desirable that a D.F. be metric even when the assumption of the Euclidean structure of the embedding space is omitted.

Some computed D.F. and almost all dissimilarity data collected directly fail to satisfy the axioms of a metric. In these cases, transformations may help in "aiding in the analysis of data by bending the data nearer to the Procrustean bed of the assumptions underlying conventional analysis". (Tukey, 1962)

Using simple isotonic transformations we showed that the given D.F. may be made metric and even more Euclidean metric. The four families of isotonic transformations are:

$$f_\alpha(t) = \begin{cases} t^{+\alpha}, & \text{if } t > 0 \\ 0, & \text{if } t = 0 \end{cases} \quad f_\beta(t) = \begin{cases} \log \beta t, & \text{if } t > 0 \\ 0, & \text{if } t = 0 \end{cases}$$

$$f_\gamma(t) = t^\gamma, \text{ for } t \geq 0, \quad f_\zeta(t) = \begin{cases} e^{\zeta t}, & \text{if } t > 0, \\ 0, & \text{if } t = 0. \end{cases}$$

where $\alpha > 0, \gamma > 0$ and $\zeta > 0$.

It is shown that (cf. Thu Hoang (1978)) the set of parameters α (resp. β, γ , and ζ) so that $f_\alpha \circ \delta$ (resp. $f_\beta \circ \delta, f_\gamma \circ \delta$ and $f_\zeta \circ \delta$) be a metric is an interval $[\alpha_{\min}, \infty)$ (resp. $[\beta_{\min}, \infty), (0, \gamma_{\max}]$)

and $(0, \xi_{\max}]$ provided that δ is congruent to at least one nonmetric D.F. Otherwise the above intervals are $(0, \infty)$.

For all isotonic function f satisfying certain properties, $f(\delta + \alpha)$ (resp. $f(\xi\delta)$ and $f(\delta^\gamma)$) is metric or Euclidean metric for all α (resp. ξ, γ) in some interval. The end point of this interval could be used as a good starting point to search for an optimal parameter α (resp. ξ, γ) in the sense that $f(\delta + \alpha)$ (resp. $f(\xi\delta), f(\delta^\gamma)$) is nearly Euclidean in some low dimensional space. This result is illustrated empirically by investigating the transformed distance $(\delta + \alpha)^\gamma$ on a real set of data.

With these results, it becomes feasible to propose the alternative method : transform the dissimilarity data by $\delta \rightarrow (\delta + \alpha)^\gamma$ so that the new distances are nearly Euclidean in some low dimensional space. In an example taken from Ekman, we exhibit the optimal solution $(\alpha_{\text{opt}}, \gamma_{\text{opt}})$ where $\alpha_{\text{opt}} < \alpha_{\text{min}}$ and $\gamma_{\text{opt}} > \gamma_{\text{max}}$ and with the distance $(\delta + \alpha_{\text{opt}})^{\gamma_{\text{opt}}}$, the gradient matrix has the two largest eigenvalues which cover 71.69% of the trace.

The transformation $t \rightarrow (t + \alpha)^\gamma$

Using either the additive constant transformation $t \rightarrow t + \alpha$ or the power transformation $t \rightarrow t^\gamma$ to make δ nearly Euclidean is not satisfactory when α turns out to be too large and γ too small. Since, in these cases, the configurations associated with $\delta + \alpha$ and δ^γ are almost equilateral and the dimensionality of the embedding spaces large.

In the following, we overcome such difficulty by combining these two transformations to have the transformation $t \rightarrow (t + \alpha)^\gamma$ where α and γ may be chosen so that $(\delta + \alpha)^\gamma$ is Euclidean or nearly Euclidean.

Remarks:

- a) By adding a constant α , we preserve the order of the $\delta(i, j)$'s but decrease the ratio $\max \delta(i, j) / \min \delta(i, j)$. Therefore roughly speaking, emphasis is put rather on the main body of the data than on the tails.
- b) By powering with $\gamma < 1$, we preserve the order of the $\delta(i, j)$'s but force a greater stretch on the small distances than on the large ones, i.e., the data is compressed hopefully to a space of lower dimension.
- c) The transformation $t \rightarrow (t + \alpha)^\gamma$ is not as good as the transformation $t \rightarrow (t + \alpha)^\gamma$ at least in the case where the existence of very small distances makes γ_0 very small and the configuration of δ^{γ_0} almost equilateral.

An example: The Ekman data

By simple transformations, the Ekman data (Ekman, 1954) are made symmetric and reflexive. It is clear that the dissimilarities δ_{ij} so obtained do not satisfy the triangle inequality axiom (cf. Exhibit 1).

The D.F. δ is transformed into $(\delta + \alpha)^\gamma$. For each $\alpha > 0$, we can find the value $\gamma_{\max}(\alpha)$ so that $(\delta + \alpha)^\gamma$ is metric for all $\gamma > \gamma_{\max}(\alpha)$. The graph $\{(\alpha, \gamma_{\max}(\alpha)) : \alpha > 0\}$ is shown in Exhibit 1.

Consider the matrix (K_{ij}) with $k_{ij} = (\delta_{ij}^2 + \delta_{.j}^2 - \delta_{.i}^2 - \delta_{ij}^2)$ and $\delta_{.i}^2 = \frac{1}{n} \sum_j \delta_{ij}^2, \delta_{.j}^2 = \frac{1}{n^2} \sum_{i,j} \delta_{ij}^2$. We recognize that

for $\alpha = 9.4$ the sum of the first two eigenvalues of K gives the largest percentage of the trace.

The set of 14 colors together with the D.F. $(\delta + \alpha)^{\gamma_{\max}}$ is analyzed with $\alpha = 9.4$. In Exhibit 2, the eigenvalues of K and the coordinates of the points representing I are tabulated for 6 dimensions.

The following Exhibit 3 shows the projection of the configuration of I onto the planes (dim 1, dim 2), (dim 2, dim 3) and (dim 2, dim 4).

Exhibit 1 inserted here.

Exhibit 2 inserted here.

Exhibit 3 inserted here.

Exhibit 4 inserted here.

Transformations of metrics into Euclidean metrics
Blumenthal (1953, p. 313) showed that if (I, δ) is a finite metric space of cardinality 4, then the metric transform (I, δ^γ) of (I, δ) by power transformation is embeddable in the 3-dimensional Euclidean space E^3 if $\gamma \in [0, 1/2]$ and $1/2$ is a sharp bound.

Using Frechet's lemma to define the dimension of a finite metric space (I, δ) as the smallest integer k so that (I, δ) is isometrically embeddable in $(\mathbb{R}^k, \|\cdot\|_{\max})$, Schoenberg (1938, p. 536) generalized Blumenthal's result to any finite metric space of dimension not exceeding 2.

In this section, we show that any metric on a finite space can be transformed to Euclidean metric by $f_\alpha, f_\beta, f_\gamma,$ and f_δ for a suitable $\alpha, \beta, \gamma,$ and δ respectively. But first few further notations are introduced.

For any subset $J = \{j_1, j_2, \dots, j_k\}$ of I , the Cayley-Menger determinant of the metric transform $(J, f_\alpha \delta)$ is denoted by $D_f(J)$:

$$D_f(J) = \begin{vmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & f_\alpha \delta(j_1, j_2) & \dots & f_\alpha \delta(j_1, j_k) \\ 1 & f_\alpha \delta(j_2, j_1) & 0 & \dots & f_\alpha \delta(j_2, j_k) \\ \dots & \dots & \dots & \dots & \dots \\ 1 & f_\alpha \delta(j_k, j_1) & f_\alpha \delta(j_k, j_2) & \dots & 0 \end{vmatrix}$$

Let $D_0(J)$ be the determinant of order $k+1$ filled with 0 on the main diagonal and 1 elsewhere, and $A_0(J)$ be the determinant obtained from $D_0(J)$ by replacing 0 by 1 in the first entry of the first row. $D_0(J)$ and $A_0(J)$ are also denoted $D_0(k)$ and $A_0(k)$ respectively.

$$D_0(J) = \begin{vmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & 1 & \dots & 1 \\ 1 & 1 & 0 & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots \\ 1 & 1 & 1 & \dots & 0 \end{vmatrix} \quad A_0(J) = \begin{vmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & 0 & 1 & \dots & 1 \\ 1 & 1 & 0 & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots \\ 1 & 1 & 1 & \dots & 0 \end{vmatrix}$$

Also denote the Cayley-Menger determinant of (J, \cdot) by $D_1(J)$, and the signum function by $\text{sgn}(\cdot)$

Lemma $D_0(k) = (-1)^k \cdot k$ and $A_0(k) = (-1)^k$.

Proof. Expanding the two determinants $D_0(k)$ and $A_0(k)$ by the first row, we have

$$D_0(k) = -k.A_0(k-1)$$

and

$$A_0(k) = D_0(k-1) - k.A_0(k-1)$$

Hence

$$D_0(k) = -k[D_0(k-2) - (k-1)A_0(k-2)].$$

Direct computations yield $D_0(1)=-1$, $D_0(2)=2$, $D_0(3)=-3$, and $A_0(1)=-1$, $A_0(2)=1$, and $A_0(3)=-1$. By induction, the proof is completed. \square

To embed a finite metric space in Euclidean space, we may use the following theorem from Blumenthal (1953, p. 99).

Theorem 1 (Blumenthal). *A metric space I of n points is embeddable in the $(n-1)$ dimensional Euclidean space iff $\text{sgn}(D_c(J))=(-1)^{|J|}$ or $=0$, for all subset $J \subset I$ of cardinality $|J|$.

**The dimension of the smallest embedding space is precisely $n-1$ iff in addition $D_1(J) \neq 0$, for all $J \subset I$. This dimension is less than or equal to $(n-2)$ if D_1 vanishes for some subset $J \subset I$.

Corollary The smallest Euclidean embedding space equipped with the constant metric d_c , with $d_c(i, j)=c$ for all $i \neq j$ and $d_c(i, i)=0$, for all i , is of dimension $(n-1)$.

Proof. If $c=1$, the corollary follows obviously from Lemma and Theorem 1.

If $0 < c \neq 1$, take in E^{n-1} the equilateral configuration whose points are at unit distance from each other and perform on it a similarity transformation of ratio c . Hence we obtain an Euclidean representation of d_c . It is clear that E^{n-1} is the smallest embedding space. \square

Theorem 2 Any metric δ can be transformed to a Euclidean metric by one of the functions f_α , f_β , f_γ , and f_ζ , for all

$$\alpha \in (\alpha_1, \infty) ; \quad \beta \in (\beta_1, \infty), \text{ with } \beta_1 > 0 ; \quad \gamma \in (0, \gamma_1), \text{ with } \gamma_1 > 0$$

and

$$\zeta \in (0, \zeta_1), \text{ with } \zeta_1 > 0 \quad \text{respectively.}$$

Proof. (a) Consider the metric $(\delta + \alpha)/\alpha = 1 + \delta/\alpha$ on I , and for each $J \subset I$, denote $D(J)$ the Cayley-Menger determinant of $(J, 1 + \delta/\alpha)$. The limit of $D(J)$ as $\alpha \rightarrow \infty$ is $D_0(J)$. Hence by Lemma, there is an interval (α_J, ∞) with $\alpha_J > 0$ so that for all $\alpha \in (\alpha_J, \infty)$, the two determinants $D(J)$ and $D_0(J)$ are of the same sign, i.e.,

$$(1) \quad D_\alpha(J) > 0, \text{ if } |J| \text{ even,} \\ < 0, \text{ if } |J| \text{ odd.}$$

The power set of the finite set I being finite, it suffices to take the intersection of all such intervals (α_J, ∞) . This intersection is again an interval, say (α, ∞) . Therefore, the inequalities in (1) hold for all $\alpha \in (\alpha, \infty)$. Theorem 1 then gives the embeddability of $(J, (\delta/\alpha)+1)$ in E^{n-1} , hence of $(J, \delta + \alpha)$ by change of scale as in the proof of Corollary (b). Same method of proof, using the continuity (in parameters β, γ and ζ) of the Cayley-Menger determinant, may be applied to f_β, f_γ , and f_ζ respectively.

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Exhibit 1: (a) The original dissimilarity data $\{\delta_{ij} ; i,j=1,\dots,14\}$
 (b) The table of transformed distances $ij \quad \left\{ \begin{matrix} \delta + \alpha\delta \\ \delta \end{matrix} ; i,j=1,\dots,14 \right\}$
 where $\delta = 0.8662720$ and $\alpha = 9.4$

(a) The original dissimilarity data

A	0.00														
B	0.50	00.00													
C	44.50	36.00	00.00												
D	44.50	42.00	5.00	00.00											
E	68.50	64.00	39.00	32.00	00.00										
F	80.50	77.00	69.00	61.00	55.00	00.00									
G	79.50	79.00	76.00	76.00	55.00	24.00	00.00								
H	82.50	79.00	78.00	77.00	60.00	41.00	13.00	00.00							
I	84.50	84.00	84.00	84.00	79.00	72.00	64.00	53.00	00.00						
J	79.50	82.00	85.00	85.00	84.00	78.00	72.00	67.00	28.00	00.00					
K	77.50	79.00	84.00	86.00	84.00	84.00	81.00	82.00	49.00	12.00	00.00				
L	74.50	75.00	85.00	85.00	85.00	84.00	84.00	83.00	59.00	36.00	10.00	00.00			
M	73.50	73.00	81.00	84.00	84.00	84.00	84.00	84.00	66.00	45.00	24.00	01.00	00.00		
N	70.50	72.00	83.00	82.00	86.00	85.00	86.00	84.00	63.00	58.00	11.00	18.00	10.00	00.00	

GAMMA= 0.8662720E+00

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
A	00.00													
B	07.29	00.00												
C	31.62	27.26	00.00											
D	31.62	30.35	15.00	00.00										
E	43.51	41.32	28.81	25.16	00.00									
F	49.26	47.59	43.75	39.86	21.43	00.00								
G	48.78	48.55	47.12	47.12	36.90	20.89	00.00							
H	50.21	48.55	48.47	47.59	39.37	29.84	14.78	00.00						
I	51.15	52.92	50.92	50.92	48.55	45.20	41.32	35.90	00.00					
J	48.78	49.97	51.39	51.39	50.92	48.07	45.20	42.78	23.04	00.00				
K	47.83	48.55	50.92	51.86	50.92	49.50	49.97	33.90	14.21	00.00				
L	46.40	46.64	51.39	51.39	51.39	50.92	50.92	50.44	38.87	27.26	13.05	00.00		
M	45.92	45.88	49.50	50.92	50.92	52.92	50.92	50.92	42.30	31.88	20.89	07.60	00.00	
N	44.48	45.20	50.44	49.97	51.86	51.39	51.86	50.92	40.84	38.38	24.64	17.60	13.05	00.00

Exhibit 2: The table of eigenvalues and the table of coordinates

(a) Table of eigenvalues:

#	Inter	Eigenvalues	%age	Histogram of the eigenvalues
1	0	375.36865	43.123	*****
2	1	248.27443	28.522	*****
3	1	90.62272	10.499	*****
4	2	77.81252	8.939	*****
5	1	33.99341	3.905	****
6	2	23.96532	2.753	***
7	1	8.99486	1.033	*
8	2	6.46948	0.743	*
9	4	4.70712	0.541	*
10	2	1.31832	0.151	*
11	4	0.05826	0.110	*
12	2	0.00010	0.000	*
13	2	1.00000	0.115	*
14	2	-1.00002	-0.115	*

(b) Table of coordinates:

Lable	Axis 1	Axis 2	Axis 3	Axis 4	Axis 5	Axis 6
A	11.352717	21.774704	12.668971	-10.066490	5.075399	-4.031044
B	13.398633	-21.275391	11.009748	-9.172412	2.599362	-2.459863
C	21.195480	15.994116	0.965671	9.899796	4.796741	7.995027
D	22.432190	-14.115020	-3.938821	10.764769	-3.854238	2.029480
E	22.317719	4.020763	-14.522429	8.280353	2.559093	-4.642523
F	17.156891	19.449567	-11.895028	-3.003985	6.066266	-6.901677
G	12.483197	24.864761	1.707663	-10.954304	2.266757	5.159155
H	9.750073	25.228607	7.7119870	-7.880297	-6.547161	5.849097
I	-12.107060	14.972086	14.964095	11.817791	-8.789591	-8.448952
J	-20.556229	7.662084	10.158557	11.710624	8.472367	2.543828
K	25.772949	1.474460	1.100596	5.887628	7.203251	2.283828
L	-25.711975	-5.402475	-6.881705	-2.540895	1.938488	1.545890
M	-23.781158	7.528996	10.022672	-6.002810	-1.903905	3.431932
N	-22.157593	-8.621627	-8.853886	-8.739642	-10.289339	-4.314269

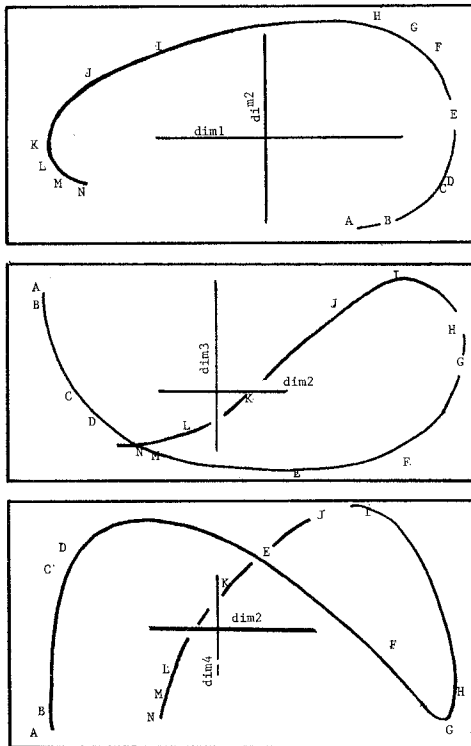


Exhibit 3: The configurations of I on dim1, dim2; dim2, dim3; dim2, dim4.

Exhibit 4: (a) the graph of γ_{max}
(b) the percentage of the trace for $c=0, 2, \text{ or } 9$.

