PSYCHOMETRIKA—VOL. 35, NO. 2
JUNE, 1970

FITTING ONE MATRIX TO ANOTHER UNDER CHOICE OF A CENTRAL DILATION AND A RIGID MOTION

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A least squares method is presented for fitting a given matrix A to another given matrix B under choice of an unknown rotation, an unknown translation, and an unknown central dilation. The procedure may be useful to investigators who wish to compare results obtained with nonmetric scaling techniques across samples or who wish to compare such results with those obtained by conventional factor analytic techniques on the same sample.

1. *Introduction*

The presently popular nonmetric multidimensional scaling techniques, such as Shepard's [1962], Kruskal's [1964a, 1964b], McGee's [1966], those of the Guttman–Lingoes series [1967, 1968], and, presumably, several others, produce configurations of points which are obtained by transforming sets of similarity or dissimilarity measures into distances. Goodness of fit is assessed in terms of the degree of monotonicity between the observed similarity measures and the interpoint distances of the reproduced configuration. The coordinates of the reproduced configuration are arbitrary in the sense of being only defined up to a central dilation (a uniform expansion or contraction along the coordinate axes), a translation (a shift of the origin), and a rotation, as these transformations in no way affect the monotonicity measure of goodness of fit. Under "rotation" we include both proper and improper rotations where improper rotations consist of proper rotations followed by an odd number of reflections.

Some investigators (*e.g.*, Kruskal, 1964a, Guttman, 1968) have pointed out the possibility of using correlation coefficients as measures of similarity. This raises the question of how results obtained with nonmetric scaling techniques would compare with results obtained by the more traditional factor analytic techniques. Yet before a meaningful comparison could be made, it would be necessary to rotate, translate, and stretch or shrink the nonmetric scaling configuration so as to obtain maximal agreement with the

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factor solution. This would become a difficult and laborious task however, as the number of dimensions increased.

The purpose of this paper, therefore, is to present a least squares technique which is readily programmed for analysis by computers for fitting a given matrix A to another given matrix B under choice of a rotation, a translation (*i.e.*, together, a "rigid motion"), and a central dilation.

The present problem is a generalization of the "orthogonal Procrustes" problem which has been solved by Green]1952] for the full rank case and by Cliff]1966] and Schönemann [1966] for the deficient rank case.

2. *Mathematical Derivation*

As a model we chose

$$B = cAT + J\gamma' + E \tag{2.1}$$

where $J' = (1, 1, \cdots, 1)$ A and B are two known $p \times q$ matrices. and where the orthogonal $q \times q$ matrix T, the $q \times 1$ vector γ, and the scalar c are to be chosen so as to minimize the sum of squared elements e_{ij} of the residual matrix E.

We note that this particular formulation of the least squares problem is as good as any of the other five which can be obtained by permuting the sequence of the unknown transformations, because the parameter triples of all six formulations are related by 1–1 transformations, so that [Anderson, 1958, p. 47] the solution triples relate by these same transformations. To illustrate, the parameters R, ω, d in $B = d(A + J\omega')R + E$ are related by $d = c$, $R = T$, and $d\omega'R = \gamma'$ to the unknowns in (2.1).

To obtain the solution for the present formulation (2.1) we differentiate

$$f = f_1 + f_2 , \tag{2.2}$$

where

$$f_1 = \operatorname{tr} E'E = \text{const} + c^2 \operatorname{tr} T'A'AT + p\gamma'\gamma - 2c \operatorname{tr} B'AT - 2 \operatorname{tr} B'J\gamma' + 2c \operatorname{tr} T'A'J\gamma',$$

and

$$f_2 = \operatorname{tr} L(T'T - I)$$

and where L is a $q \times q$ matrix of unknown Lagrange multipliers, with respect to the unknowns T, γ, and c.

Upon setting the derivatives (*e.g.*, Schönemann, 1965) equal to zero one obtains

$$\partial f/\partial T = 2c^2A'AT - 2cA'B + 2cA'J\gamma' + TM = \phi \tag{2.3}$$

where

$M = L + L' = M'$ is an unknown symmetric matrix,

$$\partial f/\partial \gamma = 2p\gamma - 2B'J + 2cT'A'J = \phi, \tag{2.4}$$

$$\partial f/\partial c = 2c \operatorname{tr} T'A'AT - 2 \operatorname{tr} B'AT + 2 \operatorname{tr} T'A'J\gamma' = 0. \tag{2.5}$$

From (2.4) one obtains

$$\gamma = (B - cAT)'J/p \tag{2.6}$$

and from (2.3)

$$T'A'B - T'A'J\gamma' = \text{a symmetric matrix,} \tag{2.7}$$

which reduces in view of (2.6) to

$$T'A'B - T'A'(JJ'/p)(B - cAT) = \text{symmetric,}$$

so that

$$T'A'(I - JJ'/p)B = \text{symmetric,} \tag{2.8}$$

since $cT'A'(JJ'/p)AT$ certainly is.

Note that (2.8) is free from γ and c and can be solved for T at once by use of the same symmetry argument which Schönemann [1966] employed to solve the "orthogonal Procrustes" problem: since (2.8) is of the form

$$T'C = C'T \tag{2.9}$$

$$T = VW' \tag{2.10}$$

where

$$VDW' = C = A'(I - JJ'/p)B \tag{2.11}$$

is the Eckart–Young decomposition of $C = A'(I - JJ'/p)B$, a matrix which is proportional to the (sample) covariance matrix of (the columns of) A with B. Care should be exercised in choosing the correct orientation for the columns in V and W in (2.10). As was shown in more detail in Schönemann [1966], the orientation should be such that $V'CW$ is a non-negative diagonal matrix.

Having computed T one can use it to solve (2.5) for the contraction factor c after eliminating γ by means of (2.6):

$$c \operatorname{tr} T'A'AT - \operatorname{tr} B'AT + \operatorname{tr} T'A'(JJ'/p)(B - cAT) = 0$$

i.e.,

$$c = \operatorname{tr} T'A'(I - JJ'/p)B/\operatorname{tr} A'(I - JJ'/p)A. \tag{2.12}$$

Eqs. (2.6) and (2.12) combine to give the translation vector γ. This vector need not be computed explicitly, however, since both

$$\begin{aligned}\hat{B} = cAT + J\gamma' &= cAT + (JJ'/p)(B - cAT) \\ &= (JJ'/p)B + c(I - JJ'/p)AT,\end{aligned} \tag{2.13}$$

the matrix of best fit, as well as

$$E = B - \hat{B} = (I - JJ'/p)(B - cAT), \tag{2.14}$$

the matrix of residuals, do not involve γ. In other words, the fit is the same regardless of the relative location of the origins of both configurations.

The procedure is easily programmed:

(i) Compute the vectors of column means $\bar{\alpha} = A'J/p$ and $\bar{\beta} = B'J/p$ and subtract these from the rows of A and B, respectively, to obtain the two column-centered matrices $A^* = A - J\bar{\alpha}'$, $B^* = B - J\bar{\beta}'$. Save $\bar{\beta}$.

(ii) Enter a standard orthogonal Procrustes subroutine [Green, 1952; Cliff, 1966; Schönemann, 1966] with the column-centered matrices A^*, B^* to obtain, upon return, the transformation matrix T and the matrix A^*T.

(iii) Compute the scalar $c = \text{tr}\,[(T'A^{*\prime})B^*]/\text{tr}\,A^{*\prime}A^*$,

(iv) and the matrix of best fit $\hat{B} = c(A^*T) + J\bar{\beta}'$.

If the contraction factor c is not wanted, one simply sets $c = 1$ in (iii) to obtain the least squares solution under variation of T and γ alone.

3. A Symmetric Measure of Fit

For many practical purposes the simple error sum of squares $\text{tr}\,E'E = \sum_i^p \sum_j^q e_{ij}^2$ (perhaps divided by pq, the number of elements in E) will suffice as a measure of fit. If, however, the objective is to interpret this measure as an index of similarity between A and B, and if there is no reason to single out one matrix as error-free, *i.e.*, if both matrices are based on fallible data, then one may prefer a symmetric measure of fit.

Bargmann [1960] has pointed out that $\text{tr}\,E'E$ is not a symmetric measure of fit if T (in $B = AT + E$) is unrestrained (unconditional oblique Procrustes problem). On the other hand, if T is constrained to be orthogonal (orthogonal Procrustes problem) then $\text{tr}\,E'E$ is a symmetric measure of fit since $\text{tr}\,E'E = \text{tr}\,T'E'ET$. That is to say, one obtains the same error sum of squares whether one fits A to B (solves $B = AT + E$ for T) or B to A (solves $A = BS + E$ for S), and the solution matrices are simply related ($S = T'$).

In the present instance the transformation matrices T and S in

$$B = cAT + J\gamma' + E \qquad \text{and} \qquad A = dBS + J\delta' + E^* \tag{3.1}$$

are also simply related, as

$$S = T' \tag{3.2}$$

since either one is obtained as the solution of an orthogonal Procrustes problem on A and B after removing the column means.

To see how the error sums of squares tr $E'E$ and tr $E^{*\prime}E^*$ relate, we recall that

$$E = B - cAT - J\gamma' \tag{3.3}$$

simplifies to

$$E = (I - JJ'/p)(B - cAT) = Q(B - cAT), \quad \text{say} \tag{3.4}$$

where

$$c = \text{tr } C'T/\text{tr } A'QA \qquad \text{and} \qquad Q = I - JJ'/p = Q^2. \tag{3.5}$$

Upon substituting c one finds for tr $E'E$

$$\text{tr } E'E = \frac{(\text{tr } B'QB)(\text{tr } A'QA) - (\text{tr } T'C)^2}{\text{tr } A'QA}. \tag{3.6}$$

Thus it appears that both c, d and tr $E'E$, tr $E^{*\prime}E^*$ are related by the same constant of proportionality

$$u = \text{tr } B'QB/\text{tr } A'QA \tag{3.7}$$

since

$$c\text{tr } A'QA = \text{tr } C'T = d \text{ tr } B'QB, \quad i.e., \quad c = ud$$

from (2.12) and also

$$(\text{tr } E'E)(\text{tr } A'QA) = (\text{tr } E^{*\prime}E^*)(\text{tr } B'QB), \quad i.e., \quad \text{tr } E'E = u \text{ tr } E^{*\prime}E^*$$

from (3.6). Note that u is independent of the unknowns T, c, and γ.

Therefore, the measure

$$e = \text{tr } E'E\sqrt{\text{tr } A'QA/\text{tr } B'QB} = (\text{tr } E'E)u^{-1/2} \tag{3.8}$$

could serve as a symmetric measure of fit, if such is desired, since

$$\begin{aligned} e = (\text{tr } E'E)u^{-1/2} &= (\text{tr } E^{*\prime}E^*)u \cdot u^{-1/2} = (\text{tr } E^{*\prime}E^*)u^{1/2} \\ &= (\text{tr } E^{*\prime}E^*)v^{-1/2} = e^* \end{aligned} \tag{3.9}$$

where $v = u^{-1}$ follows from (3.7) upon interchanging A and B. Using this measure of fit amounts to carrying out the least squares fit on the scaled matrices $u^{-1/4}A$ and $u^{-1/4}B$, or, equivalently, to solving a weighted least squares problem, minimizing tr $E'(u^{-1/2})E$, rather than tr $E'E$.

4. Illustrative Examples

A FORTRAN IV program was written to carry out the computations described in the preceding sections. A statement listing is available upon request from the junior author. Here we present three illustrative examples: one based on artificial data generated without error, another based on artificial data generated with random error, and a third based on empirical data which we took from the literature.

Table 1

Data Generated Without Error

Matrix A

$$A = \begin{bmatrix} 4.000 & 0.000 \\ 3.000 & 1.414 \\ 0.000 & 1.414 \\ 0.000 & 0.000 \end{bmatrix}$$

Target Matrix B

$$B = \begin{bmatrix} 3.828 & 1.828 \\ .414 & 2.414 \\ -3.828 & -1.828 \\ -1.828 & -3.828 \end{bmatrix}$$

Matrix of best fit $\hat{B}$

$$\hat{B} = \begin{bmatrix} 3.828 & 1.828 \\ .414 & 2.414 \\ -3.828 & -1.828 \\ -1.828 & -3.828 \end{bmatrix}$$

Residual Matrix E

$E = \emptyset$

Transformation Matrix T

$$T = \begin{bmatrix} .707 & .707 \\ -.707 & .707 \end{bmatrix}$$

Translation Vector γ'

$$\gamma' = \begin{bmatrix} -1.828 & -3.828 \end{bmatrix}$$

Contraction factor c	trE'E/pq	Normalized Symmetric Error
2.000	.000	.000

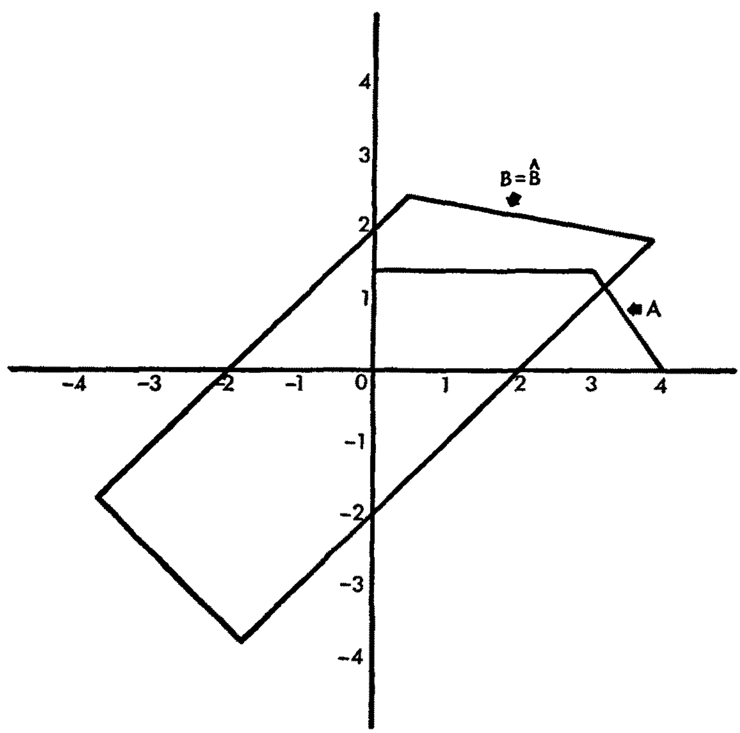

FIGURE 1
Graphical representation of matrices A, B, and $\hat{B}$ for data generated without error.

Table 2

Data Generated with Random Error

Matrix A

$$\begin{bmatrix} 4.000 & 0.000 \\ 3.000 & 1.414 \\ 0.000 & 1.414 \\ 0.000 & 0.000 \end{bmatrix}$$

Target Matrix B

$$\begin{bmatrix} 4.456 & 1.688 \\ .165 & 1.646 \\ -3.230 & -2.045 \\ -1.114 & -4.235 \end{bmatrix}$$

Matrix of best fit $\hat{B}$

$$\begin{bmatrix} 4.046 & 1.596 \\ .684 & 2.003 \\ -3.252 & -2.345 \\ -1.202 & -4.200 \end{bmatrix}$$

Residual Matrix E

$$\begin{bmatrix} .410 & .092 \\ -.519 & -.357 \\ .022 & .300 \\ .088 & -.035 \end{bmatrix}$$

Transformation Matrix T

$$\begin{bmatrix} .671 & .741 \\ -.741 & .671 \end{bmatrix}$$

Translation Vector γ'

$$\begin{bmatrix} -1.202 & -4.200 \end{bmatrix}$$

Contraction Factor c	trE'E/pq	Normalized Symmetric Error
1.955	.084	.042

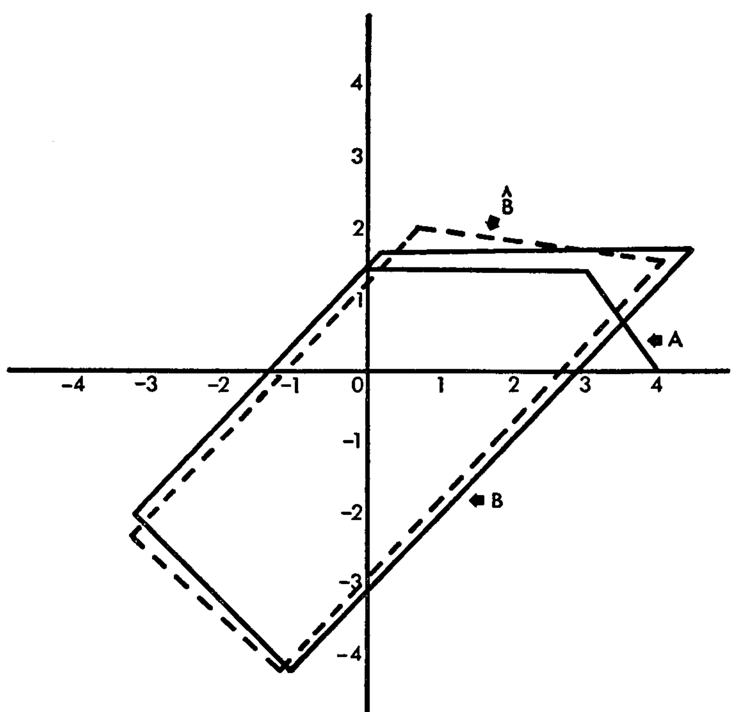

FIGURE 2
Graphical representation of matrices A, B, and $\hat{B}$ for data generated with random error.

For the error-free case we derived the "target matrix" B from A by rotating A through an angle of 45 degrees, then translating the origin by 1.828 and 3.828 units, and multiplying all interpoint distances by two. Thus $\hat{B}(=cAT + J\gamma')$ should equal B exactly, as indeed it did (see Table 1 and Figure 1).

The second set of data was identical to the first except that random normal deviates with mean zero and variance unity were added to the target matrix yielding a new matrix B which no longer allows for a perfect fit. The actually obtained fit (see Figure 2 and Table 2) was fairly good, how-

Table 3

Empirical Data Reported by Prien and Liske (1962)

Matrix A (Scaling Solution)

1.409	1.066	-1.378	0.390	0.104
1.541	0.683	-0.251	-0.856	-0.467
1.365	0.781	-0.905	-0.923	-0.275
0.586	1.706	-0.190	-0.097	-0.482
0.225	1.418	-0.871	-0.303	-0.407
1.213	1.109	0.081	-0.061	0.830
1.813	-0.148	0.002	-1.014	0.880
1.076	1.223	-0.175	-0.791	0.484
-1.809	-0.499	-1.615	-0.459	0.857
-0.767	-1.281	1.108	-0.831	0.519
-1.188	-1.950	-0.186	-0.349	0.071
-1.012	-0.944	1.206	1.398	-0.800
-1.102	-0.241	0.729	0.178	-1.730
-0.628	-0.749	0.922	1.726	1.599
0.119	-2.214	-0.675	0.840	0.907
-0.145	-1.829	0.690	0.945	-1.205

Matrix B (Factor Solution)

0.233	-0.198	0.350	0.582	0.219
0.360	0.012	0.347	0.616	0.109
0.241	0.053	0.354	0.785	-0.010
0.867	0.053	0.137	0.365	0.063
0.501	0.078	0.221	0.547	0.099
0.474	0.030	0.486	0.336	0.242
0.234	0.289	0.927	0.036	0.008
0.524	0.083	0.508	0.415	0.113
0.031	0.220	0.063	0.237	0.340
-0.043	0.496	0.161	0.229	0.369
-0.148	0.589	0.058	0.306	0.371
0.112	0.420	-0.166	0.123	0.460
0.341	0.574	-0.228	0.278	0.151
0.049	0.111	0.043	0.026	0.644
0.017	0.319	0.215	0.012	0.482
0.174	0.531	-0.025	-0.006	0.402

Matrix of best fit Â

0.607	0.964	-1.502	-0.070	0.656
0.632	1.028	-0.937	-0.607	0.049
0.514	0.909	-1.490	-1.226	-0.204
0.973	1.863	0.478	0.412	-0.973
0.510	1.183	-0.449	-0.304	-0.431
1.129	0.847	-0.005	-0.119	0.624
2.551	-0.839	0.497	-1.084	0.989
1.308	1.002	-0.036	-0.537	0.235
-0.391	-0.794	-0.436	0.438	0.139
-0.605	-1.395	0.114	-0.277	0.227
-1.132	-1.673	-0.065	-0.477	-0.008
-1.146	-1.028	0.390	0.859	-0.308
-0.864	-0.462	0.611	0.138	-1.609
-0.627	-0.856	0.010	1.435	0.999
-0.155	-1.335	0.335	0.578	0.789
-0.609	-1.282	0.977	0.635	-0.288

Matrix of best fit B̂

0.336	-0.158	0.299	0.391	0.083
0.416	0.177	0.403	0.398	-0.018
0.336	0.095	0.396	0.490	-0.009
0.559	0.080	0.207	0.486	0.159
0.411	0.060	0.177	0.573	0.155
0.463	0.045	0.451	0.332	0.279
0.262	0.202	0.627	0.275	0.132
0.446	0.114	0.461	0.473	0.196
-0.120	0.203	0.083	0.618	0.485
0.132	0.602	0.275	0.251	0.437
-0.110	0.491	0.083	0.275	0.352
0.295	0.426	-0.152	0.028	0.398
0.362	0.502	-0.162	0.313	0.201
0.200	0.181	0.153	-0.016	0.706
-0.170	0.186	0.209	0.026	0.340
0.143	0.449	-0.064	-0.032	0.160

Table 3 continued

Residual Matrix E*

0.801	0.101	0.124	0.460	-0.552
0.908	-0.345	0.686	-0.249	-0.516
0.850	-0.128	0.585	0.303	-0.070
-0.387	-0.157	-0.668	-0.509	0.491
-0.285	0.234	-0.421	0.001	0.024
0.083	0.261	0.086	0.058	0.205
-0.738	0.691	-0.495	0.070	-0.109
-0.232	0.220	-0.138	-0.254	0.248
-1.417	0.295	-1.178	-0.897	0.718
-0.161	0.114	0.994	-0.553	0.292
-0.055	-0.276	-0.120	0.128	0.079
0.134	0.084	0.815	0.538	-0.491
-0.237	0.221	0.117	0.039	-0.120
-0.000	0.107	0.911	0.290	0.599
0.274	-0.878	-1.010	0.261	0.117
0.464	-0.546	-0.287	0.309	-0.916

Residual Matrix E

-0.103	-0.039	0.050	0.190	0.135
-0.056	-0.165	-0.056	0.217	0.127
-0.095	-0.042	-0.042	0.294	-0.000
0.307	-0.027	-0.070	-0.121	-0.096
0.089	0.017	0.043	-0.026	-0.056
0.010	-0.015	0.035	0.003	-0.037
-0.028	0.086	0.299	-0.239	-0.124
0.077	-0.031	0.046	-0.058	-0.083
0.151	0.016	-0.020	-0.381	-0.145
-0.175	-0.106	-0.114	-0.022	-0.068
-0.038	0.097	-0.025	0.030	0.018
-0.183	-0.006	-0.013	0.094	0.061
-0.021	0.071	-0.065	-0.035	-0.050
-0.151	-0.070	-0.110	0.042	-0.062
0.187	0.132	0.005	-0.014	0.141
0.031	0.082	0.039	0.026	0.241

Transformation Matrix S

0.200	0.751	0.575	0.101	-0.231
-0.319	-0.393	0.613	-0.543	-0.266
0.591	0.005	0.122	-0.513	0.609
-0.408	0.516	-0.438	-0.611	-0.035
-0.583	0.117	0.292	0.239	0.709

Transformation Matrix T

0.200	-0.319	0.591	-0.408	-0.583
0.751	-0.393	0.005	0.516	0.117
0.575	0.613	0.122	-0.438	0.292
0.101	-0.543	-0.513	-0.611	0.239
-0.231	-0.266	0.609	-0.035	0.709

Translation Vector δ'

0.785	-1.158	-1.005	1.213	-0.610

Translation Vector γ'

0.273	0.243	0.189	0.322	0.275

Contraction Factor d

3.651

trE*'E*/pq

0.246

Normalized Symmetric Error

0.058

Contraction Factor c

0.205

trE'E/pq

0.013

Normalized Symmetric Error

0.058

ever. The measures of fit were .084 for tr $E'E/pq$ and .042 for the normalized symmetric measure.

Our final example is based on the results of a factor analysis and a scale analysis of a 16 $\times$ 16 correlation matrix which was reported by Prien and Liske [1962]. The factors are in a varimax position and the scaling solution was obtained with a modification of Kruskal's [1964] program written by Robert J. Wherry. We decided to carry out the fit both ways so as to be able to compare the goodness of fit obtained when fitting A to B with that obtained when fitting B to A. The results (using the notation $B = cAT + J\gamma' + E$ and $A = dBS + J\delta' + E^*$) are shown in Table 3. Note that $S = T'$ and also that tr $E'E/pq <$ tr $E^{*\prime}E^*/pq$ while the normalized symmetric error measures are the same (.058) for both solutions.

In practice one would probably prefer to fit the more general nonmetric solution to the factor solution, especially if the latter has been rotated to a simple structure position. Upon comparing the factor solution (Table 3, matrix B) with the fitted scaling solution (Table 3, matrix $\hat{B}$) and the associated residual matrix E, one finds that the first three dimensions are in fairly close agreement between both methods while the last two factors disagree more noticeably with their counterparts in the fitted scaling solution. For instance, variable 9 (self rating on social skills) received only a moderate weight on factor 4 but it received the highest weight on the fourth dimension of the fitted scaling solution. Roughly the converse is true for variable 16 (self rating on overall efficiency) with regard to the fifth dimension of both solutions.

It is quite possible that one might be interested in fitting a multidimensional scaling solution to a factor analytic solution having more dimensions than the scaling solution. This situation can be handled by the present method by augmenting the scaling solution with columns of zeros bringing its column order up to that of the factor solution. More extensive illustrations of some practical applications of fitting nonmetric scaling solutions to factor analytic solutions, including some where the scaling solution has fewer dimensions than the factor solution, are described in Carroll [1969].

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Manuscript received 3/8/69
Revised manuscript received 8/5/69