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ORTHOGONAL PROCRUSTES ROTATION FOR TWO OR MORE MATRICES

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Necessary and sufficient conditions for rotating matrices to maximal agreement in the least-squares sense are discussed. A theorem by Fischer and Roppert, which solves the case of two matrices, is given a more straightforward proof. A sufficient condition for a best least-squares fit for more than two matrices is formulated and shown to be not necessary. In addition, necessary conditions suggested by Kristof and Wingersky are shown to be not sufficient. A rotation procedure that is an alternative to the one by Kristof and Wingersky is presented. Upper bounds are derived for determining the extent to which the procedure falls short of attaining the best least-squares fit. The problem of scaling matrices to maximal agreement is discussed. Modifications of Gower's method of generalized Procrustes analysis are suggested.

Key words: factor matching, least-squares rotation.

The Orthogonal Procrustes Problem

The problem of rotating m matrices ($m \geq 2$) toward a best least-squares fit is known as the orthogonal Procrustes problem. If A_i ($i = 1, 2, \cdots m$) is a set of m matrices of order $n \times k$ ($n \geq k$), then the problem is to find orthonormal matrices T_i ($i = 1, 2, \cdots m$) for which the function

$$f(T_1, \cdots T_m) = \sum_{i<j} \operatorname{tr} (A_iT_i - A_jT_j)'(A_iT_i - A_jT_j),$$

is minimized, or equivalently, for which the function

$$g(T_1, \cdots T_m) = \sum_{i<j} \operatorname{tr} T_i'A_i'A_jT_j$$

is maximized. Since postmultiplying each T_i by the same orthonormal T does not affect the value of f or g, any one of the matrices T_i can be taken as the $k \times k$ identity matrix. Therefore when $m = 2$, the problem can be reduced to finding an orthonormal matrix T_1 for which the function

$$f(T_1) = \operatorname{tr} (A_1T_1 - A_2)'(A_1T_1 - A_2),$$

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is minimized, or equivalently, for which

$$g(T_1) = \text{tr } T_1'A_1'A_2$$

is maximized. The solution to this problem is well known [Green, 1952; Kristof, 1964; Fischer & Roppert, 1965; Cliff, 1966; Schönemann, 1966]. It will be worthwhile to analyze this solution in detail since it has important implications for the general case of $m > 2$. The solution is most conveniently based on the so-called Eckart–Young decomposition of a real matrix [Eckart & Young, 1936].

Theorem 1. If X is a real $n \times k$ matrix of rank r ($n \geq k \geq r$), then matrices $P_r(n \times r)$, $D_r(r \times r)$ and $Q_r(k \times r)$ can be constructed which satisfy the equation

(1) $$X = P_r D_r Q_r', \quad \text{where}$$

(2) $$P_r'P_r = Q_r'Q_r = I_r,$$

and D_r is diagonal and positive definite.

Proof. Let Q_r contain any orthonormal set of eigenvectors corresponding to the non-zero eigenvalues of $X'X$. Then Q_r satisfies

(3) $$X'X = Q_r D_r^2 Q_r',$$

and

(4) $$Q_r'Q_r = I_r.$$

Obviously, D_r^2 is a diagonal matrix of positive eigenvalues of $X'X$. Let D_r be the diagonal matrix of positive square roots of these eigenvalues. Finally, let P_r be constructed as

(5) $$P_r = XQ_r D_r^{-1}.$$

Then $P_r'P_r = Q_r'Q_r = I_r$, D_r is diagonal and positive definite, and

(6) $$P_r D_r Q_r' = XQ_r Q_r'.$$

Schönemann, Bock and Tucker [Note 2, Lemma 1] proved that

(7) $$XQ_r Q_r' = X,$$

for any Q_r satisfying (3) and (4). This completes the proof of Theorem 1. The case of multiple zero or non-zero eigenvalues has been implicitly covered [see also Schönemann, Bock & Tucker, Note 2, pp. 11–12].

By adding orthonormal columns to P_r and Q_r and zeros to D_r, one can construct matrices $P(n \times k)$, $Q(k \times k)$ and $D(k \times k)$ satisfying

(8) $$X = P_r D_r Q_r' = PDQ',$$

with $P'P = Q'Q = QQ' = I_k$ and D diagonal and positive semidefinite. Equation (8) is known as the Eckart–Young decomposition of X.

A Necessary and Sufficient Condition for Maximum Agreement when $m = 2$

Theorem 2. The function $g(T_1) = \text{tr } T_1'A_1'A_2$, where T_1 varies without restriction over the set of orthonormal matrices of order $k \times k$, is maximized if and only if $T_1'A_1'A_2$ is symmetric and positive semi-definite (SPSD).

Proof. Let $T_1'A_1'A_2 = P_rD_rQ_r' = PDQ'$ be an Eckart–Young decomposition of $T_1'A_1'A_2$. Let it be given that, for any orthonormal $k \times k$ matrix N,

$$\text{tr } T_1'A_1'A_2 \geq \text{tr } N'A_1'A_2. \tag{9}$$

Suppose, contrary to what is to be proved, that $T_1'A_1'A_2$ is not *SPSD;* then $Q_r \neq P_r$ and

$$\text{tr } T_1'A_1'A_2 = \text{tr } P_rD_rQ_r' = \text{tr } Q_r'P_rD_r < \text{tr } D_r. \tag{10}$$

But taking $N = T_1PQ'$ would yield

$$\text{tr } N'A_1'A_2 = \text{tr } QP'PDQ' = \text{tr } D = \text{tr } D_r. \tag{11}$$

Clearly, (10) and (11) jointly contradict (9). Therefore, $T_1'A_1'A_2$ is *SPSD* if (9) holds.

Conversely, let $T_1'A_1'A_2$ be *SPSD*. Then

$$T_1'A_1'A_2 = PDQ' = PDP' \tag{12}$$

and

$$\text{tr } T_1'A_1'A_2 = \text{tr } PDP' = \text{tr } P'PD = \text{tr } D. \tag{13}$$

Again, if N is an arbitrary orthonormal matrix of order $k \times k$, then

$$\text{tr } N'A_1'A_2 = \text{tr } N'T_1T_1'A_1'A_2 = \text{tr } N'T_1PDP' = \text{tr } P'N'T_1PD \leq \text{tr } D, \tag{14}$$

since the product $P'N'T_1P$ is orthonormal and has no diagonal entries greater than one. This completes the proof of Theorem 2.

Theorem 2 is essentially due to Fischer and Roppert [1965]. Our proof, however, is shorter and does not require the aid of calculus. The theorem solves the Procrustes problem at once, when $m = 2$. Let $A_1'A_2 = PDQ'$ be an Eckart–Young decomposition of $A_1'A_2$. Then if we let $T_1 = PQ'$, we obtain $T_1'A_1'A_2 = QDQ'$. But QDQ' is *SPSD,* which is both necessary and sufficient for attaining the best least-squares fit.

The General Case of $m > 2$

We have been discussing the case of $m = 2$ in some detail. This offers a useful starting point for dealing with the general case of $m > 2$. For notational convenience we will write S_{ij} for $T_i'A_i'A_jT_j$, S_i for $T_i'A_i' \sum A_jT_j$, $S_{i.}$ for $T_i'A_i' \sum_{j \neq i} A_jT_j$ and g for $g(T_1, T_2, \cdots, T_m) = \sum_{i<j} \text{tr } S_{ij}$.

When more than two matrices are involved, g must be maximized. The following condition is *sufficient* for a maximum: *If each product S_{ij} is SPSD, then g is maximal.* The proof of this is fairly obvious. If each S_{ij} is SPSD, then

TABLE 1
Artificial Data for Which Not Every S_{ij} can be *SPSD*

A_1	A_2	A_3
I	$-I$	0
I	0	I
0	I	I

Note that $A_1'A_2 = -I$; $A_1'A_3 = I$; $A_2'A_3 = I$.

rotation could not increase the trace of any of the S_{ij} (Theorem 2) and therefore the sum of traces g must be maximal.

It may be noted that this sufficient condition cannot generally be satisfied. This follows from the example in Table 1, where I and O denote the identity matrix and zero matrix, respectively, both of order $k \times k$.

For the data of Table 1, S_{13} will be *SPSD* if and only if $T_1 = T_3$. Similarly, S_{23} will be *SPSD* if and only if $T_2 = T_3$. But the implication $T_1 = T_2$ will leave S_{12} negative definite. Therefore, for these data, no set of matrices T_1, T_2, T_3 can satisfy the sufficient condition for a maximum. Since g does assume a maximum value [Kristof & Wingersky, 1971, p. 89], the sufficient condition is not *necessary* for a maximum.

Kristof and Wingersky [1971] formulated a *necessary* condition for maximal agreement which is: *If g is maximal, then* $S_{i.}$ *is SPSD*, $i = 1, 2, \cdots m$.

Proof. The expression g can always be rewritten as

$$g = \text{tr } S_{i.} + \text{a sum independent of } T_i, \tag{15}$$

for any value of $i(i = 1, 2 \cdots m)$. Now suppose that, for some i, $S_{i.}$ is not *SPSD*. Then by Theorem 2, one can still increase tr $S_{i.}$ by changing T_i without affecting the terms independent of T_{i}. Therefore g cannot be maximal if $S_{i.}$ is not *SPSD* for $i = 1, 2 \cdots m$.□

It may be noted that Kristof and Wingersky [1971] proved an overly restrictive version of the necessary condition, requiring that each S_i be nonsingular. Since Theorem 2 deals with singular matrices as well, the necessary condition has been shown to hold regardless of singularity of the matrices S_i.

Above, a sufficient condition was shown to be not necessary; conversely, the necessary condition just stated can be shown to be not sufficient. One may consult the data of Table 2. It is clear that each $S_{i.}$ is *SPSD*. While it is apparent that the attained value of g is k, changing signs in A_2T_2 and A_3T_3 jointly would yield a value as high as $3k$. This would also be the maximum since upon reflecting A_2T_2 and A_3T_3 each S_{ij} would be *SPSD*. Obviously, the necessary condition for a maximum is *not sufficient* for $m > 2$.

Kristof and Wingersky [1971] weakened their necessary condition to the

TABLE 2
Artifical Data for Which the Necessary Condition is Satisfied, but Maximum Agreement has not been Attained

A_1T_1	A_2T_2	A_3T_3	A_4T_4
I	$-I$	0	0
I	0	0	I
0	I	I	0
$S_{1.}$	$S_{2.}$	$S_{3.}$	$S_{4.}$
0	0	I	I

following effect: If g is maximal, then S_i is *SPSD*, $i = 1, 2, \cdots m$. This *weak* necessary condition follows from the original *strong* necessary condition since $T_i'A_i'A_iT_i$ is *SPSD* and so is the sum of any two quadratic forms both of which are *SPSD*.

Satisfaction of the weak necessary condition does not imply satisfaction of the strong necessary condition. An example can be found in Table 2. After deleting the matrix A_4T_4, the remaining data will only satisfy the weaker condition.

Before examining procedures for the implementation of the necessary conditions, it may be instructive to summarize the necessary and sufficient conditions for a maximum when $m > 2$. The following four statements form a hierarchy, in which each statement implies all statements below it, but is not implied by the statements below it.

1. (Sufficient condition) S_{ij} is *SPSD* for $i, j = 1, 2, \cdots m$.
2. g is maximal.
3. (Strong necessary condition) $S_{i.}$ is *SPSD* for $i = 1, 2, \cdots m$.
4. (Weak necessary condition) S_i is *SPSD* for $i = 1, 2, \cdots m$.

Kristof and Wingersky [1971] succeeded in constructing an iterative algorithm that satisfies their weak necessary condition. Their procedure runs as follows.

Step 1. Take $A_m = B^{(1)}$. Rotate each A_i to maximal agreement with $B^{(1)}$, thus yielding $A_iT_i^{(1)}$, $i = 1, 2 \cdots m$.

Step 2. Compute $1/m \sum A_iT_i^{(1)} = B^{(2)}$. Rotate each $A_iT_i^{(1)}$ to $B^{(2)}$, thus yielding $A_iT_i^{(2)}$, $i = 1, 2, \cdots m$.

Step p. Compute $1/m \sum A_iT_i^{(p-1)} = B^{(p)}$. Rotate each $A_iT_i^{(p-1)}$ to $B^{(p)}$, thus yielding $A_iT_i^{(p)}$, $i = 1, 2 \cdots m$.

It can be shown that g will increase at each step after Step 1 until the procedure converges, which occurs if and only if the weak necessary condition has been satisfied (Theorem 2). Convergence can be shown to occur [Kristof & Wingersky, 1971, p. 90], and is rapid in practice.

Kristof and Wingersky iteratively rotate each matrix to the average, or equivalently, to the sum of the matrices. An obvious modification of their procedure, needed to satisfy the strong necessary condition, would be to rotate each matrix iteratively to the sum of all other matrices. This procedure, however, would clearly fail in the case of $m = 2$. If $A_1'A_2 = PDQ'$, then we would obtain $T_1 = PQ'$ and $T_2 = QP'$. After rotation we would have

$$g = \text{tr } T_1'A_1'A_2T_2 = \text{tr } QDP' = \text{tr } A_1'A_2; \tag{16}$$

that is, the function to be maximized would not have taken a higher value. Therefore, the following procedure is to be preferred.

Step 1. Rotate A_1 to $\sum_{j=2}^{m} A_j$, thus yielding $A_1T_1^{(1)}$.

Step 2. Rotate A_2 to $A_1T_1^{(1)} + \sum_{j=3}^{m} A_jT_j$, thus yielding $A_2T_2^{(1)}$.

Step m. Rotate A_m to $\sum_{j=1}^{m-1} A_jT_j^{(1)}$, thus yielding $A_mT_m^{(1)}$.

Step m + 1. Rotate $A_1T_1^{(1)}$ to $\sum_{j=2}^{m} A_jT_j^{(1)}$, thus yielding $A_1T_1^{(2)}$.

The procedure is terminated if m steps jointly fail to raise g above some threshold value. It can be readily seen that g increases at each step. The sum of terms that depend on the matrix being rotated increases, while the remaining terms are left unchanged. The procedure will converge if and only if the *strong* necessary condition has been satisfied (Theorem 2). Again, convergence can be shown to occur and is rapid in practice.

Haven [Note 1] compared our procedure to the Kristof and Wingersky method for 52 sets of matrices. Our procedure yielded equal or higher values of g, requiring on the average a smaller number of rotations. The differences were substantial for random matrices, and consistent although less impressive for empirical matrices.

Our procedure attains the maximum of g if $m = 2$. The same holds for the Kristof and Wingersky procedure, owing to the awkward first step. It does not hold for the Kristof and Wingersky logic: Rotating two matrices to their sum need not satisfy the necessary and sufficient condition for a maximum. One may compare the data of Table 2, after deleting A_3T_3 and A_4T_4. Either A_1T_1 or A_2T_2 needs to be reflected; nothing will happen if both matrices are rotated to $A_1T_1 + A_2T_2$.

Two Upper Bounds

Our procedure satisfies only a necessary condition for a maximum of g; it need not necessarily arrive at the maximum. The same holds true a fortiori for the Kristof and Wingersky procedure. Therefore, it may be wise to compute the following two upper bounds. Let

$$A_i'A_j = P_{ij}D_{ij}Q_{ij}', \tag{17}$$

be an Eckart–Young decomposition of $A_i'A_j$. Then tr D_{ij} is the maximum of $g(T_i, T_j) = \text{tr } S_{ij}$ (Theorem 2). Summing yields the first upper bound

$$g \leq \sum_{i<j} \text{tr } D_{ij}. \tag{18}$$

Let $\overline{A'A}$ denote the $km \times km$ supermatrix

$$\overline{A'A} = \begin{bmatrix} 0 & A_1'A_2 & \cdots & A_1'A_m \\ A_2'A_1 & 0 & \cdots & A_2'A_m \\ \vdots & \vdots & & \vdots \\ A_m'A_1 & A_m'A_2 & \cdots & 0 \end{bmatrix}. \tag{19}$$

Let

$$\overline{A'A} = P\Delta P' \qquad (PP' = I;\ \delta_i \geq \delta_j \text{ for } i < j), \tag{20}$$

be an eigenvector-eigenvalue decomposition of $\overline{A'A}$. We then obtain the second upper bound

$$g \leq \frac{m}{2} \sum_{i=1}^{k} \delta_i. \tag{21}$$

Proof. Let T be the column supervector containing the matrices T_1, T_2, $\cdots$, T_m, with $T_i'T_i = I_k$. We then have

$$g = \tfrac{1}{2} \text{ tr } T'\overline{A'A}T = \frac{m}{2} \text{ tr } U'P\Delta P'U \tag{22}$$

where $U = m^{-1/2}T$, with $U'U = I_k$. Substituting $V = P'U$, with $V'V = I_k$, yields

$$g = \frac{m}{2} \text{ tr } V'\Delta V = \frac{m}{2} \text{ tr } VV'\Delta \leq \frac{m}{2} \sum_{i=1}^{k} \delta_i, \tag{23}$$

since $VV_{ii}' \leq 1$ and tr $VV' = k$. This completes the proof of the second upper bound.

Neither upper bound can be shown to be superior. Therefore, in practical applications, one may compare the value of g obtained with that upper bound which is the lowest. When a small difference occurs, the value obtained must be close to or equal to the maximum. When a large difference occurs, the value obtained may be far below the maximum. In that case one might resort to a successive method of rotation, that is, a method which first yields column one of each T_i, then column two, etc. The author obtained excellent results for artificial data, using Kettenring's SUMCOR-rotation [Kettenring, 1971]. For real world data, values of g tend to be very close to the lowest upper bound, so no further precautions need to be taken. If a large difference should occur, however, one might profitably insert Kettenring's rotation as a start for a new set of rotations by our procedure.

Haven [Note 1] found the first upper bound to be the lower one in nearly all cases examined. In addition, he never observed a difference of more than four percent between this upper bound and the value of g attained by our procedure.

Gower's Generalized Procrustes Analysis

Gower [1975] derived a method of generalized Procrustes analysis which includes scaling constants and translations for two or more matrices. His method starts with an initial centering and scaling of the matrices, so that all column sums are zero and $\sum \text{tr } A_i'A_i = m$ [Gower, 1975, p. 43, Step 2]. From then on, rotation matrices (Gower's Steps 3 and 4) and scaling constants (Steps 6 and 7) are adjusted in turn. Gower has adopted the Kristof and Wingersky procedure for steps 3 and 4. This part of his method can be improved by inserting our procedure. Moreover, Gower's solution to the scaling problem (Step 6) is not correct. The correct solution will be outlined next, using our own notation.

Let A_i, $i = 1, 2, \ldots m$ be m matrices of order $n \times k$, with $\sum \text{tr } A_i'A_i = m$, for which scaling constants $c_1, c_2 \ldots c_m$ are desired to maximize

$$h(c_1, c_2, \cdots, c_m) = \sum_{i<j} c_i c_j \text{ tr } A_i'A_j, \tag{24}$$

under the constraint

$$\sum c_i^2 \text{ tr } A_i'A_i = \sum \text{tr } A_i'A_i = m. \tag{25}$$

This constraint safeguards the equivalence of maximizing (24) and minimizing the least-squares function $\sum_{i<j} \text{tr } (c_iA_i - c_jA_j)'(c_iA_i - c_jA_j)$. Let the $m \times m$ matrix Y be defined as

$$Y = \begin{bmatrix} \text{tr } A_1'A_1 & \text{tr } A_1'A_2 & \cdots & \text{tr } A_1'A_m \\ \text{tr } A_2'A_1 & \text{tr } A_2'A_2 & \cdots & \text{tr } A_2'A_m \\ \vdots & \vdots & & \vdots \\ \text{tr } A_m'A_1 & \text{tr } A_m'A_2 & \cdots & \text{tr } A_m'A_m \end{bmatrix}; \tag{26}$$

$Y_d = \text{Diag }[Y]$. Let $\Phi = Y_d^{-1/2} Y \, Y_d^{-1/2}$, the matrix of coefficients of congruence [Tucker, Note 3] between matrices $A_1, A_2, \cdots, A_m$ after arranging their elements in a $nk \times 1$ vector.

Let

$$\Phi = P\Delta P' \; (PP' = I; \; \delta_i \geq \delta_j \text{ for } i < j), \tag{27}$$

be an eigenvector-eigenvalue decomposition of Φ, and p_1 be the first column of P. Then (24) is maximized subject to (25) by taking

$$c_i = \left(\frac{m}{\text{tr } A_i'A_i}\right)^{1/2} p_{i1}. \tag{28}$$

Proof. Without loss of generality each matrix A_i can be rescaled to

$$A_i^* = (\text{tr } A_i'A_i)^{-1/2}A_i, \text{ with tr } A_i^{*\prime}A_i^* = 1 \text{ for } i = 1, 2, \cdots, m. \tag{29}$$

Then scalars d_i are needed to maximize

$$h^*(d_1, d_2, \cdots, d_m) = \sum_{i<j} d_i d_j \text{ tr } A_i^{*\prime}A_j^*, \tag{30}$$

under the constraint

$$\sum d_i^2 \text{ tr } A_i^{*\prime}A_i^* = \sum d_i^2 = \sum \text{tr } A_i'A_i = m. \tag{31}$$

Let the d_i be arranged in a vector d. Then (30) can be written as

$$h_*(d) = \tfrac{1}{2}d'(\Phi - I)d, \tag{32}$$

which is to be maximized subject to (31), that is, subject to

$$d'd = m. \tag{33}$$

Combining (27), (32) and (33), and substituting $u = P'd$ yields

$$\begin{aligned} h^*(d) &= \tfrac{1}{2}d'(\Phi - I)d = \tfrac{1}{2}d'(P\Delta P' - I)d \\ &= \tfrac{1}{2}(u'\Delta u - m) \leq \tfrac{1}{2}(\delta_1 u'u - m) = \tfrac{1}{2}m(\delta_1 - 1). \end{aligned} \tag{34}$$

Taking $d = m^{1/2}p_1$, which clearly satisfies (33), yields

$$\begin{aligned} h^*(m^{1/2}P_1) &= \tfrac{1}{2}mp_1'(\Phi - I)p_1 = \tfrac{1}{2}mp_1'(P\Delta P' - I)p_1 \\ &= \tfrac{1}{2}m(e_1'\Delta e_1 - p_1'p_1) = \tfrac{1}{2}m(\delta_1 - 1). \end{aligned} \tag{35}$$

Therefore, (32) is maximized subject to (33) when $d = m^{1/2}p_1$. This result and the prior rescaling (29) completes the proof of (28). It can be used to improve Step 6 of Gower's computation scheme [Gower, 1975, p. 43]. Gower [1975, p. 39, Equation 13] derived an equation in scalar notation which, if put in matrix notation, shows that the optimal scaling constants are elements of the principal right-hand eigenvector of $Y^{-1}{}_dY$. This is equivalent to our result (28). However, Gower applies an iterative algorithm (Step 6) with unknown convergence properties to solve his Equation 13. It would be safer to compute the scaling constants by our result (28) which is guaranteed to yield the correct solution.

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