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#### ABSTRACT

An algorithm is presented for the best least-squares fitting correlation matrix approximating a given missing value or improper correlation matrix. The proposed algorithm is based on a solution for C. I. Mosier's oblique Procrustes rotation problem offered by J. M. F. ten Berge and K. Nevels (1977). It is shown that the minimization problem belongs to a certain class of convex programs in optimization theory. A necessary and sufficient condition for a solution to yield the unique global minimum of the least-squares function is derived from a theorem by A. Shapiro (1985). A computer program was implemented to yield the solution of the minim zation problem with the proposed algorithm. This empirical verification of the condition indicates that the occurrence of non-optimal solutions with the proposed algorithm is very unlikely. Two tables present values using J. de Leeuw's target matrix. (Author/SLD)

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## Least-squares Approximation of an Improper by a Proper Correlation Matrix Using a Semi-infinite Convex Program

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Research Report

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Jos M.F. ten Berge



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#### Abstract

An algorithm is presented for the best least-squares fitting correlation matrix approximating a given missing value or improper correlation matrix. The proposed algorithm is based upon a solution for Mosier's oblique Procrustes rotation problem offered by Ten Berge and Nevels. It is shown that the minimization problem belongs to a certain class of convex programs in optimization theory. A necessary and sufficient condition for a solution to yield the unique global minimum of the least-squares function is derived from a theorem by Shapiro. Empirical verification of the condition indicates that the occurrence of non-optimal solutions with the proposed algorithm is very unlikely.

Key words: missing value correlation, tetrachoric correlation, indefinite correlation matrix, constrained least-squares approximation, semi-infinite program, convex program.



Least-squares Approximation of an Improper by a Proper Correlation Matrix Using a Semi-infinite Program

When product-moment correlations of a set of n variables are computed by any of the missing value correlation methods described by Frane (1978), it may happen that the resulting missing value correlation Eatrix is indefinite, and hence improper. This can be a serious problem in various multivariate data analysis techniques, e.g., in regression and factor analysis.

One possible approach to this problem consists of avoiding an (indefinite) improper correlation matrix entirely by estimating the missing data themselves. Missing data can be estimated by maximum likelihood estimation from incomplete data (Beale & Little, 1975; Dempster, Laird & Rubin, 1977; Orchard & Woodbury, 1972) and by pragmatic procedures (Frane, 1976, 1978; Gleason & Staelin, 1975; Timm, 1970).

Another possible approach to the problem is to render the improper correlation matrix non-negative definite by some smoothing procedure (Devlin, Gnanadesikan & Kettenring, 1975, p. 543; Dong, 1985; Frane, 1978).

The purpose of the present paper is to offer a least-squares smoothing procedure. That is, one may seek the best fitting (in the sense of least-squares) symmetric, unitdiagonal, non-negative definite matrix G to the given improper missing value correlation matrix R. Specifically, the function



#### (1) $e(G) = \frac{1}{2} tr (G - R)^2$

can be minimized subject to the constraints G = G', Diag (G) = I<sub>n</sub> and  $G \ge 0$ . For convenience we write  $Y \ge 0$  and Y > 0 to denote that a symmetric matrix Y is non-negative definite and positive definite, respectively.

The minimization problem (1) can be generalized in three ways. Firstly, the problem can be applied to any improper correlation matrix, e.g., an indefinite tetrachoric correlation matrix or a correlation matrix obtained by elementwise robust estimation (Devlin, Gnanadesikan & Kettenring, 1975, 1931, Gnanadesikan & Kettenring, 1972). Secondly, the problem can be generalized to handle indefinite matrices with fixed diagonal elements not necessary equal to one. For example, the scope of the problem can be extended to missing value covariance matrices with known variances or to productmoment correlation matrices with known communalities. Thirdly, it is possible to exclude those product-moment correlations or covariances which are computed between complete variables (no missing values) from the minimization procedure. That is, the excluded elements of R can be held constant in (1). Without loss of generality these elements can be collected in the  $n_1 \ge n_1$  ( $0 \le n_1 < n$ ) submatrix  $R_{11} \ge 0$  of R, where R is partitioned as



$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} \\ \hline \mathbf{R}_{21} & \mathbf{R}_{22} \end{bmatrix}$$

In order to incorporate these three generalizations, we shall address the generalized problem of minimizing (1) subject to the constraints

(2a) G = G',

(2b) G≥0,

(2c)  $G_{11} = R_{11} \ge 0$ 

and

(2d) Diag  $(G_{22}) = Diag (R_{22}) \ge 0$ ,

where G is partitioned as

$$G = \begin{bmatrix} G_{11} & G_{12} \\ \hline & \\ G_{21} & G_{22} \end{bmatrix}$$



LS Approximation

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and  $G_{11}$  is of order  $n_1 \ge n_1$ . Note that the constraints (2c) and (2d) for the problems with  $n_1 = 0$  and  $n_1 = 1$  are equivalent. In the next section a computational solution will be offered for the generalized problem of minimizing (1) subject to the constraints (2).

#### An algorithm

The constraints G = G' (2a) and  $G \ge C$  (2b) can equivalently be expressed by the constraint

(3) G = AA'

for some n x m ( $n_1 \le m \le n$ ) matrix A. Consider the partitioning

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

where  $A_1$  is of order  $n_1 \ge m$ ,  $A_{11}$  is of order  $n_1 \ge n_1$ , and  $A_1$  is fixed in advance as

(4) 
$$A_1 = [R_{11}^{\aleph} | 0]$$
.



This choice of  $A_1$  satisfies the constraint  $G_{11} = R_{11}$  (2c) and can be adopted without loss of generality, because every matrix A satisfying (3) is determined up to an orthogonal rotation.

Upon substitution of (3) and (4) for G in (1), the problem of minimizing (1) subject to the constraints (2) can be reduced to the problem of minimizing the function

(5) 
$$f(A_2) = W \operatorname{tr} (A_2A_2 - R_{22})^2$$
  
+ tr  $(A_1A_2 - R_{12})'(A_1A_2 - R_{12})$ 

subject to the constraint Diag  $(A_2A_2) = Diag(R_{22})$ .

In order to simplify the notation, let for any positive integer  $\ell$  the index set  $\mathbb{N}_{\ell}^2$  be defined by the Cartesian product

$$\mathbb{N}^2_{\mu} = \{1, \ldots, \ell\} \times \{1, \ldots, \ell\}$$

and let  $\tau$  be the symmetric subset of  $\mathbb{N}_n^2$  defined by

$$τ = {(i,j): i ≠ j & (i,j) ∈  $\mathbb{N}_n^2 - \mathbb{N}_{n_1}^2$  }.$$

Then the minimization problem (5) can be written as minimizing

(6) 
$$f(\mathbf{A}) = \frac{1}{2} \sum_{\substack{(i_+,j) \in T \\ i_+ j \in T}} (a'a - r)^2$$

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subject to the constraints  $a_k'a_k = r_{kk}$   $(k = n_1+1, ..., n)$ , where  $R = [r_{ij}]$  and  $a_i'$  is row i (i = 1, ..., n) of A. For each k  $(k = n_1+1, ..., n)$ , (6) can be written as

(7) 
$$f(\underline{A}_{2}) = \underbrace{\mathbb{M}}_{(i,k)\in T} \underbrace{\sum_{i=k}^{\infty} (a_{i}^{*}a_{i} - r_{i})^{2}}_{i,k} \\ + \underbrace{\mathbb{M}}_{(k,j)\in T} \underbrace{\sum_{k=j}^{\infty} (a_{k}^{*}a_{j} - r_{j})^{2}}_{i,j\neq k} \\ + \underbrace{\mathbb{M}}_{(i,j)\in T} \underbrace{\sum_{i=j}^{\infty} (a_{i}^{*}a_{j} - r_{j})^{2}}_{i,j\neq k} \\ = \underbrace{\sum_{i=k}^{\infty} (a_{i}^{*}a_{k} - r_{i}^{*})^{2} + L_{k}}_{i=k} \\ = \underbrace{\sum_{i\neq k}^{\infty} (a_{i}^{*}a_{k} - r_{i}^{*})^{2} + L_{k}}_{k} \\ = (A_{k}^{(0)}a_{k} - r_{k}^{(0)})'(A_{k}^{(0)}a_{k} - r_{k}^{(0)}) + L_{k}$$

where  $L_k$  is a constant with respect to  $a_k$ ,  $A_k^{(0)}$  is the matrix A with row k replaced by zeroes, and  $r_k^{(0)}$  is column k of [R - Diag(R)].

In the context of Mosier's (1939) oblique Procrustes problem, Ten Berge and Nevels (1977) have given a solution



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for the global minimum of  $f_k(a_k)$  subject to the constraint  $\mathbf{a_k}'\mathbf{a_k} = 1$ . With some minor adjustments, their solution can be generalized to minimize  $f_k(a_k)$  subject to any arbitrary constraint  $a_k a_k = r_{kk} \ge 0$ . After taking a suitable initial choice for  $A_2$ , and row-wise minimization of '7) for  $k = n_1 + 1, \dots, n$  with the adjusted Ten Berge and Nevels solution, an algorithm for solving (5) is obtained. For each k  $(k = n_1+1, ..., n)$ ,  $f(A_2)$  decreases with the row-wise minimization, alfecting only elements of row k and column k of AA'. The  $n_2 = n - n_1$  minimization steps can be repeated until no significant decrease of  $f(\lambda_2)$  between two succeeding iteration cycles occurs. Because f(Ar decreases monotonically and  $f(\lambda_2)$  is bounded below, convergence of the algorithm is guaranteed. In the next section we shall describe a necessary and sufficient condition for a global minimum of  $f(\lambda_2)$ .

## A necessary and sufficient condition for a global minimum

After minimizing  $f_k(a_k)$  with the adjusted Ten Berge and Nevels algorithm, there exists a Lagrange multiplier  $\theta_k$  such that

(8) 
$$A_{k}^{(0)}, A_{k}^{(0)} = \theta_{k} = A_{k}^{(0)}, r_{k}^{(0)}$$



(Mulaik, 1972, p. 505). The Lagrange multiplier  $\theta_k$  can be evaluated directly from the equations (11), (12) and (13) in Ten Berge and Nevels (1977, p. 595) for their cases 1, 2 and 3 respectively. Rewriting (8) yields

$$(\mathbf{A}_{\mathbf{k}}^{(0)},\mathbf{A}_{\mathbf{k}}^{(0)} + \mathbf{a}_{\mathbf{k}}\mathbf{a}_{\mathbf{k}}^{*})\mathbf{a}_{\mathbf{k}} - (\mathbf{A}_{\mathbf{k}}^{(0)},\mathbf{r}_{\mathbf{k}}^{(0)} + \mathbf{a}_{\mathbf{k}}\mathbf{r}_{\mathbf{k}\mathbf{k}}) - \mathbf{\theta}_{\mathbf{k}}\mathbf{a}_{\mathbf{k}} = 0$$

and hence

(9) 
$$\mathbf{A}'\mathbf{A}\mathbf{a}_{\mathbf{k}} - \mathbf{A}'\mathbf{r}_{\mathbf{k}} - \mathbf{\theta}_{\mathbf{k}}\mathbf{a}_{\mathbf{k}} = 0$$

where  $r_k$  is column k of R. It should be noted that during the iteration process, (9) holds for the index k only immediately after the minimization of row  $k - n_1$  of A<sub>2</sub>. However, after convergence of the proposed algorithm, (9) holds simultaneously for all k ( $k = n_1+1,...,n$ ). Denote for convenience a solution of the proposed algoritm by A. Then the  $n_2$  equations (9) can be collected in the matrix equation

(10) 
$$A'AA_2' - A'R_2' - A_2'\Theta_{22} = 0$$

where  $\mathbb{P}_2 = [\mathbb{R}_{21} | \mathbb{R}_{22}]$  and  $\Theta_{22} = \text{Diag}(\theta_{n_1+1}, \dots, \theta_n)$ . Transposing (10) and rewriting yields the first-order necessary conditions for a minimum of (5)

(11a) 
$$(\mathbb{A}_2\mathbb{A}_1^{\prime} - \mathbb{R}_{21})\mathbb{A}_{11} + (\mathbb{A}_2\mathbb{A}_2^{\prime} - \mathbb{R}_{22} - \Theta_{22})\mathbb{A}_{21} = 0$$



and

(11b)  $(\mathbf{A}_2\mathbf{A}_2' - \mathbf{R}_{22} - \mathbf{\Theta}_{22})\mathbf{A}_{22} = 0$ .

It should be noted that the first-order necessary conditions (11) for a minimum of (5) have been obtained from standard partial differentiation of a constrained function (cf. Luenberger, 1984, chap. 10). Additional results can be obtained from a reformulation of the problem in terms of a semi-infinite convex program (Shapiro, 1985). This will be pursued next.

Let  $\Omega(\tau)$  denote the set of symmetric n x n matrices X = [x<sub>ij</sub>] such that  $x_{ij} = 0$  whenever (i,j)  $\notin \tau$ . Then the matrix G can be written as

$$(12) \quad G = C + \mathbf{X}$$

where  $X \in \Omega(\tau)$  and  $C = [c_{ij}]$  such -it  $c_{ij} = 0$  whenever (i,j)  $\in \tau$  and  $c_{ij} = r_{ij}$  otherwise. In (12) G is decomposed as the sum of a matrix C containing the  $(n_1)^2 + n_2$  known (fixed) elements of G, and a matrix X containing the unknown (free) elements of G. Inserting (12) in (1) leads to the restatement of the minimization problem

(13) 
$$g(X) = e(G) = X \operatorname{tr} (C + X - R)^2$$

subject to the constraints  $X \in \Omega(\tau)$  and  $(C + X) \ge 0$ .



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Replacing the constraint  $(C + \mathbf{X}) \geq 0$  by the equivalent constraint

(14)  $h(X,u) = u'(C + X)u \ge 0$ 

for all  $u \in \Psi = \{u \in \mathbb{R}^n : u'u = 1\}$  makes problem (13) a semi-infinite program.

Assuming that we have  $R_{11} > 0$  it can be verified that the semi-infinite program defined by (13) and (14) has the following nine properties:

- (P1)  $\Omega(\tau)$  is convex.
- (P2) g(X) is convex.

(P3) h(.,u) is concave for all  $u \in \Psi$ .

- (P4) The Slater (1950) condition (cf. Stoer & Witzgall, 1970, p. 247) holds, i.e. there exists a matrix  $X \in \Omega(\tau)$ , wiz.,  $X_0 = 0$ , such that  $h(X_0, u) > 0$  for all  $u \in \Psi$ .
- (P5)  $\Psi$  is compact.
- (P6) g(X) is continuously differentiable.
- (P7) h(.,u) is continuously differentiable for all  $u \in \Psi$ .
- (P8) h(X,u) is continuous.
- (P9) grady h(X,u) is continuous.

Properties (P1) through (P3) make the program a convex program and properties (P4) through (P9) are regularity conditions.

For semi-infinite programs satisfying the conditions (P1) through (P9), Theorem 2.2 of Shapiro (1985) is applicable, which states: A feasible  $\mathbf{X}^* \in \Omega(\tau)$ , i.e.  $(C + \mathbf{X}^*)$  $\geq 0$ , is a solution of the minimization problem if and only if there exists an n x n matrix B =  $[b_{1,1}]$  satisfying

(i) B = B',

(ii)  $(C + X^*)B = 0$ ,

(iii) grad  $g(X)|_{X=X^*} = P_T(B)$ ,

where  $P_{\tau}(B)$  is the projection of B onto the space  $\Omega(\tau)$  defined by

 $[P_{\tau}(B)]_{ij} = \begin{cases} b_{ij} & \text{whenever } (i,j) \in \tau \\ 0 & \text{otherwise } . \end{cases}$ 

(iv)  $B \ge 0$ .

In order to assess whether these neces ary and sufficient conditions are satisfied after convergence of the proposed algorithm, we shall use the following lemma.

Lemma 1. For the matrix

(15)  $B = W'B_{22}W$ ,

where  $W = [-A_{21}A_{11}|I_{n_2}]$  and  $B_{22} = (A_2A_2 - R_{22} - \Theta_{22})$ , the conditions (i) through (iii) are satisfied, and condition (iv) is equivalent to the condition  $B_{22} \ge 0$ .

<u>Proof</u>. Condition (i) is obviously satisfied. To prove condition (ii), note that

(16)  $B_{22}WA = [0 | B_{22}A_{22}]$ .

**Rewriting (11b) as B\_{22}A\_{22} = 0 and transposing (16) yields** 

$$A'W'B_{22} = 0$$

and hence

(17)  $AA'W'B_{22}W = 0$ .

Substituting (C +  $X^*$ ) = AA' and (15) in (17) proves condition (ii).

To prove condition (iii), the matrix B is written out as

$$B = \begin{bmatrix} \frac{(B_{22}A_{21}A_{11}^{-1}) \cdot A_{21}A_{11}^{-1}}{-(B_{22}A_{21}A_{11}^{-1}) \cdot A_{21}A_{11}^{-1}} \\ -B_{22}A_{21}A_{11}^{-1} \\ B_{22} \end{bmatrix}$$



From (11a) it follows

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(19) 
$$B_{22}A_{21}A_{11}^{-1} = -(A_2A_1 - R_{21})$$
.

Inserting (19) in (18) yields

$$B = \begin{bmatrix} -(A_1A_2 - R_{12})A_{21}A_{11}^{-1} & A_1A_2 - R_{12} \\ \hline \\ A_2A_1 - R_{21} & A_2A_2 - R_{22} - \Theta_{22} \end{bmatrix}$$

which can be written as

 $(20) \qquad B = AA' - R - \Theta$ 

 $= C + X^* - R - \Theta ,$ 

where

$$\Theta = \begin{bmatrix} \frac{(A_1A_2 - R_{12})A_{21}A_{11}^{-1}}{0} \\ 0 \\ \theta_{22} \end{bmatrix}$$

From (20) it is easily shown that  $P_T(B) = (C + X^* - R)$ , which equals grad  $g(X)|_{X=X}^*$ . This proves condition (iii).



Regarding condition (iv), it is obvious from (15) that the condition  $B \ge 0$  is equivalent to the condition  $B_{22} \ge 0$ .

From our Lemma 1 and Shapiro's Theorem 2.2 it is obvious that  $B_{22} \ge 0$  is a necessary and sufficient condition for a feasible  $\mathbf{X}^{*} \in \Omega(\tau)$  to be a solution of the minimization problem (13). It should be noted that, after convergence of the proposed algorithm,  $\Theta_{22}$  can be evaluated hence the condition  $B_{22} \ge 0$  can be verified. Moreover, when  $B_{22} \ge 0$ , it follows immediately from the strict convexity of  $g(\mathbf{X})$  that  $\mathbf{X}^{*}$ is the unique solution of the minimization problem (13), which means that if and only if  $B_{22} \ge 0$  the unique global minimum of  $\mathbf{e}(\mathbf{G})$  subject to the constraints (2) has been attained for  $\mathbf{G}^{*} = (\mathbf{C} + \mathbf{X}^{*})$ .

In the derivation of the necessary and sufficient condition for a solution to yield the unique global minimum of e(G), it has to be assumed that  $R_{11} > 0$ . In the case of singular  $R_{11}$  the Slater condition (P4) does not hold and  $A_{11}^{-1}$  does not exist, hence it cannot be verified whether the obtained solution yields the unique global minimum of e(G). However, for singular  $R_{11}$ . Alexander Shapiro (personal communication, August 11, 1986) has shown that the problem of minimizing (1) subject to the constraints (2) can be transformed to a problem of (lower) dimensionality [rank  $(R_{11}) + n_2$ ], with a (transformed) fixed submatrix  $R_{11}^{*} > 0$ . For reasons of availability, we give the proof which is due to Shapiro.

Firstly, the function e(G) can be written as



(21) 
$$e(G) = % \operatorname{tr} [P(G - R)P']^2 = % \operatorname{tr} (PGP' - PRP')^2$$

for any orthogonal matrix P of order  $n \ge n$ . Secondly, let us take P in the form

$$P = \begin{bmatrix} P_{11} & 0 \\ \hline 0 & I_{n_2} \end{bmatrix}$$

such that

(22) 
$$P_{11}R_{11}P_{11} = \begin{bmatrix} 0 & 0 \\ 0 & R_{11} \end{bmatrix}$$

with  $R_{11}^* > 0$ . Then the constraints (2) become

$$(23a) PGP' = PG'P'$$



## (23c) $P_{11}G_{11}P_{11} = P_{11}R_{11}P_{11} \ge 0$

and

#### (23d) Diag $(G_{22}) = Diag (R_{22}) \ge 0$ .

From (22) and (23c) it follows that the first  $[n_1 - rank (R_{11})]$  diagonal elements of PGP' are zero. From this and (23b) it follows that the first  $[n_1 - rank (R_{11})]$  rows and columns of PGP' are zeroes. Hence the problem of minimizing (21) subject to the constraints (23) is reduced to a problem of dimensionality  $[rank (R_{11}) + n_2] < n$ .

In order to verify the necessary and sufficient condition  $B_{22} \ge 0$  for a solution  $G^* = AA'$  to yield the unique global minimum of e(G) subject to the constraints (2), a computer program has been implemented yielding the solution of the minimization problem with the proposed algorithm and evaluating the smallest eigenvalue of  $B_{22}$ . The computer program was run on 100 symmetric unit-diagonal indefinite matrices, where n ranged from 5 to 25,  $n_1$  ranged from 0 to min (10, n - 2) and the column order m of A was set equal to n. With changes in each (free) element of G between two succeeding iteration cycles less than  $10^{-4}$  as convergence criterion, the algorithm never took more than 10 iteration cycles until convergence. Computation time never exceeded 1 minute CPU time on a VAX8650 computer. In all cases, the obtained solution satisfied the condition  $B_{22} \ge 0$  within



accuracy limits. From these results, it can be concluded that the proposed algorithm tends to produce the unique globally optimal solution.

In the following lemma, another important property of the solution is stated.

Lemma 2. The rank of  $G^*$  equals n if and only if R > 0.

<u>Proof</u>. Suppose first that R > 0. Then,  $G^* = R > 0$ , and hence the rank of  $G^*$  equals n.

Conversely, let the rank of  $G^* = (C + X^*)$  equal n. From condition (ii) it follows that B = 0, and from condition (iii) that grad  $g(X)|_{X=X^*} = 0$ . From this it follows that  $P_T(B) = (C + X^* - R) = (G^* - R) = 0$  and hence  $G^* = R > 0$ .

In practice it seems to be true that the rank of  $G^*$  is always less than or equal to the number p of positive eigenvalues of R. Since computation time heavily depends upon the column order m of A, it is advised to take m = p. A further reduction of computation time can be accomplished by setting a suitable initial value for A. A reasonable initial value  $A^{(0)}$  can be based upon an eigen-decomposition of R

#### $\mathbf{R} = \mathbf{K} \Delta \mathbf{K}'$

where K is an orthogonal matrix of order n x n containing as columns the normalized eigenvectors of R and  $\Delta$  is a diagonal matrix containing the n eigenvalues of R. Let  $\Delta_p$  be the

diagonal matrix of order p with diagonal elements the p positive eigenvalues of R, and let  $\mathbf{E}_p$  be the matrix of order n x p with columns the p corresponding (normalized) eigenvectors. In the case  $n_1 = 0$ , it is advised to take as initial value for A

(24) 
$$\lambda^{(o)} = [\text{Diag } (R)]^{\frac{1}{2}} [\text{Diag } (\mathbf{K}_{p} \Delta_{p} \mathbf{K}_{p})]^{-\frac{1}{2}} \mathbf{K}_{p} \Delta_{p}^{\frac{1}{2}} T$$

where T is an arbitrary orthogonal matrix of order  $p \ge p$ . In the case  $n_1 > 0$  one can take T such that the upper  $p \ge p$ submatrix of  $A^{(0)}$  is in lower triangular form and replace the submatrix  $A_1^{(0)}$  by (4). For the 100 least-squares problems used above, total computation time could be reduced by more than 50% using (24) as initial value, and the condition  $B_{22}$ was again satisfied in all cases after convergence of the algorithm.

#### A numerical example

As an illustration and for reasons of possible checks. an indefinite 6 x 6 matrix R of polychoric correlations (smallest eigenvalue -.0626) published by De Leeuw (1983, p. 121) has been analyzed with various values of  $n_1$  ( $R_{11} > 0$  for  $n_1 \le 4$ ). In order to have  $R_{11} > 0$  for  $n_1 = 5$  too, the fifth and sixth variable have been interchanged. The matrix R is given in Table 1.



Insert Table 1 about here

Table 2 gives the residual matrices  $(G^* - R)$  for various values of  $n_1$ , together with the values of  $e(G^*)$ . Because the constraints (2) for the problems with  $n_1 = 0$  and  $n_1 = 1$  are equivalent, the solutions are equal. In all cases, the solution satisfies the condition  $B_{22} \ge 0$  within accuracy limits.

Insert Table 2 about here

It can be verified that the value of  $e(G^*)$  increases as  $n_1$  increases, as is to be expected.

#### Discussion

A monotone convergent algorithm has been constructed for the best least-squares non-negative definite approximation of an improper correlation or covariance matrix, preserving the diagonal elements. Additionally a verifiable necessary and sufficient condition for a solution to yield the unique global minimum of the least-quares function has been derived.



Moreover, this condition tends to be satisfied in practice. Thus a possibly useful alternative to existing smoothing procedures has been found.

However, the solution  $G^*$  is singular except in the trivial case R > 0 (cf. Lemma 2) hence the inverse of  $G^*$  does not exist. When inversion of  $G^*$  is required for a particular subsequent multivariate analysis, one may impose the additional constraint to (2) that all eigenvalues of G are greater than or equal to an arbitrary positive constant  $\delta$ . An algorithm for the latter optimization problem is in progress, but is beyond the scope of the present paper.



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## TABLE 1

De Leeuw's target matrix R of polychoric correlations with the fifth and sixth variable interchanged

	R							
var	1	2	3	4	5	6		
1	1.0000							
2	. 4770	1.0000						
3	.6440	.5160	1.0000					
4	. 4780	.2330	. 5990	1.0000				
5	.6510	.6820	.5810	.7410	1.0000			
6	. 8260	.7500	.7420	. 8000	.7980	1.0000		



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### TABLE 2

The values of  $e(G^*)$  and the lower-triangular parts of the residual matrices  $(G^* - R)$  using De Leeuw's target matrix. for various values of  $n_1$  (structural zeroes omitted)

	€(G <sup>*</sup> )	Var	(G <sup>+</sup> - R)				
n <sub>1</sub>			1	2	3	4	5
0.1	.002760	2	.0108				
		3	0011	0015			
		4	.0125	.0173	0017		
		5	0063	0088	.0009	0101	
		6	0178	0248	.0025	0286	.0144
2	.002884	3	0012	0016			
		4	.0131	.0180	0019		
		5	0067	0092	.0009	0105	
		6	0189	0259	.0027	0296	.0151
3	.002888	4	.0132	.0181	0020		
		5	0067	0092	.0010	0105	
		6	0189	0259	.0028	0296	.0151
4	.003515	5	0083	0116	.0016	0133	
		6	0225	0312	.0043	0359	.0185
5	.004062	6	0243	0349	.0057	0403	. 0245

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