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OBTAINING SQUARED MULTIPLE CORRELATIONS FROM A CORRELATION MATRIX WHICH MAY BE SINGULAR*

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A theorem is presented relating the squared multiple correlation of each measure in a battery with the other measures to the unique generalized inverse of the correlation matrix. This theorem is independent of the rank of the correlation matrix and may be utilized for singular correlation matrices. A coefficient is presented which indicates whether the squared multiple correlation is unity or not. Note that not all measures necessarily have unit squared multiple correlations with the other measures when the correlation matrix is singular. Some suggestions for computations are given for simultaneous determination of squared multiple correlations for all measures.

For over thirty years the squared multiple correlation of a measure with the other measures in a battery has been known to be the lower bound of the communality of that measure [Roff, 1936; Guttman, 1940]. For a number of years the squared multiple correlation of each measure with the other measures has been used as an estimate of the measure's communality. When the matrix of intercorrelations, R, among the measures is non-singular, these squared multiple correlations are easy to compute from the inverse of the correlation matrix. Let c_k^2 be the squared multiple correlation of the k'th measure with the other measures in the battery and r^{kk} be the k'th diagonal entry in R^{-1}, then

$$c_k^2 = 1 - \frac{1}{r^{kk}}. \tag{1}$$

This procedure is not possible, of course, when R is singular. An alternative procedure, but little used due to amount of time required for the solutions,

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has been to make a separate solution of the regression system for each measure in turn as predicted from the remaining measures. In each such solution a step-wise procedure might be used which discarded measures from the predictor set which were dependent on measures already employed. This report concerns a theorem which provides a basis for simultaneous computation of the squared multiple correlations for all measures in a battery even when the correlation matrix is singular.

Let R be the $n \times n$ correlation matrix for n measures and be of rank r greater than zero and equal to or less than n. Let k be any one of the measures and j represent all other measures. Also, let R_{jj} be the matrix of intercorrelations of the measures j, R_{jk} be a column vector of correlations of measures j with measure k, R_{kj} be the transpose of R_{jk} . When k is the n'th measure matrix R may be represented as:

$$R = \begin{bmatrix} R_{jj} & R_{jk} \\ R_{kj} & 1 \end{bmatrix}.$$

In general, R_{jj} may be obtained by deleting the k'th row and column of R; R_{jk} may be obtained from the k'th column of R by deleting the k'th element. Normal equations for prediction of the k'th measure from the j measures may be written as

$$R_{jj}\tilde{B}_k = R_{jk} \tag{2}$$

where $\tilde{B}_k$ is a column vector containing the regression weights. When R_{jj} is singular, the normal equations are consistent and solutions for (2) exist; however, $\tilde{B}_k$ is not uniquely determined. The squared multiple correlation, c_k^2 , is given by

$$R_{kj}\tilde{B}_k = c_k^2 \tag{3}$$

and is unique even when R_{jj} is singular. Every solution for $\tilde{B}_k$ yields the same value of c_k^2 . Consider k to be the n'th measure. A permissible construction is given in (4).

$$\begin{bmatrix} R_{jj} & R_{jk} \\ R_{kj} & 1 \end{bmatrix} \begin{bmatrix} \tilde{B}_k \\ 0 \end{bmatrix} = \begin{bmatrix} R_{jk} \\ c_k^2 \end{bmatrix} = \begin{bmatrix} R_{jk} \\ 1 \end{bmatrix} - \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \begin{bmatrix} 0 \\ c_k^2 \end{bmatrix}. \tag{4}$$

The construction of (4) to any measure k by letting B be an $n \times n$ matrix with zero diagonal entries,

$$b_{kk} = 0, \tag{5}$$

and with the $\tilde{B}_k$ in the remaining cells of the k'th column. Let C^2 be a diagonal matrix containing the squared multiple correlations c_k^2 . Equation (4) is generalized to any measure k by (6).

$$RB_k = R_k - I_k + C_k^2 \tag{6}$$

where B_k , R_k , I_k and C_k^2 are the k'th columns of the indicated matrices.

Before stating the basic theorem of this report two constructions must be defined. Let the matrix R (with unities in the diagonal cells) be factored to an $n \times r$ matrix F of full column rank so that:

$$R = FF' \tag{7}$$

and

$$|F'F| \neq 0. \tag{8}$$

Let matrices P and Q be defined as in (9) and (10).

$$P = F(F'F)^{-2}F'; \tag{9}$$

$$Q = RP = F(F'F)^{-1}F'. \tag{10}$$

P is the unique generalized inverse of R as defined by Penrose [1955]. (For discussion of generalized inverses see Searle, [1966, pages 144–145], and Graybill, [1969, chapter 6].) The basic theorem may be stated in terms of the diagonal entries p_{kk} and q_{kk} of the matrices P and Q.
Theorem:

$$\text{If } q_{kk} < 1, \quad c_k^2 = 1; \tag{11}$$

$$\text{if} \quad q_{kk} = 1, \qquad c_k^2 = 1 - \frac{1}{p_{kk}}. \tag{12}$$

A first step in the proof of the theorem is a demonstration that the theorem covers all possible values of q_{kk} . The two parts of the theorem will be proven by development of possible column vectors B_k which satisfy (6) and establishment of the values of c_k^2 determined by these column vectors B_k .

Two properties of the matrix Q are important in the proof of the theorem. From (7) and (10), Q is symmetric, idempotent.

$$Q = Q', \tag{13}$$

$$QQ' = QQ = Q, \tag{14}$$

$$RQ = QR = R. \tag{15}$$

Proof that the theorem covers all possible values of q_{kk} involves (14) from which

$$q_{kk} = \sum_i q_{ik}^2 = q_{kk}^2 + \sum_{i \neq k} q_{ik}^2 \tag{16}$$

or

$$q_{kk}(1 - q_{kk}) = \sum_{i \neq k} q_{ik}^2 . \tag{17}$$

Note that the term on the left of (17) will be negative for values of q_{kk} less than zero or greater than unity and will be non-negative between these values of q_{kk}. However, the term on the right of (17) necessarily is non-negative, being the sum of squared real numbers. Therefore, the permissible range of values for q_{kk} is:

$$0 \leqq q_{kk} \leqq 1. \tag{18}$$

Consequently, the theorem covers all possible values of q_{kk}.

Consider the first case when $q_{kk} < 1$. Define a diagonal matrix D_Q containing the diagonal entries of Q. Then, the matrix $(Q - D_Q)$ has zero diagonal entries. A column vector of regression weights, B_k, may be developed from the following series of operations.

$$R(Q - D_Q) = RQ - RD_Q = R - RD_Q = R(I - D_Q) \tag{19}$$

in which the transition between the second term and the third term is by (15). Let $(Q - D_Q)_k$ be a column vector composed of the k'th column of $(Q - D_Q)$. Then by (19)

$$R(Q - D_Q)_k = R(I - D_Q)_k = R_k(1 - q_{kk}) \tag{20}$$

where $(I - D_Q)_k$ is the k'th column of $(I - D_Q)$. Since $(I - D_Q)$ is a diagonal matrix, $(I - D_Q)_k$ contains all zero entries except for the k'th entry which is $(1 - q_{kk})$, this observation resulting in the transition from the second to third term in (20). Then

$$R(Q - D_Q)_k \frac{1}{(1 - q_{kk})} = R_k . \tag{21}$$

Comparison of (21) with (6) leads to the possibility of defining

$$B_k = (Q - D_Q)_k \frac{1}{(1 - q_{kk})} \tag{22}$$

with

$$-I_k + C_k^2 = 0 \tag{23}$$

which yields

$$c_k^2 = 1. \tag{24}$$

This completes the proof of the first part of the theorem.

Consider the second case when $q_{kk} = 1$. A first point is that p_{kk} must be greater than zero. Let F_k be a row vector composed of the k'th row of F. Note that F_k can not be a null vector since its length is unity, the diagonal entry in R. Note also that $(F'F)^{-2}$ is positive, definite since $(F'F)$ is non-singular. The product $F_k\,(F'F)^{-2}F_k^{1}$ is a quadratic form which must be positive for a non-null F_k and positive, definite $(F'F)^{-2}$. This product, however, by

(9), is p_{kk}. Consider the column vector $(I_k = P_k(1/p_{kk}))$ where P_k is the k'th column of P. Note that the k'th entry is zero. Note that

$$R\left(I_k - P_k \frac{1}{p_{kk}}\right) = R_k - Q_k \frac{1}{p_{kk}}. \tag{25}$$

Equation (10) was used in establishing this equality. A further point is derived from (17). When $q_{kk} = 1$, the left term of (17) equals zero; consequently, the sum of squares on the right equals zero and all q_{jk} for $j \neq k$ equal zero. Then, Q_k is the k'th column of an identity matrix, I_k. Equation (25) becomes

$$R\left(I_k - P_k \frac{1}{p_{kk}}\right) = R_k - I_k \frac{1}{p_{kk}}. \tag{26}$$

Comparison of (26) with (6) leads to the possibility of defining

$$B_k = \left(I_k - P_k \frac{1}{p_{kk}}\right) \tag{27}$$

with

$$-I_k + C_k^2 = -I_k \frac{1}{p_{kk}}. \tag{28}$$

This yields

$$c_k^2 = 1 - \frac{1}{p_{kk}}. \tag{29}$$

This completes the proof of the second part of the theorem.

Some interesting results when the factoring of R is by a principal axes method. Let V_r be an $n \times r$ section of an orthonormal matrix containing the first r characteristic roots of R, and let Λ_r be a diagonal matrix containing the first r characteristic roots in decreasing order. Since R is of rank r, all roots not included in Λ_r are zero and

$$R = V_r \Lambda_r V_r' . \tag{30}$$

Then

$$F = V_r \Lambda_r^{1/2} \tag{31}$$

and

$$F'F = \Lambda_r . \tag{32}$$

This factoring results in

$$P = V_r \Lambda_r^{-1} V_r' , \tag{33}$$

$$Q = V_r V_r' . \tag{34}$$

Then

$$p_{kk} = \sum_{p=1}^{r} v_{kp}^2/\lambda_p \,, \tag{35}$$

$$q_{kk} = \sum_{p=1}^{r} v_{kp}^2 \,. \tag{36}$$

Thus the test coefficient, q_{kk}, is a sum of squared coefficients in the characteristic vectors. The coefficient p_{kk} needs be calculated only when q_{kk} is less than unity.

Implementation of calculations for the squared multiple correlations using principal axes of R may involve use of two very small values, ϵ_λ and ϵ_q, set according to computational inaccuracies of the computer in use. The first problem involves the number of principal axes factors to be utilized. Let the roots be in decreasing algebraic order. A suggestion is to establish r such that

$$\lambda_r > \epsilon_\lambda \geqq \lambda_{r+1} \,. \tag{37}$$

A suggestion for the test coefficient is to compare it with $1 - \epsilon_q$. Thus,

$$\text{when} \quad q_{kk} < 1 - \epsilon_q \,, \qquad c_k^2 = 1; \tag{38}$$

$$\text{when} \quad q_{kk} \geqq 1 - \epsilon_q \,, \qquad c_k^2 = 1 - \frac{1}{p_{kk}}. \tag{39}$$

The computational scheme based on the theorem is applicable whether or not the correlation matrix is non-singular. It would not be as rapid as the procedure involving the inverse of the correlation matrix for non-singular matrices. However, it has an advantage over the separate solutions for the various measures when the correlation matrix is singular. The theorem does yield a way to compute all of the squared multiple correlations in a single solution and should involve fairly rapid calculations with modern computers.

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