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Generalized correlations in the singular case

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Abstract: A unified approach to obtain multiple, partial, canonical and some generalized canonical correlation is presented. These may all be obtained as roots of a certain determinantal equation involving a transformation of the original dispersion matrix specific to the generalized correlation under consideration. We extend this representation to the singular case using generalized inverses. The numbers of critical correlations are also obtained.

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1. Introduction

The concept of canonical correlations for two sets of random variables is well known. There exist various generalizations of canonical correlations to more than two sets of random variables. Here we first present a unified representation, using the original covariance matrix, of the defining equations for various generalizations of canonical correlations. This representation is then extended to cover the cases of the corresponding appropriate singular covariance matrices, thereby generalizing the previous results, e.g. Rao (1981), on multiple, partial and canonical correlations for two sets of variables in the singular case. The numbers of various critical generalized correlations are also derived for the general case.

2. Multiple, partial and canonical correlations: singular case

Let $R=(R_1:\ldots:R_p)$ be the correlation matrix of p variables. Further, let $R^-=(r^{ij})=(T_1:\ldots:T_p)$ by any g-inverse of R. Define $RR^-=Q=(Q_1:\ldots:Q_p)$. Let I_p have the unit vector e_i as its i-th column, $i=1,\ldots,p$.

Result 1. *The squared multiple correlation of X_1 on $X_2,\ldots,X_p$ is*

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$$R^2_{1\cdot(2\ldots p)} = \begin{cases} 1 & \textit{if } Q_1 \neq e_1, \\ 1-(r^{11})^{-1} & \textit{if } Q_1 = e_1. \end{cases}$$

Result 2. *The partial correlation between X_1 and X_2 eliminating $X_3, X_4, \ldots, X_p$ is*

$$r_{12\cdot(34\ldots p)} = \begin{cases} 0 & \textit{if } Q_1 \neq e_1 \textit{ and } Q_2 = e_2 \textit{ or if } Q_1 = e_1 \textit{ and } Q_2 \neq e_2, \\ 1 & \textit{if } Q_1 \neq e_1 \textit{ and } Q_2 \neq e_2, \\ -r^{12}/(r^{11}r^{22})^{1/2} & \textit{if } Q_1 = e_1 \textit{ and } Q_2 = e_2. \end{cases}$$

Let X_1 and X_2 be two sets of variables with the joint dispersion matrix Dispersion$(X_1', X_2')' \equiv$ Dispersion$(X) = \Sigma$, partitioned accordingly.

Result 3. *The squared canonical correlations are the non-zero roots of the determinantal equation $|\Sigma_{11}^- \Sigma_{12} \Sigma_{22}^- \Sigma_{21} - \varrho^2 I| = 0$ where Σ_{11}^- and Σ_{22}^- are any g-inverses of Σ_{11} and Σ_{22} respectively.*

For proofs and discussions see Rao (1981).

3. Generalized canonical correlations

3.1. A general representation

Several generalizations of canonical correlations for the case of $k>2$ sets have been proposed. Edgerton and Kolbe (1936), Horst (1961), Lord (1958), Wilks (1938) - all with one observation per set - and McKeon (1965), in the general situation, used generalizations of some association measures. Extensions of tests of independence for two sets led to partial, part and bipartial (Timm and Carlson, 1976) and g_1-, g_2-bipartial (Lee, 1978, 1979) canonical correlations. SenGupta (1983) chose the criterion of minimum generalized variance. For a review, see SenGupta (1983).

Let $X = (X_1', \ldots, X_k')'$, X_i: $p_i \times 1$, $p_1 + \cdots + p_k = p$, Dispersion$(X) = {}_k\Sigma > 0$, Covariance$(X_i, X_j) = \Sigma_{ij}$. Let ${}_k\Sigma^* > 0$ be a modification of ${}_k\Sigma$, modified by a particular generalization under consideration, and ${}_k\Sigma_{\mathrm{d}}^*$ be the diagonal $(\Sigma_{11}^*, \ldots, \Sigma_{kk}^*)$, a diagonal super matrix with elements Σ_{ii}^*, $i = 1, \ldots, k$. Also let ϱ^* be an eigen value of ${}_k\Sigma^*$ in the metric of ${}_k\Sigma_{\mathrm{d}}^*$. Starting with the defining equations, we see that a general representation can be given to cover all the above cases. The generalized canonical correlations, non-zero ϱ-values, are then given by

$$(k-1)\varrho + 1 = \varrho^* \quad \text{where } \varrho^* \text{ satisfies } |{}_k\Sigma^* - \varrho^* {}_k\Sigma_{\mathrm{d}}^*| = 0. \tag{3.1}$$

Specifically, in the notation of Lee, ${}_k\Sigma^*$, with $k=2$, is the dispersion matrix of the residual vectors, $\tilde{E} = (\tilde{e}_{1\cdot 34}', \tilde{e}_{2\cdot 35}')'$ and $E = (e_{1\cdot 34}', e_{2\cdot 35}')'$ for the g_1- and g_2-bipartial canonical correlations, respectively. In the notation of Timm and Carlson,

${}_k\Sigma^* = \Sigma_{\cdot 3}, \Sigma_{1(2\cdot 3)}$ and $\Sigma_{(1\cdot 3)(2\cdot 4)}$ with $k=2$ for partial, part and bipartial canonical correlations respectively. Also for McKeon's and SenGupta's generalized canonical correlations, ${}_k\Sigma^* = {}_k\Sigma$.

3.2. *The singular case*

Consider the case when ${}_k\Sigma_{\mathrm{d}}^*$ is singular. In practice, with a large number of variables, this singularity may arise, e.g., when one (or more) of the variables is (are) linear functions of the other variables. Let ${}_k\Sigma_{\mathrm{d}}^-$ be a g-inverse (Rao, 1981, p. 1) of ${}_k\Sigma_{\mathrm{d}}^*$. Let ϱ^* be a proper value (Mitra and Rao, 1968, p. 317; see also Puntanen, 1987 and Scott and Styan, 1985) of ${}_k\Sigma^*$ with respect to ${}_k\Sigma_{\mathrm{d}}^*$, i.e. ${}_k\Sigma^*\omega = \varrho^*{}_k\Sigma_{\mathrm{d}}^*\omega$ with ω such that, ${}_k\Sigma_{\mathrm{d}}^*\omega \neq 0$. Thus,

$$|{}_k\Sigma^*{}_k\Sigma_{\mathrm{d}}^{*-} - \varrho^* I| = 0. \tag{3.2}$$

Theorem. *The generalized canonical correlations, for all the methods quoted above, are given by* $\varrho = (\varrho^* - 1)/(k-1)$, *where* ϱ^* *is a non-zero proper value of* ${}_k\Sigma^*$ *with respect to* ${}_k\Sigma_{\mathrm{d}}^*$.

Proof. Consider the following lemma which is a direct consequence of Theorem 3.1 of Mitra and Rao (1968, p. 315).

Lemma. *Let A be a symmetric matrix of order n and rank s, and B be a symmetric, non-negative definite matrix of order n and rank r such that $S(A) \subset S(B)$, where $S(M)$ represents the vector space spanned by the column vectors of M. Then*:

(i) *There exists a matrix L of order $n \times r$ such that $L'AL = \Lambda$, $L'BL = I_r$ where Λ is a diagonal matrix with s non-zero elements, some of which may be repeated, and I_r is the identity matrix of order r.*

(ii) *The non-zero elements of Λ are the same as the roots of the determinantal equation $|AB^- - \lambda I| = 0$ with repetitions allowed, for any g-inverse B^- of B.*

By (ii), ϱ^* is a non-zero proper value of (3.1) iff (3.2) holds, provided $S({}_k\Sigma^*) \subset S({}_k\Sigma_{\mathrm{d}}^*)$. This follows from the identity $AB^-B = A$. But it is well known, e.g. from properties of Schur complements of partitioned matrices, that $S(\Sigma_{ij}) \subset S(\Sigma_{ii})$ which implies that the above-mentioned required condition is satisfied.

Note. For $k=2$, if $p_1 = 1$, $p_2 > 1$ and if $p_1 > 1$, $p_2 > 1$ then we have the cases of multiple and canonical correlations respectively. Further, with $k=2$, consideration of residual variables leads to partial, part and various bipartial canonical correlations. Thus, the above theorem unifies the Results 1 through 3, considers simple, and not squared, multiple, partial and canonical correlations and uses the representation in terms of the original dispersion matrix. The theorem now, for $k>2$, also extends the above results for the singular case to various part, bipartial, McKeon's, and SenGupta's generalized canonical correlations.

4. Numbers of critical generalized correlations

In the context of Lemma 1, the elements of Λ are called the proper values and the corresponding columns of L, the proper vectors of A with respect to B. For the generalized correlations, we consider from (3.1) only the proper values of ${}_k\Sigma^*$ with respect to ${}_k\Sigma_{\mathrm{d}}^*$. Note that for $k \geq 2$, 1 and $-1/(k-1)$ are the maximum and minimum possible values, respectively, for the generalized correlations. Let ${}_k\Sigma_{\mathrm{od}}^*$ be the off-diagonal super matrix such that ${}_k\Sigma^* = {}_k\Sigma_{\mathrm{d}}^* + {}_k\Sigma_{\mathrm{od}}^*$. Also let $R(M)$ denote the rank of the matrix M.

Result. *The numbers of zero, unit and* $-1/(k-1)$ *-valued generalized correlations are given by* $r - R({}_k\Sigma_{\mathrm{od}}^*)$, $r - R[{}_k\Sigma_{\mathrm{od}}^* - (k-1)\,{}_k\Sigma_{\mathrm{d}}^*]$ *and* $r - R({}_k\Sigma^*)$ *respectively, where* $r = R({}_k\Sigma_{\mathrm{d}}^*)$.

Proof. The proof follows by rewriting (3.1) as $|{}_k\Sigma_1^* - \lambda\,{}_k\Sigma_{\mathrm{d}}^*| = 0$ where $({}_k\Sigma_1^*, \lambda) = ({}_k\Sigma_{\mathrm{od}}^*, (k-1)\varrho)$, $({}_k\Sigma_{\mathrm{od}}^* - (k-1)\,{}_k\Sigma_{\mathrm{d}}^*, (k-1)(\varrho - 1))$ and $({}_k\Sigma^*, (k-1)\varrho + 1)$ for the zero, unit and $-1/(k-1)$ -valued generalized correlations respectively, and noting the one-one relationship between λ and ϱ.

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