Inference in Canonical Correlation Analysis

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The asymptotic behavior, for large sample size, is given for the distribution of the canonical correlation coefficients. The result is used to examine the Bartlett-Lawley test that the residual population canonical correlation coefficients are zero. A marginal likelihood function for the population coefficients is obtained and the maximum marginal likelihood estimates are shown to provide a bias correction.

1. INTRODUCTION

Let $r_1, \ldots, r_p$ be the sample canonical correlation coefficients between variates $y_1, \ldots, y_p$ and $x_1, \ldots, x_q$ ($p \leq q$) calculated from a sample of size $N = n + 1$ observations from a $(p + q)$-variate normal distribution. The exact joint density function of $r_1^2, \ldots, r_p^2$ is (see Constantine [5], James [9])

$$
\prod_{i=1}^{p} (1 - r_i^2) \frac{1}{n} \frac{P(\alpha)}{(\frac{1}{2} n; \frac{1}{2}; P^2, R^2)} \times k_1 \prod_{i=1}^{p} (r_i^2)^{1(q-p-1)} (1 - r_i^2)^{1(q-p-1)} \prod_{i<j}^{p} (r_i^2 - r_j^2)
$$

(1 > r_1^2 > r_2^2 > \cdots > r_p^2 > 0),

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where $1 \geq \rho_1 \geq \rho_2 \geq \cdots \geq \rho_p \geq 0$ are the population canonical correlation coefficients, $R = \text{diag}(r_1, \ldots, r_p)$, $P = \text{diag}(\rho_1, \ldots, \rho_p)$,

$$k_1 = \Gamma_p(\frac{1}{2}n)^{1/2} \frac{1}{[\Gamma_p(\frac{1}{2}(n - q)) \Gamma_p(\frac{1}{2}q) \Gamma_p(\frac{1}{2}p)]},$$

and $_2F_1^{(p)}$ is a hypergeometric function with the matrices $P^2$ and $R^2$ as arguments. The distribution of $r_1^2, \ldots, r_p^2$ depends only on $\rho_1, \ldots, \rho_p$ and hence that part of the distribution involving $\rho_1, \ldots, \rho_p$ can be regarded as a marginal likelihood. From (1.1) we see that the marginal likelihood function is

$$\prod_{i=1}^{n} (1 - \rho_i^2)^{1/n} _2F_1^{(p)}(\frac{1}{2}n, \frac{1}{2}n; \frac{1}{2}q; P^2, R^2).$$

In Section 2 we derive an asymptotic representation for the $_2F_1^{(p)}$ function, and hence for the distribution (1.1) and marginal likelihood (1.3), for large sample size $n$. This is done by expressing $_2F_1^{(p)}$ as a complicated multiple integral and using a multivariate extension of Laplace's method for integrals to obtain its asymptotic behavior. In Section 3 the asymptotic distribution is used to examine the Bartlett-Lawley test of the null hypothesis that the last $p - k$ population canonical correlation coefficients are zero. Maximum marginal likelihood estimates of certain transformed population coefficients are also obtained and are shown to provide a bias correction.

2. ASYMPTOTIC DISTRIBUTIONS

Before deriving the asymptotic behavior of the $_2F_1^{(p)}$ function in (1.1) we first note Hsu's extension [8] of Laplace's method for obtaining the asymptotic behavior of integrals. If the function $f(x) = f(x_1, \ldots, x_m)$ has an absolute maximum at an interior point $\xi$ of a domain $\mathcal{S}$ in real $m$-dimensional space, then under suitable conditions, as $n \to \infty$

$$\int_{\mathcal{S}} f(x)^n \varphi(x) \, dx \sim (2\pi/n)^{1/2} f(\xi)^n \varphi(\xi) \Delta(\xi)^{-1},$$

where $a \sim b$ means that $\lim_{n \to \infty} a/b = 1$ and $\Delta(x) = \det(-\partial^2 \log f/\partial x_i \partial x_j)$. We begin by looking at the $_2F_1$ function with one $k \times k$ matrix $T^2$ as argument (see [9]). Without loss of generality $T$ can be assumed diagonal, $T = \text{diag}(t_1, \ldots, t_k)$, and we will assume that the roots are distinct with $1 > t_1 > t_2 > \cdots > t_k > 0$. The integrals involved in the subsequent development can be found in James [9] and Herz [7].
Theorem 1. As \( n \to \infty \)

\[
_2F_1\left(\frac{1}{2}n, \frac{1}{2}n; \frac{1}{2}; T^2\right) \sim c_1 \prod_{i=1}^{k} t_i^{(k-q)(1 - t_i)^{-1}} \prod_{i < j}^{k} (t_i + t_j)^{-\frac{1}{2}},
\]

(2.2)

where

\[
c_1 = \left(\frac{n}{2}\right)^{\frac{1}{2}(k-1)} \Gamma_k(\frac{1}{2}) \prod_{i=1}^{k} \frac{\Gamma_i(\frac{1}{2})}{\Gamma_i(\frac{1}{2}) - i} (1 + O(n^{-1})).
\]

Proof. The idea here is to express \( _2F_1 \) as a multiple integral to which Hsu’s result (2.1) can be applied. We can write

\[
_2F_1\left(\frac{1}{2}n, \frac{1}{2}n; \frac{1}{2}; T^2\right) = c_2 \int_{O(k)} \int_{D_U} \int_{O(k)} \int_{D_V} \exp\{-\frac{1}{2}n \text{tr}(U^2 + V^2)\}
\]

\[
\times UV \exp\{n \text{tr}([TH_1U'H_2H_2'VH_2': O]Q_1)\}
\]

\[
\times \prod_{i < j}^{k} (u_i^2 - u_j^2)(v_i^2 - v_j^2)(dQ_1)(dV)(dH_2)(dU)(dH_1),
\]

(2.3)

where

\[
c_2 = \left(\frac{n}{2}\right)^{k/2} \frac{1}{\pi^{k/2}} \frac{1}{\Gamma_k(1/2) \Gamma_{k-k}(1/2 - k)}.
\]

\( O(k) \) is the group of \( k \times k \) orthogonal matrices, \( (dH_i) \) \((i = 1, 2) \) is the unnormalized measure on \( O(k) \), so that the volume of \( O(k) \) is \( 2^{k/2} \pi^{k^2/4} \Gamma_k(1/2) \), \( U = \text{diag}(u_1, ..., u_k) \), \( V = \text{diag}(v_1, ..., v_k) \), \( D_u = \{(u_1, ..., u_k); u_1 > u_2 > ... > u_k > 0\} \), and \( V(k, q) \) is the Stiefel manifold consisting of all \( q \times k \) matrices \( Q_1 \) with orthonormal columns. The integral (2.3) is of the form \( c_2 \int_{\mathcal{S}} f^k_\phi \), where

\[
f = \exp\{-\frac{1}{2} \text{tr}(U^2 + V^2) + \text{tr}([TH_1U'H_2H_2'VH_2': O]Q_1)\} \quad |UV|
\]

and

\[
\varphi = |UV|^{-k} \prod_{i < j}^{k} (u_i^2 - u_j^2)(v_i^2 - v_j^2).
\]

It can be shown that \( f \) achieves its maximum value at the \( 2^{2k} \) points in \( \mathcal{S} \) of the form
U = V = \text{diag}((1 - t_1)^{-1}, \ldots, (1 - t_k)^{-1})

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and the maximum value of \( f \) is

\begin{equation}
f^* = e^{-k} \prod_{i=1}^{k} (1 - t_i)^{-1}.
\end{equation}

At these maxima \( \phi \) has the value

\begin{equation}
\phi^* = \prod_{i=1}^{k} (1 - t_i)^{2-k} \prod_{i<j} (t_i - t_j)^2
\end{equation}

and it can be shown that the Hessian is

\begin{equation}
\Delta = 2(2-k) \prod_{i=1}^{k} (1 - t_i)^{2-k} \prod_{i<j} (t_i - t_j)^2(t_i + t_j).
\end{equation}

The number of variables \( m \) in Hsu's result being integrated is \( \frac{1}{2}k(k + 2q + 1) \). Substitution of (2.4), (2.5), and (2.6) in (2.1), together with an obvious simplification of \( \epsilon_2 \), yields the theorem. As a check on some very tedious algebra it can be noted that when \( k = 1 \), (2.2) agrees with the known asymptotic behavior of the classical hypergeometric function (see Luke [13, Sect. 7.2]).

The asymptotic behavior of the two-matrix \( _2F_1 \) function follows from Theorem 1. Let

\begin{equation}
R = \text{diag}(r_1, \ldots, r_p), \text{ where } 1 > r_1 > \cdots > r_p > 0
\end{equation}

and let \( P \) be a \( p \times p \) diagonal matrix of the form

\begin{equation}
P = \begin{bmatrix} P_1 & 0 \\ 0 & 0 \end{bmatrix},
\end{equation}

where \( P_1 = \text{diag}(\rho_1, \ldots, \rho_k) \) with \( 1 > \rho_1 > \cdots > \rho_k > 0 \). Then we have
Theorem 2. As $n \to \infty$,

\begin{equation}
\mathcal{I}_n \sim c_3 \prod_{i=1}^{k} \prod_{j=1}^{p} C_{ij}^{-\frac{1}{2}},
\end{equation}

where

\begin{equation}
c_3 = (\frac{1}{2}n)^{-\frac{3}{2}} \pi^{-\frac{1}{2}} \Gamma_k(\frac{1}{2}p) \Gamma_k(\frac{1}{2}q) 2^{-\frac{1}{4}} [1 + O(n^{-1})]
\end{equation}

and

\begin{equation}
C_{ij} = (r_i^2 - r_j^2)(\rho_i^2 - \rho_j^2) \quad i = 1, \ldots, k; \quad j = 1, \ldots, p.
\end{equation}

Proof. This follows from (2.1), (2.2), and the fact that

\begin{equation}
\mathcal{I}_n \sim c_4 \prod_{i=1}^{k} \prod_{j=1}^{p} (\delta_i^\frac{1}{2}(1 - \delta_i)^{-n+\frac{1}{4}}) \prod_{i<j}^{k} (\delta_i + \delta_j)^{-\frac{1}{4}} (dH_1),
\end{equation}

where $c_4 = c_1 \Gamma_k(\frac{1}{2}p) \pi^{-\frac{1}{2}} \rho_k$ and $\delta_1 > \cdots > \delta_k$ are the positive square roots of the latent roots of $P_1H_1R^2H_1P_1$. This integral is of the form $c_4 \int_{V(k, p)} f^n \phi$, where

\begin{equation}
f = \prod_{i=1}^{k} (1 - \delta_i)^{-\frac{1}{2}}
\end{equation}

and

\begin{equation}
\phi = \prod_{i=1}^{k} \delta_i^\frac{1}{2}(1 - \delta_i)^{\frac{1}{4}} \prod_{i<j}^{k} (\delta_i + \delta_j)^{-\frac{1}{4}}.
\end{equation}

It can be shown that $f$ has $2^k$ maxima which are obtained when $H_1$ has the form

\begin{equation}
H_1 = \begin{bmatrix}
\pm \frac{1}{2} & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & \pm \frac{1}{2} & 0 \\
k & p - k
\end{bmatrix} k.
\end{equation}
At these values for $H_1, \delta_i = r_i\rho_i$ for $i = 1, \ldots, k$, and the maximum value of $f$ is

$$f = \prod_{i=1}^{k} (1 - r_i\rho_i)^{-1}.$$  

The value of $\varphi$ at these maxima is

$$\varphi = \prod_{i=1}^{k} (r_i\rho_i)^{1/(k-q)}(1 - r_i\rho_i)^{1/q} \prod_{i<j}^{k} (r_i\rho_i + r_j\rho_j)^{-1},$$

and it can be shown that the Hessian is

$$\Delta = \prod_{i=1}^{k} (r_i\rho_i)^{k-p}(1 - r_i\rho_i)^{p} \prod_{i<j}^{k} \frac{(r_i^2 - r_j^2)(\rho_i^2 - \rho_j^2)}{(r_i\rho_i + r_j\rho_j)} \prod_{i=1}^{k} \prod_{j=k+1}^{p} [\rho_i^2(r_i^2 - r_j^2)].$$

The theorem now follows from a straightforward application of (2.1).

Substitution of (2.7) in (1.1) gives an asymptotic representation for the distribution of $r_1^2, \ldots, r_p^2$ under the assumption that the population canonical correlation coefficients satisfy

$$1 > \rho_1 > \cdots > \rho_k > \rho_{k+1} = \cdots = \rho_p = 0.$$  

This is summarized in the following

**Theorem 3.** The asymptotic density function of $r_1^2, \ldots, r_p^2$ for large $n$, when the population coefficients satisfy (2.9), is

$$k_2 \prod_{i=1}^{k} (1 - r_i\rho_i)^{-n+1/(p+q-1)}(r_i^2)^{1/(q-p)-1}(1 - r_i^2)^{1/(n-p-q-1)} \prod_{i<j}^{k} \left( \frac{r_i^2 - r_j^2}{\rho_i^2 - \rho_j^2} \right)^{1/2}$$

$$\times \prod_{i=1}^{k} \prod_{j=k+1}^{p} (r_i^2 - r_j^2)^{1/2}$$

$$\times \prod_{i=k+1}^{p} (r_i^2)^{1/(q-p-1)}(1 - r_i^2)^{1/(n-q-p-1)} \prod_{i<j}^{k+1} (r_i^2 - r_j^2),$$

where

$$k_2 = k_1(\frac{3}{2}n)^{-1/4(k+p-q-k-1)}n^{-1/2(k+1)}\Gamma(k/4) \Gamma(k/4)p2^{-k}$$

$$\times \prod_{i=1}^{k} (1 - \rho_i^2)^{1/2} \rho_i^{k-4/(p+q)}[1 + O(n^{-1})]$$

and $k_1$ is given by (1.2).
An alternative asymptotic result has been given by Chattopadhyay and Pillai [3] and Chattopadhyay, Pillai, and Li [4]; however the asymptotic behavior given by these authors involves a $2F_1$ function with the matrix $P_2R_2$ as argument and appears to be incorrect. From Theorem 3 it is easy to obtain the following:

**Corollary.** The asymptotic conditional density function of the $p - k$ smallest sample coefficients $r_{k+1}^2, ..., r_p^2$ given the first $k$ coefficient $r_1^2, ..., r_k^2$ is proportional to

$$\prod_{i=1}^{k} \prod_{j=k+1}^{p} (r_i^2 - r_j^2) \prod_{i=k+1}^{p} (r_i^2)^{(q-p-1)} \prod_{i=1}^{p} (r_i^2)^{(q-p)(n-q-p-1)} \prod_{i<j} (r_i^2 - r_j^2). \tag{2.11}$$

From this we see that the largest $k$ sample coefficients $r_1^2, ..., r_k^2$ are asymptotically sufficient for $\rho_1^2, ..., \rho_k^2$. This suggests the use of (2.11) as a basis for testing the null hypothesis that the smallest $p - k$ population coefficients are all zero; this approach will be followed in the next section.

### 3. Testing and Estimation

We first investigate the Bartlett-Lawley test of the null hypothesis $H_0: \rho_k^2 \geq \cdots \geq \rho_p^2 = 0$ against $H: \rho_k^2 \geq \cdots \geq \rho_p^2 \geq \rho_1^2 \geq \cdots \geq \rho_p^2 > 0$ and $\rho_k^2 > 0$ using the distribution (2.11) of $r_{k+1}^2, ..., r_p^2$ given $r_1^2, ..., r_k^2$ which does not depend on the nuisance parameters $\rho_1, ..., \rho_k$. The approach given here is similar to that used by James [10] in another context.

The likelihood ratio statistic is

$$T_k = -\log \prod_{j=k+1}^{p} (1 - r_j^2)$$

and under $H_0$ Bartlett [1, 2] showed that $\{n - \frac{1}{2}(p + q + 1)\} T_k$ has an asymptotic $\chi^2$ distribution with $(p - k)(q - k)$ degrees-of-freedom. Lawley [12] obtained a correction to Bartlett's multiplying factor which makes the moments equal to those of the asymptotic $\chi^2$ distribution, apart from errors of order $n^{-2}$. Fujikoshi [6] has obtained an expansion for the asymptotic distribution of Lawley's statistic. This statistic involves the $k$ largest population coefficients and since these will usually be unknown, Lawley suggested, somewhat tentatively, that they be replaced by the $k$ largest sample coefficients. Here we attempt to provide some information about the accuracy of the approximation when this is done.

The appropriate multiplier of $T_k$ can be obtained by finding its expected value. For notational convenience let $E_n$ denote expectation taken with respect to the conditional distribution (2.11) of $r_{k+1}^2, ..., r_p^2$ given $r_1^2, ..., r_k^2$ and let $E_N$
denote expectation with respect to the null distribution obtained by ignoring the linkage factor

\[
\prod_{i=1}^{k} \prod_{j=k+1}^{p} (r_{ij}^2 - r_j^2)^{1/2}
\]

in (2.11). In order to obtain \(E_\varepsilon(T_k)\) we first find \(E_\varepsilon(e^{-HT_k})\). This can obviously be done by finding

\[
E_N \left[ \prod_{i=1}^{k} \prod_{j=k+1}^{p} \left( 1 - \frac{r_{ij}^2}{r_j^2} \right)^{1/2} e^{-HT_k} \right]. 
\]

(3.1)

Writing

\[
\prod_{i=1}^{k} \prod_{j=k+1}^{p} \left( 1 - \frac{r_{ij}^2}{r_j^2} \right)^{1/2} = 1 - \frac{\alpha}{2} \sum_{j=k+1}^{p} r_j^2 + O(n^{-2}),
\]

where

\[
\alpha = \sum_{i=1}^{k} r_i^2,
\]

and substituting this in (3.1) it is seen that we need the following:

**Lemma.**

\[
E_N \left( e^{-HT_k} \sum_{j=k+1}^{p} r_j^2 \right) = \frac{(p - k)(q - k)}{n - 2k + 2h} E_\theta(h),
\]

(3.2)

where \(E_\theta(h) = E_N(e^{-HT_k})\).

The proof of this follows easily from the fact that

\[
\sum_{j=k+1}^{p} r_j^0 = \text{tr}(I - U),
\]

where \(U\) is a \((p - k) \times (p - k)\) matrix having a multivariate Beta\(\left( \frac{1}{2} (n - q - k), \frac{1}{2} (q - k) \right)\) distribution (see Kshirsagar [11, Chap. 8]). Using the lemma we can then show, from (3.1), that

\[
E_\varepsilon(e^{-HT_k}) = \theta(h)/\theta(0),
\]
where \( \theta(h) = E_0(h) f(h) \) with \( f(h) = 1 - \alpha(p - k)(q - k)/(2(n - 2k + 2h)) \).

Now

\[
E_c(T_k) = -\frac{d}{dh} \left\{ \frac{\theta(h)}{\theta(0)} \right\}_{h=0}
= -E'_0(0) - \frac{\alpha(p - k)(q - k)}{(n - 2k)^2} + O(n^{-3}).
\]

But \(-E'_0(0) = E_N(T_k)\) and when \( H_0 \) is true we know that

\[
[n - k - \frac{1}{2}(p + q + 1)]T_k
\]

has an asymptotic \( \chi^2 \) distribution with \( (p - k)(q - k) \) degrees-of-freedom and
the means agree to \( O(n^{-2}) \) so that

\[
-E'_0(0) = (p - k)(q - k)[n - k - \frac{1}{2}(p + q + 1)] + O(n^{-3}).
\]

Hence it follows that

\[
E_c(T_k) = (p - k)(q - k)/[(n - k - \frac{1}{2}(p + q + 1) + \alpha] + O(n^{-1}).
\]

Thus the appropriate multiplier of \( T_k \) is \( n - k - \frac{1}{2}(p + q + 1) + \alpha \). Summarizing this, together with Lawley's result [12] we have the following theorem.

**Theorem 4.** The statistic

\[
L_k = \left( n - k - \frac{1}{2}(p + q + 1) + \frac{1}{2} \sum \limits_{i=1}^{k} T_i^2 \right) T_k
\]

has an asymptotic \( \chi^2 \) distribution with \( (p - k)(q - k) \) degrees-of-freedom and
\( E_c(L_k) = (p - k)(q - k) + O(n^{-2}) \).

We now turn to the problem of estimating the parameters \( \xi_1, \ldots, \xi_p \) defined via
the familiar transformation

\[
\xi_i = \tanh^{-1} \rho_i - \frac{1}{2} \log \frac{1 + \rho_i}{1 - \rho_i}.
\]

Let \( z_i = \tanh^{-1} r_i \) \((i = 1, \ldots, p)\), the usual maximum likelihood estimate of \( \xi_i \),
which has a bias term of order \( n^{-1} \). We will show that the maximum marginal likelihood estimate of \( \xi_i \) provides a bias correction.
From (1.3) and (2.7) with \( k = p \) we see that the asymptotic marginal log likelihood function is

\[
\log L = \frac{1}{2} n \sum_{i=1}^{p} \log(1 - \rho_i^2) + \left\{ \frac{1}{2}(p + q - 1) - n \right\} \sum_{i=1}^{p} \log(1 - r_i \rho_i) \\
+ \frac{1}{2}(p - q) \sum_{i=1}^{p} \log \rho_i - \frac{1}{2} \sum_{i<j}^{p} \log(\rho_i^2 - \rho_j^2)
\]

from which it follows easily that the maximum marginal likelihood estimate of \( \xi \) is

\[
\hat{\xi}_i = z_i - \frac{1}{2nr_i} \left\{ p + q - 2 + r_i^2 + 2(1 - r_i^2) \sum_{j \neq i} \frac{r_j^2}{r_i^2 - r_j^2} \right\} + O(n^{-2}).
\]

Using expressions for the mean and variance of \( r_i \) given by Lawley [12] it can readily be verified

\[
E(\hat{\xi}_i) = \xi_i + O(n^{-2})
\]

and

\[
\text{Var}(\hat{\xi}_i) = 1/n + O(n^{-2})
\]

so that these estimates stabilize the variance to order \( n^{-1} \) and also provide a correction for bias.

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**References**


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