SOME DISTRIBUTION THEORY RELATING TO CONFIDENCE REGIONS IN MULTIVARIATE CALIBRATION

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(Received June 8, 1985; revised Oct. 23, 1985)

Summary

In the problem of multivariate calibration, Williams (1959, Regression Analysis, Wiley) and Wood (1982, to appear in Proc. 11th Internat. Bio. Conf.) have proposed a decomposition of the usual Hotelling's T^2 statistic into the sum of two statistics for use in constructing confidence regions. This paper presents general results for the moment terms basic to Fujikoshi and Nishii's (1984, Hiroshima J. Math., 14, 215-225) approach to the distributions of these statistics, and presents simple alternative approximations to their percentiles.

1. Introduction

We assume that a set of p dependent variables $y = (y_1, \dots, y_p)'$ is linearly determined by a set of q independent variables $x=(x_1,\dots,x_q)'$, and that a calibration sample of N observations of x and y are available. A new observation y is made at a single unknown vector x, and it is required to make inference about x. If, as is assumed here, the x's in the calibration sample were chosen at fixed preassigned values rather than at random, then this is the problem of controlled multivariate calibration (Brown [1]). In the case p=q, Williams [13] proposed fiducial limits based on a Hotelling's generalized T^2 statistic, which yields elliptical confidence regions for x under a certain condition. When p>q, this approach may lead to empty confidence regions even when the condition is fulfilled, and Williams [13] defined a statistic R for testing the consistency of the new y with the model, and a statistic Q for constructing a confidence region for x. Williams also conjectured approximations to the distributions of Q and R. Wood [14] pointed out that the Hotelling's T^2 statistic may be decomposed into the sum of Q and R, and called attention once more to the problem of the distri-

Key words and phrases: Multivariate calibration, decomposition of Hotelling T^2 , Laplace transform, invariant polynomials, asymptotic expansion.

butions of these statistics. Fujikoshi and Nishii [7] showed that the required distribution theory may be related to results of Gleser and Olkin [8] on regression with an unknown covariance matrix. They obtained early terms in the asymptotic expansion of the distribution of Q in terms of central chi-squared distributions, and gave the corresponding expansion of the percentile point of Q up to order $1/N^2$.

In the present paper we obtain general expressions for the moments which are fundamental to the approach of Fujikoshi and Nishii [7], and consider the asymptotic expansion of the distributions of Q and R in terms of central F distributions. The associated expansions of the percentile points of Q and R in terms of F percentiles yield simple first order approximations which reduce to the exact result for Q when p=q, and may be compared with the proposals of Williams [13]. The problem is raised of a multivariate extension of Watson's lemma for loop integrals, required for the justification of the asymptotic expansions.

2. Decomposition of T^2

In the multivariate regression model it is assumed that

$$(2.1) Y=1_{N}a'+XB+E$$

where $Y=[y_1,y_2,\cdots,y_N]'$ is an $N\times p$ observation matrix, $X=[x_1,\cdots,x_N]'$ is a known $N\times q$ design matrix with rank q, 1_N is an $N\times 1$ vector of ones, a is an unknown $p\times 1$ location vector, and B is a $q\times p$ matrix of unknown regression coefficients. E is an $N\times p$ error matrix whose rows are independently distributed as $N_p(0, \Omega)$. Without loss of generality we shall assume that $\overline{x}=\sum\limits_{i=1}^N x_i/N=0$. The usual maximum likelihood estimators of a, B and Ω are

$$\hat{a} = \overline{y} = \sum_{i=1}^{N} y_i / N$$

$$\hat{B} = (X'X)^{-1}X'Y$$

$$\hat{Q} = S/n , \qquad S = Y'[I_N - 1_N 1_N' / N - X(X'X)^{-1}X']Y ,$$

where $n=N-q-1 \ge p$ and I_N is the $N \times N$ unit matrix.

In the calibration problem a new p-dimensional observation y having the same structure as (2.1) is observed,

$$y=a+B'x+e$$
,

where x is an unknown $q \times 1$ vector, and e is distributed as $N_p(0, \Omega)$, independently of E. Following Williams [13], Brown suggested that a $1-\alpha$ confidence region for x may be constructed from

$$(2.2) T^2 = (y - \bar{y} - \hat{B}'x)'S^{-1}(y - \bar{y} - \hat{B}'x) \le \sigma^2(x)K,$$

where

$$K = \frac{q}{n-p+1} F_{q,n-p+1}(\alpha)$$

(2.3)
$$\sigma^2(x) = 1 + N^{-1} + x'(X'X)^{-1}x$$

and $F_{q,n-p+1}(\alpha)$ is the upper α -point of F with q and n-p+1 degrees of freedom.

In order for the confidence region to be a closed set, it is required that $\hat{B}S^{-1}\hat{B}'-K(X'X)^{-1}$ be positive definite, but when p>q the region may be empty even when this condition holds.

Wood [14] showed that T^2 could be decomposed as

$$T^2 = (\hat{x} - x)'\hat{B}S^{-1}\hat{B}'(\hat{x} - x) + (y - \bar{y} - \hat{B}'\hat{x})'S^{-1}(y - \bar{y} - \hat{B}'\hat{x}) = Q + R$$

say, where $\hat{x} = (\hat{B}S^{-1}\hat{B}')^{-1}\hat{B}S^{-1}(y-\bar{y})$ is the natural estimator of x. Williams [13] proposed R as a test for the consistency of y with the model (2.1), and Q as the basis for a confidence region for x when p>q. (When p=q, $R\equiv 0$ and $T^2\equiv Q$).

If we write $u=y-\bar{y}-\hat{B}'x$, and let $P_x=X(X'X)^{-1}X'$ denote the orthogonal projection onto the linear subspace $\mathcal{L}(X)$ spanned by the columns of X, with complement $\bar{P}_x=I-P_x$, then T^2 , Q and R may be expressed as follows,

$$T^2 = (S^{-1/2}u)'(S^{-1/2}u) ,$$
 (2.4) $Q = (S^{-1/2}u)'P_{S^{-1/2}\hat{B}'}(S^{-1/2}u) ,$ $R = (S^{-1/2}u)'ar{P}_{S^{-1/2}\hat{B}'}(S^{-1/2}u) .$

Wood's [14] decomposition may thus be represented geometrically as in Fig. 1.

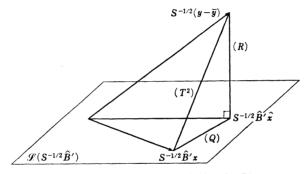


Fig. 1. Decomposition of $T^2=Q+R$.

3. Distributions of Q and R

Fujikoshi and Nishii [7] have shown that certain conditional distributions of Q and R may be obtained from Gleser and Olkin [8]. A concise derivation of these results using (2.4) is as follows.

Let $B_0 = B \Omega^{-1/2}$ and $\bar{B} = \hat{B} \Omega^{-1/2}$. Then we may assume without loss of generality that $\Omega = I_p$. If the columns of the $p \times (p-q)$ matrix H_2 form an orthonormal basis of the orthogonal complement of \hat{B}' , then we may write

$$R = (S^{-1/2}u)'P_{S^{1/2}H_2}(S^{-1/2}u) = u'H_2(H_2'SH_2)^{-1}H_2'u$$
.

Let $H=[H_1, H_2] \in O(p)$, the group of $p \times p$ orthogonal matrices. Then, conditional upon \bar{B} , $\bar{u}=(1+N^{-1})^{-1/2}H'u$ is distributed as $N_p(H'(B_0-\bar{B})'\bar{x}, I_p)$, where $\tilde{x}=(1+N^{-1})^{-1/2}x$, and $\tilde{S}=H'SH$ is independently distributed as $W_p(n, I_p)$, the central Wishart distribution with n degrees of freedom. Partitioning \tilde{u} and \tilde{S} as

$$egin{aligned} & ilde{u} = \left[egin{aligned} & ilde{u}_1 \\ & ilde{u}_2 \end{array}
ight]_{p-q}^q = \left[egin{aligned} & H_1'u \\ & H_2'u \end{aligned}
ight] (1+N^{-1})^{-1/2} \;, \ & ilde{S} = \left[egin{aligned} & ilde{S}_{11} & ilde{S}_{12} \\ & ilde{S}_{21} & ilde{S}_{22} \end{array}
ight] \;, \qquad & ilde{S}_{ij} = H_i'SH_j \;, \quad i, \, j = 1, \, 2 \;, \end{aligned}$$

we have

(3.1)
$$\tilde{R} = \frac{R}{1 + N^{-1}} = \tilde{u}_2' \tilde{S}_{22}^{-1} \tilde{u}_2$$

where $\tilde{S}_{22} \sim W_{p-q}(n, I_{p-q})$. Hence the conditional distribution of $((n-(p-q)+1)/(p-q))\tilde{R}$ given \bar{B} is a non-central F distribution with p-q and n-(p-q)+1 degrees of freedom, and non-centrality parameter

(3.2)
$$\mu = \tilde{x}'(\bar{B} - B_0)\bar{P}_{\bar{B}'}(\bar{B} - B_0)\tilde{x} ,$$

noting that the columns of H_2 span the orthogonal complement of \bar{B}' . Q may be expressed as

$$(3.3) \quad \tilde{Q} = \frac{Q}{1 + N^{-1}} = \tilde{u}' \tilde{S}^{-1} \tilde{u} - \tilde{u}'_{2} \tilde{S}_{22}^{-1} \tilde{u}_{2} = (\tilde{u}_{1} - \tilde{S}_{12} \tilde{S}_{22}^{-1} \tilde{u}_{2})' \tilde{S}_{11.2}^{-1} (\tilde{u}_{1} - \tilde{S}_{12} \tilde{S}_{22}^{-1} \tilde{u}_{2}) ,$$

where $\tilde{S}_{11,2} = \tilde{S}_{11} - \tilde{S}_{12}\tilde{S}_{21}^{-1}\tilde{S}_{21} \sim W_q(n-(p-q), I_q)$. Following Gleser and Olkin [8], we note that $\tilde{S}_{11,2}$, \tilde{S}_{22} and $T = \tilde{S}_{22}^{-1/2}\tilde{S}_{21}$ are independently distributed, the q(p-q) elements of T being independently N(0,1). Hence,

$$E[\tilde{u}_1\!-\! ilde{S}_{\!\scriptscriptstyle 12}\! ilde{S}_{\!\scriptscriptstyle 22}^{-1}\! ilde{u}_{\!\scriptscriptstyle 2}|ar{B},\, ilde{u}_{\scriptscriptstyle 2},\, ilde{S}_{\!\scriptscriptstyle 22}]\!=\!H_{\!\scriptscriptstyle 1}'(B_{\scriptscriptstyle 0}\!-\!ar{B})' ilde{x}$$
 ,

$$\cos \left[\tilde{u}_1 - \tilde{S}_{12}\tilde{S}_{22}^{-1}\tilde{u}_2 | \bar{B}, \tilde{u}_2, \tilde{S}_{22}\right] = (1 + \tilde{u}_2'\tilde{S}_{22}^{-1}\tilde{u}_2)I_a = (1 + \tilde{R})I_a$$

and so the conditional distribution of $((n-p+1)/q)(\tilde{Q}/(1+\tilde{R}))$ given \bar{B} and \tilde{R} is non-central F with q and n-p+1 degrees of freedom and non-centrality parameter

(3.4)
$$\lambda = (1 + \tilde{R})^{-1} \tilde{x}' (\bar{B} - B_0) P_{\bar{R}} (\bar{B} - B_0)' \tilde{x} = (1 + \tilde{R})^{-1} \lambda^*.$$

say. The above results agree with Fujikoshi and Nishii [7]. These authors proceeded to develop the asymptotic expansion of the unconditional distribution of Q in terms of central chi-squared distributions. In the present paper we shall consider a rather simpler approach to the unconditional distributions of Q and R in terms of central F-distributions. This is based on the distribution of non-central F with ν_1 and ν_2 degrees of freedom and non-centrality parameter τ (Tiku [12]),

$$(3.5) P\{F_{\nu_{1},\nu_{2}}(\tau) \leq F\} = \Phi_{\nu_{1},\nu_{2}}(F) + \phi_{\nu_{1},\nu_{2}}(F) \sum_{r=1}^{\infty} \frac{(-\tau/2)^{r}}{r!} \sum_{j=0}^{r-1} (-1)^{j} {r-1 \choose j} \cdot \frac{((\nu_{1}+\nu_{2})/2)_{j}(\nu_{1}/\nu_{2})^{j}F^{j+1}}{(\nu_{1}/2)_{j+1}(1+(\nu_{1}/\nu_{2})F)^{j}}$$

where $(a)_j = a(a+1)\cdots(a+j-1)$, and $\Phi_{\nu_1,\nu_2}(F)$ and $\phi_{\nu_1,\nu_2}(F)$ are the cumulative distribution function and probability density function, respectively, of a central F variable with ν_1 and ν_2 degrees of freedom.

The unconditional distribution of \tilde{R} is seen to require the evaluation of moments $\overline{\mu^r} = E_{\bar{B}}[\mu^r]$, where μ is defined by (3.2), while for the unconditional distribution of \tilde{Q} we have

$$(3.6) P\left\{\frac{n-p+1}{q}\tilde{Q} \leq F|\bar{B}, \tilde{R}\right\} = P\left\{F_{q,n-p+1}(\lambda) \leq F+F\Delta\right\}$$

where $\Delta = 1/(1+R)-1$. If we were to substitute in (3.5) and carry out a Taylor expansion in terms of Δ , we should require terms

$$E\left[\frac{\lambda^r}{(1+\tilde{R})^s}\right] = E_{\bar{B}}\left[\lambda^{*r}E\left[\frac{1}{(1+\tilde{R})^{r+s}}\middle|\bar{B}\right]\right].$$

Since

$$E\left[\frac{1}{(1+\tilde{R})^s}\Big|\,\bar{B}\,
ight] = \frac{((n-(p-q)+1)/2)_s}{((n+1)/2)_s} {}_{\scriptscriptstyle 1}F_{\scriptscriptstyle 1}\!\!\left(s, \frac{n+1}{2}\!+\!s\,;\, -\frac{1}{2}\,\mu
ight)$$
 ,

where $_{1}F_{1}$ denotes the confluent hypergeometric function, we ultimately require the product moments

(3.7)
$$\zeta_{rs} = E_{\bar{B}}(\lambda^{*r}\mu^{s}), \quad r, s = 0, 1, 2, \cdots.$$

Fujikoshi and Nishii [7] obtained asymptotic expansions of early ζ_{rs} to order N^{-2} , using the perturbation method. In the next section we

shall consider the general case.

4. The Laplace transform of ζ_{rs}

Setting

$$U = \bar{B}'(X'X)^{1/2}$$
, $U_0 = B'_0(X'X)^{1/2}$, $\Psi = (X'X)^{-1/2}\tilde{x}\tilde{x}'(X'X)^{-1/2}$.

we have

(4.1)
$$\zeta_{rs} = (2\pi)^{-pq/2} \int_{U} \operatorname{etr} \left\{ -\frac{1}{2} (U - U_0)'(U - U_0) \right\} C_{[r]} \{ P_U(U - U_0) \Psi(U - U_0)' \}$$

$$\cdot C_{[s]} (\bar{P}_U U_0 \Psi U_0') dU$$

where $C_{[r]}(A)$ is the zonal polynomial (James [11]) corresponding to the partition [r] of the integer r into a single part, noting that rank $\Psi=1$.

We first show that ζ_{r} is a function of $U_0'U_0$. Let $U_0 = H_1(U_0'U_0)^{1/2}$, $H = [H_1, H_2] \in O(p)$, and $V = H'U = [V_1', V_2']'$. Then

which is a function of $U_0'U_0$.

We now consider the Laplace transform $L_{r,s}(W/2)$ of $|U_0'U_0|^{(p-q-1)/2}\zeta_{rs}$ with respect to $U_0'U_0$. This may be written as an integral with respect to U_0 ,

$$egin{split} L_{r,s}\!\left(rac{1}{2}W
ight) &= c \int_{U_0} \mathrm{etr} \left(-rac{1}{2}WU_0'U_0
ight) &\zeta_{rs}(U_0'U_0) dU_0 \ &= (2\pi)^{-pq/2} c \int_{U_0} \int_{U} \mathrm{etr} \left\{-rac{1}{2}WU_0'U_0 - rac{1}{2}(U-U_0)'(U-U_0)
ight\} \ &\cdot C_{[r]}(\cdot) C_{[s]}(\cdot) dU_0 dU \,, \end{split}$$

where $c=\pi^{-pq/2}\Gamma_q(p/2)$ and the arguments of the zonal polynomials are as in (4.1). If we complete the square and let

$$Z = \{U_0 - U(I+W)^{-1}\}(I+W)^{1/2}, \qquad V = U\left(\frac{W}{I+W}\right)^{1/2},$$
 $\Psi^* = (I+W)^{-1/2}\Psi(I+W)^{-1/2}.$

then

$$L_{r,\imath}\!\!\left(\!\frac{1}{2}W\right)\!=\!(2\pi)^{pq/2}c\,|\,W|^{-p/2}\int\int {\rm etr}\left(-\frac{1}{2}Z'Z\!-\!\frac{1}{2}V'V\right)\,.$$

$$\cdot C_{[r]} \{ P_{V}(Z - VW^{1/2}) \varPsi * (Z - VW^{1/2})' \}$$

 $\cdot C_{[s]} \{ \bar{P}_{V}Z \varPsi * Z') dZ dV .$

Making the transformation $V=H_1(V'V)^{1/2}$, $H=[H_1, H_2] \in O(p)$, we have

$$egin{aligned} P_{v} = & H_{1}H_{1}' \;, \qquad ar{P}_{v} = & H_{2}H_{2}' \;, \qquad ext{and} \ & L_{r,s} \Big(rac{1}{2}W\Big) = & (2\pi)^{-pq/2} |W|^{-p/2} \int \int \int \operatorname{etr} \Big(-rac{1}{2}Z'Z - rac{1}{2}V'V\Big) |V'V|^{(p-q-1)/2} \ & \cdot C_{[r]} [\{H_{1}'Z - (V'V)^{1/2}W^{1/2}\}\varPsi * \{H_{1}'Z - (V'V)^{1/2}W^{1/2}\}'] \ & \cdot C_{r,s} (H_{s}'Z\varPsi * Z'H_{s}) dZ d(V'V) dH \;. \end{aligned}$$

where dH is the invariant Haar measure on O(p). Putting

$$X=H'Z=\begin{bmatrix}H_1'Z\\H_2'Z\end{bmatrix}=\begin{bmatrix}X_1\\X_2\end{bmatrix}_{p-q}^q$$

the integral is decomposed into three factors,

$$egin{aligned} L_{r,s}(W/2) &= (2\pi)^{-pq/2} |W|^{-p/2} \int \operatorname{etr} \left(-V'V/2\right) |V'V|^{(p-q-1)/2} d(V'V) \\ & \cdot \int \operatorname{etr} \left(-X_2'X_2/2\right) C_{[s]}(X_2'X_2 \mathcal{F}^*) dX_2 \\ & \cdot \int \operatorname{etr} \left(-X_1'X_1/2\right) C_{[r]} [\{X_1 - (V'V)^{1/2} W^{1/2}\} \mathcal{F}^* \\ & \cdot \{X_1 - (V'V)^{1/2} W^{1/2}\}'] dX_1 \ . \end{aligned}$$

Using Constantine's [2] result on the Laplace transform of a zonal polynomial, and Hayakawa's [9] definition of the polynomial $P_{\epsilon}(T, A)$, we obtain

$$egin{split} L_{r,s}\!\left(rac{1}{2}W
ight) &= 2^{r+s}\!\left(rac{p-q}{2}
ight)_{\!s}\!|W|^{-p/2}C_{\![s]}\!({f T}^*)\int \mathrm{etr}\left(-rac{1}{2}V'V
ight)\!|V'V|^{(p-q-1)/2} \ &\cdot \left\{(-2)^rP_{[r]}\!\left(rac{1}{\sqrt{2}\,i}(V'V)^{1/2}W^{1/2},\,{f T}^*
ight)
ight\}\!d(V'V) \;. \end{split}$$

 P_{ϵ} may be expanded in terms of a class of invariant polynomials $C_{\epsilon}^{i,\lambda}(X,Y)$ with two matrix arguments using equation (4.2) of Davis [6]. Thus finally

$$(4.2) \qquad L_{r,s}\left(\frac{1}{2}W\right) = \Gamma_{q}\left(\frac{1}{2}p\right)2^{r+s}\left(\frac{q}{2}\right)_{r}\left(\frac{p-q}{2}\right)_{s}\left|\frac{1}{2}W\right|^{-p/2}C_{[s]}(\mathcal{T}(I+W)^{-1}) \\ \qquad \qquad \cdot \sum_{j=0}^{r}\binom{r}{j}\left(\frac{p}{2}\right)_{j}C_{r}^{r-j,j}(\mathcal{T}(I+W)^{-1},\mathcal{T}W(I+W)^{-1})/\left(\frac{q}{2}\right)_{j}.$$

5. Inversion of the Laplace transform

The asymptotic expansions of Fujikoshi and Nishii [7] assumed that

$$\frac{1}{m}X'X=\theta=O(1) ,$$

where m=n-p-1. Thus we require to invert $L_{r,s}(W/2)$ to obtain an asymptotic expansion of ζ_{rs} for large values of $U_0'U_0=m\Theta^{1/2}B\Omega^{-1}B'\Theta^{1/2}$, noting also that $\mathcal{T}=m^{-1}\Theta^{-1/2}\tilde{x}\tilde{x}'\Theta^{-1/2}$.

Considering first the moments of μ , it follows from Davis [6] equation (6.19) that for $W < I_q$,

$$(5.1) L_{0,s}\left(\frac{1}{2}W\right) = \Gamma_{q}\left(\frac{1}{2}p\right)2^{s}\left(\frac{p-q}{2}\right)_{s}\left|\frac{1}{2}W\right|^{-p/2}C_{[s]}(\varPsi(I+W)^{-1})$$

$$= \Gamma_{q}\left(\frac{1}{2}p\right)2^{s}\left(\frac{p-q}{2}\right)_{s}\left|\frac{1}{2}W\right|^{-p/2}$$

$$\cdot \sum_{k=0}^{\infty} \sum_{s} \sum_{\phi \in \epsilon + s} \psi_{s}^{\phi}\theta_{\phi}^{\epsilon,s}C_{\phi}^{\epsilon,s}(-W, \varPsi)/k!$$

where $\theta_{\phi}^{\epsilon,\lambda} = C_{\phi}^{\epsilon,\lambda}(I, I)/C_{\phi}(I)$ and for a partition $\phi = [f_1, f_2, \dots, f_q], f_1 \ge f_2 \ge \dots \ge f_q \ge 0$,

$$\psi_{s}^{\phi} = \lim_{\beta \to 0} \frac{(\beta)_{\phi}}{(\beta)_{s}} = \frac{(f_{1} - 1)!}{(s - 1)!} \prod_{i=1}^{q-1} \left(-\frac{1}{2}i \right)_{f_{i+1}}$$

which is zero if $f_3 \ge 2$. The notation " $\phi \in \kappa \cdot s$ " means that the irreducible representation $[2\phi]$ of the real linear group of nonsingular matrices occurs in the decomposition of the Kronecker product $[2\kappa] \otimes [2s]$ into irreducible representations.

Formally inverting (5.1) by the analogue of Constantine [3] equation (10) for invariant polynomials, we obtain the asymptotic expansion of $\overline{\mu^s} = E_{\bar{B}}[\mu^s]$ for large m,

$$(5.2) \quad \overline{\mu^{\mathfrak{s}}} \sim 2^{\mathfrak{s}} \left(\frac{p-q}{2}\right)_{\mathfrak{s}} \sum_{k=0}^{\infty} \sum_{\mathfrak{s}} \sum_{\phi \in \mathfrak{s}, \mathfrak{s}} 2^{k} \left(\frac{q+1-p}{2}\right)_{\mathfrak{s}} \psi_{\mathfrak{s}}^{\phi} \theta_{\phi}^{\mathfrak{s}, \mathfrak{s}} C_{\phi}^{\mathfrak{s}, \mathfrak{s}} ((U_{0}U_{0})^{-1}, \boldsymbol{\varPsi})/k!$$

$$\sim 2^{\mathfrak{s}} \left(\frac{p-q}{2}\right)_{\mathfrak{s}} \sum_{k=0}^{\infty} \sum_{\mathfrak{s}} \sum_{\phi \in \mathfrak{s}, \mathfrak{s}} 2^{k} \left(\frac{q+1-p}{2}\right)_{\mathfrak{s}} \psi_{\mathfrak{s}}^{\phi} \theta_{\phi}^{\mathfrak{s}, \mathfrak{s}}$$

$$\cdot C_{\mathfrak{s}, \mathfrak{s}}^{\mathfrak{s}} ((\boldsymbol{\Theta}^{1/2}B\Omega^{-1}B'\boldsymbol{\Theta}^{1/2})^{-1}, \boldsymbol{\Theta}^{-1/2} \tilde{x} \tilde{x}' \boldsymbol{\Theta}^{-1/2})/m^{k+s} k! = O(m^{-s}).$$

The question arises as to the validity of this procedure, which inverts an expansion of the Laplace transform for small argument to yield an asymptotic expansion of the required function for large argument. In particular, Constantine's result has only been derived for $k_1 < (p-q+1)/2$, where $\kappa = [k_1, k_2, \dots, k_q]$. In the univariate situation, the procedure may be justified under certain conditions by Watson's lemma for loop integrals (Davies [5], Section 6.3). A multivariate extension for this result is obviously highly desirable, but remains to be proved.

An alternative approach is to note that in virtue of its product

form, $L_{0,s}$ may be regarded as the limit as $\beta \rightarrow 0$ of the Laplace transform of the convolution (Constantine [2]).

$$\begin{split} & \left[\left(\frac{p-q}{2} \right)_{s} \middle/ 2^{\beta q/2} \varGamma_{q}(\beta)(\beta)_{s} \right] \int_{0 < Z < U_{0}'U_{0}} |U_{0}'U_{0} - Z|^{(p-q-1)/2} \\ & \cdot \operatorname{etr} \left(-\frac{1}{2} Z \right) |Z|^{\beta - (q+1)/2} C_{[s]}(\varPsi Z) dZ \; . \end{split}$$

The expansion (5.2) may be derived from (5.3) by a similar procedure to Constantine and Muirhead [4], Theorem 3.2. It should of course be observed that the integral (5.3) is convergent only for $\beta > (q-1)/2$, but it is reasonable to argue that (5.2) holds by analytic continuation.

It is difficult to give an explicit expansion of $\zeta_{r,t}$ in general, but since (4.2) may be developed in a series of $C_{\xi}^{r,t}(W, \mathbb{F})$, the early terms may be derived by formal inversion. The results agree with those of Fuji-koshi and Nishii [7], Section 5, Lemma 1. In particular, the tables of Davis [6] may be used to obtain, to $o(m^{-3})$,

$$\begin{split} \overline{\mu} &= \frac{1}{m} (p-q) \widetilde{x}' \theta^{-1} \widetilde{x} - \frac{1}{m^2} (p-q) (p-q-1) \widetilde{x}' (\theta B \mathcal{Q}^{-1} B' \theta)^{-1} \widetilde{x} \\ &+ \frac{1}{m^3} (p-q) (p-q-1) [(p-q-2) \widetilde{x}' (\theta B \mathcal{Q}^{-1} B' \theta B \mathcal{Q}^{-1} B' \theta)^{-1} \widetilde{x} \\ &- \widetilde{x}' (\theta B \mathcal{Q}^{-1} B' \theta)^{-1} \widetilde{x} \cdot \operatorname{tr} \left(B \mathcal{Q}^{-1} B' \theta^{-1} \right)] \end{split} ,$$

$$\begin{split} (5.4) \qquad \overline{\mu^{2}} &= \frac{1}{m^{2}} (p-q) (p-q+2) (\tilde{x}' \theta^{-1} \tilde{x})^{2} - \frac{2}{m^{3}} (p-q) (p-q+2) \\ &\qquad \cdot (p-q-1) \tilde{x}' (\theta B \Omega^{-1} B' \theta)^{-1} \tilde{x} \cdot \tilde{x}' \theta^{-1} \tilde{x} \ , \\ \overline{\mu^{3}} &= \frac{1}{m^{3}} (p-q) (p-q+2) (p-q+4) (\tilde{x}' \theta^{-1} \tilde{x})^{3} \ . \end{split}$$

6. Percentile expansions

From (3.5) writing $\nu_1=p-q$, $\nu_2=n-(p-q)+1$, we have

$$\begin{split} P\left\{\frac{\nu_{2}}{\nu_{1}}\tilde{R} \leq F\right\} = & \varPhi_{\nu_{1},\nu_{2}}(F) + \varPhi_{\nu_{1},\nu_{2}}(F) \\ & \cdot \left[-\frac{\bar{\mu}}{\nu_{1}}F + \frac{\bar{\mu}^{2}}{4}\left\{\frac{F}{\nu_{1}} - \frac{(\nu_{1} + \nu_{2})F^{2}}{\nu_{2}(\nu_{1} + 2)(1 + (\nu_{1}/\nu_{2})F)}\right\} \right] + o(m^{-2}) \; . \end{split}$$

Using (5.4) and the general inverse expansion of Hill and Davis [10] we obtain for the upper α -point of \tilde{R} .

$$\frac{n-(p-q)+1}{(p-q)}\tilde{R}_{\alpha} = F_{1,\alpha} \left\{ 1 + \frac{1}{m} \tilde{x}' \Theta^{-1} \tilde{x} - \frac{1}{m^2} (p-q-1) \right\}$$

$$\left.\cdot \ \widetilde{x}'(\Theta B \Omega^{-1} B' \Theta)^{-1} \widetilde{x} \right\} + o(m^{-2})$$
 ,

where $F_{1,\alpha} = F_{p-q,n-(p-q)+1}(\alpha)$. Hence

(6.1)
$$\frac{n-(p-q)+1}{(p-q)}R_{\alpha} = F_{1,\alpha} \left\{ \sigma^{2}(x) - \frac{1}{m^{2}} (p-q-1)x'(\Theta B \Omega^{-1} B' \Theta)^{-1} x \right\} + o(m^{-2}),$$

where $\sigma^2(x)$ was defined in (2.3). The unknown parameters B and Ω occur in the $O(m^{-2})$ term, which vanishes when p=q+1. In practical use, they may be replaced by their estimates. Equation (6.1) may be compared with the approximation suggested by Williams [13].

$$\frac{n-p+1}{p-q}R_{\alpha}\approx\sigma^{2}(x)F_{p-q,n-p+1}(\alpha).$$

Similarly, from (3.6),

$$\begin{split} P\left\{\frac{\nu_2}{\nu_1}\tilde{Q} \!\leq\! F\right\} &= \varPhi_{\nu_1,\nu_2}(F) \!+\! \phi_{\nu_1,\nu_2}\!(F) \Big[F\Big(\overline{\boldsymbol{J}} \!-\! \frac{\overline{\boldsymbol{\lambda}}}{\nu_1}\Big) \!+\! F\Big(\!\frac{1}{4}\,\overline{\boldsymbol{\lambda}}^2 \!-\! \overline{\boldsymbol{\lambda}}\overline{\boldsymbol{J}}\Big)\Big/\nu_1 \\ &+ F^2\Big\{\!\frac{\phi'}{\phi}\Big(\!\frac{1}{2}\,\overline{\boldsymbol{J}}^2 \!-\! \frac{\overline{\boldsymbol{\lambda}}\overline{\boldsymbol{J}}}{\nu_1}\Big) \!-\! \frac{\overline{\boldsymbol{\lambda}}^2(\nu_1\!+\!\nu_2)}{4\nu_2(\nu_1\!+\!2)(1\!+\!(\nu_1\!/\nu_2)F)}\!\Big\}\,\Big] \\ &+ o(m^{-2}) \ , \end{split}$$

where $\nu_1 = q$, $\nu_2 = n - p + 1$. To $o(m^{-2})$,

$$\begin{split} \overline{\lambda} &= \frac{1}{m} q \widetilde{x}' \Theta^{-1} \widetilde{x} + \frac{1}{m^2} (p-q) \{ -q \widetilde{x}' \Theta^{-1} \widetilde{x} + (p-q-1) \widetilde{x}' (\Theta B \mathcal{Q}^{-1} B' \Theta)^{-1} \widetilde{x} \} \;, \\ \overline{\lambda}^2 &= \frac{1}{m^2} q (q+2) (\widetilde{x}' \Theta^{-1} \widetilde{x})^2 \;, \\ \overline{\mathcal{A}} &= -\frac{1}{m} (p-q) + \frac{1}{m^2} (p-q) (p+2-\widetilde{x}' \Theta^{-1} \widetilde{x}) \;, \\ \overline{\mathcal{A}}^2 &= \frac{1}{m^2} (p-q) (p-q+2) \;, \\ \overline{\lambda} \overline{\mathcal{A}} &= \overline{\lambda} \overline{\mathcal{A}} &= -\frac{1}{m^2} q (p-q) \widetilde{x}' \Theta^{-1} \widetilde{x} \;, \end{split}$$

and we obtain from the inversion formula

(6.2)
$$\frac{n-p+1}{q}Q_{\alpha} = F_{2,\alpha} \left[\sigma^{2}(x) + \frac{1}{m} (p-q) + \frac{1}{m^{2}} (p-q) \right] \cdot \left\{ x' \theta^{-1} x + \frac{1}{2} q (F_{2,\alpha} - 3) + \frac{(p-q-1)}{q} \right\}$$

$$\cdot x'(\Theta B \Omega B'\Theta)^{-1}x$$
 $\Big\}\Big]+o(m^{-2})$,

where $F_{2,\alpha} = F_{q,n-p+1}(\alpha)$. Williams [13] gave

$$\frac{n-p+1}{q}Q_{\scriptscriptstyle\alpha}\!\approx\!\sigma^{\scriptscriptstyle2}(x)F_{\scriptscriptstyle2,\alpha}\;.$$

Equation (6.2) reduces to the exact result for T^2 when p=q, and is simpler in form than Fujikoshi and Nishii [7] equation (4.10). Again, the unknown parameters occur in the $O(m^{-2})$ term, and may be replaced by their estimates for the construction of confidence regions.

When a and B are known, let Q^* denote the statistic Q with \overline{y} and \hat{B} replaced by a and B, respectively. Corresponding to Fujikoshi and Nishii (equation (3.4)) it may be shown that

| Table 1. Comparison of approximations to | nQ_{*}^{*} | for | $\alpha = 0.05$ | 0.01 |
|------------------------------------------|--------------|-----|-----------------|------|
|------------------------------------------|--------------|-----|-----------------|------|

| | | | • | | · · · · · · | • |
|---|---|----|----------------------|------------|-------------|-----------------|
| p | q | n | Fujikoshi- Nishii | Eqn. (6.3) | Eqn. (6.4) | Exact |
| 2 | 1 | 20 | 6.259 | 6.265 | 6.161 | 6.237 |
| | | | 11.898 | 12.082 | 11.626 | 11.918 |
| | | 35 | 4.985 | 4.985 | 4.963 | 4.982 |
| | | | 9.036 | 9.056 | 8.971 | 9.040 |
| | 2 | 20 | 9.530 | 9.547 | 9.445 | 9.489 |
| | | | 16.302 | 16.570 | 16.073 | 16. 29 7 |
| | | 35 | 7.675 | 7.676 | 7.657 | 7.668 |
| | | | 12.458 | 12.487 | 12.403 | 12.455 |
| 4 | 2 | 20 | 17.720 | 17.984 | 17.114 | 17.386 |
| | | | 31.291 | 34.626 | 30.135 | 31.548 |
| | | 35 | 10.217 | 10.229 | 10.141 | 10.193 |
| | | | 16.761 | 16.954 | 16.553 | 16.792 |
| | 4 | 20 | 25.849 | 26.263 | 25.583 | 25.176 |
| | | | 42.357 | 42.292 | 41.889 | 42.021 |
| | | 35 | 15.520 | 15.532 | 15.509 | 15.467 |
| | | | 23.384 | 23.642 | 23.280 | 23.374 |
| | 6 | 20 | 31.072 | 31.245 | 31.051 | 30.347 |
| | | | 49.149 | 53.126 | 49.211 | 48.538 |
| | | 35 | 19.614 | 19.606 | 19.650 | 19.552 |
| | | | 28.347 | 28.538 | 28.347 | 28.313 |

The upper figures are for $\alpha=0.05$ and the lower figures are for $\alpha=0.01$.

(6.3)
$$\frac{n-p+1}{q} Q_{\alpha}^* = F_{2,\alpha} \left[1 + \frac{(p-q)}{m} + \frac{1}{m^2} (p-q) \left\{ \frac{1}{2} q(F_{2,\alpha} - 3) - 1 \right\} \right] + o(m^{-2}) .$$

As shown in Table 1, the approximation (6.3) is generally less accurate than Fujikoshi and Nishii's result, obtained from their Table 1. However, the $O(N^{-1})$ approximation

(6.4)
$$\frac{n-p+1}{q}Q_a^* \approx \frac{n-q+1}{n-p+1}F_{2,a},$$

obtained by reexpressing (6.3) as an expansion in $(n-p+1)^{-1}$, is very simple in form. It is considerably more accurate than Fujikoshi and Nishii's $O(m^{-1})$ approximation, and sometimes performs better than their $O(m^{-2})$ result. An approximation for $q^{-1}(n-p+1)Q_a$ may be obtained by multiplying (6.4) by $(1+N^{-1})$ and adding the terms involving x in (6.2).

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REFERENCES

- [1] Brown, P. J. (1982). Multivariate calibration, J. R. Statist. Soc., B44, 287-321.
- [2] Constantine, A. G. (1963). Some non-central distribution problems in multivariate analysis. Ann. Math. Statist., 34, 1270-1285.
- [3] Constantine, A. G. (1966). The distribution of Hotelling's generalized T_0^2 , Ann. Math. Statist., 37, 215-225.
- [4] Constantine, A. G. and Muirhead, R. J. (1976). Asymptotic expansions for distributions of latent roots in multivariate analysis, J. Multivar. Anal., 6, 369-391.
- [5] Davies, B. (1978). Integral Transforms and Their Applications, Springer-Verlag, New York.
- [6] Davis, A. W. (1979). Invariant polynomials with two matrix arguments extending the zonal polynomials: applications to multivariate distribution theory, Ann. Inst. Statist. Math., 31, 465-485.
- [7] Fujikoshi, Y. and Nishii, R. (1984). On the distribution of a statistic in multivariate inverse regression analysis, *Hiroshima J. Math.*, 14, 215-225.
- [8] Gleser, L. J. and Olkin, I. (1972). Estimation for a regression model with unknown covariance matrix, Proc. Sixth Berkeley Symp. Math. Statist. Prob., 1, 541-568.
- [9] Hayakawa, T. (1969). On the distribution of the latent roots of a positive definite random symmetric matrix I, Ann. Inst. Statist. Math., 21, 1-21.
- [10] Hill, G. W. and Davis, A. W. (1968). Generalized asymptotic expansions of Cornish-Fisher type, Ann. Math. Statist., 39, 1264-1273.
- [11] James, A. T. (1964). Distributions of matrix arguments and latent roots derived from normal samples, Ann. Math. Statist., 35, 475-501.
- [12] Tiku, M. L. (1965). Laguerre series forms of non-central χ² and F distributions, Biometrika, 52, 415-427.
- [13] Williams, E. J. (1959). Regression Analysis, Wiley, New York.
- [14] Wood, J. T. (1982). Estimating the age of an animal; an application of multivariate calibration, to appear in *Proc. 11th Internat. Bio. Conf.*, 1982.