ON THE MOMENTS OF THE TRACE OF A MATRIX AND APPROXIMATIONS TO ITS NON-CENTRAL DISTRIBUTION

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1. Introduction and summary. Let $\mathbf{A}_1$ and $\mathbf{A}_2$ be two symmetric matrices of order p, $\mathbf{A}_1$, positive definite and having a Wishart distribution [2], [18] with f_1 degrees of freedom and $\mathbf{A}_2$, at least positive semi-definite and having a (pseudo) non-central (linear) Wishart distribution [1], [3], [5], [18], [19] with f_2 degrees of freedom. Now let

$$\mathbf{A}_2 = \mathbf{CYY'C'}$$

where $\mathbf{Y}$ is $p \times f_2$ and $\mathbf{C}$ is a lower triangular matrix such that

$$\mathbf{A}_1 + \mathbf{A}_2 = \mathbf{CC'}.$$

Now consider the $s(=\text{minimum } (f_2, p))$ non-zero characteristic roots of the matrix $\mathbf{YY'}$. It can be shown that the density function of the characteristic roots of $\mathbf{Y'Y}$ for $f_2 \leqq p$ can be obtained from that of the characteristic roots of $\mathbf{YY'}$ for $f_2 \geqq p$ if in the latter case the following changes are made [6], [18]:

$$(f_1, f_2, p) \to (f_1 + f_2 - p, p, f_2). \tag{1.1}$$

Now define $U^{(s)} = \text{tr}\,(\mathbf{I}_p - \mathbf{YY'})^{-1} - p = \text{tr}\,(\mathbf{I}_{f_2} - \mathbf{Y'Y})^{-1} - f_2$. In view of (1.1), we only consider $U^{(s)}$ when $s = p$, i.e. $U^{(p)}$, based on the density function [9] of $\mathbf{L} = \mathbf{YY'}$ for $f_2 \geqq p$. The first four moments of $U^{(s)}$ have been studied by Pillai in the central case [11], [12], [13], [14], [17] those for $U^{(2)}$ also by Pillai [15] in the non-central (linear) case and the first two moments of $U^{(p)}$ by the authors [7]. These results are extended in the present paper, obtaining the third and fourth moments of $U^{(p)}$ and further, two approximations to the distribution of $U^{(p)}$ are suggested in the linear case.

2. Moments of $U^{(p)}$. In the previous paper by the authors [7] it has been shown that

$$1 + U^{(p)} = \{(1 - l_{11})(1 - \mathbf{u'u})\}^{-1} + (1 - \mathbf{u'u})^{-1}(\mathbf{u'Mu}) + \text{tr}\,\mathbf{M} \tag{2.1}$$

where l_{11}, $\mathbf{u}$: $(p-1) \times 1$ and $\mathbf{M}$ are independently distributed and their respective distributions are given by

$$\exp(-\lambda^2) \textstyle\sum_{j=0}^{\infty} [(\lambda^2)^j/j!]\{l_{11}^{\frac{1}{2}f_2+j-1}(1 - l_{11})^{\frac{1}{2}f_1-1}/\beta[\tfrac{1}{2}f_2 + j, \tfrac{1}{2}f_1]\}\, dl_{11} \tag{2.2}$$

$$[\Gamma(\tfrac{1}{2}f_1)/\{\Pi^{\frac{1}{2}(p-1)}\Gamma[\tfrac{1}{2}(f_1 - p + 1)]\}](1 - \mathbf{u'u})^{\frac{1}{2}(f_1-p+1)-1}\, d\mathbf{u} \tag{2.3}$$

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and

(2.4) $\prod_{i=1}^{p-1} \{\Gamma[\frac{1}{2}(f_1 + f_2 - i)]/\Gamma[\frac{1}{2}(f_1 - i + 1)]\Gamma[\frac{1}{2}(f_2 - i)]\}$

$$\cdot[|\mathbf{M}|^{\frac{1}{2}[f_2-1-(p-1)-1]}/\Pi^{\frac{1}{4}(p-1)(p-2)}|\mathbf{I}_{p-1} + \mathbf{M}|^{\frac{1}{2}(\nu-1)}]\, d\mathbf{M},$$

where

$$\mathbf{M} = (\mathbf{I}_{p-1} - \mathbf{L}_{22})^{-1} - \mathbf{I}_{p-1}, \qquad \mathbf{L}_{22} = \mathbf{L}_{11} - \mathbf{l}\mathbf{l}'/l_{11},$$

$$\mathbf{L} = \begin{pmatrix} l_{11} & \mathbf{l}' \\ \mathbf{l} & \mathbf{L}_{11} \end{pmatrix} \quad \text{and} \quad \nu = f_1 + f_2,$$

where $\mathbf{l}$ is $(p - 1) \times 1$ and $\mathbf{L}_{11}$ is $(p - 1) \times (p - 1)$. Now note that (2.3) is invariant under an orthogonal transformation of $\mathbf{u}$, $x_i = u_i^2/(1 - u_1^2 - \cdots - u_{i-1}^2)$, $i = 1, 2, \cdots, p - 1$, $u_0 = 0$, is distributed as [7]

(2.5) $$g_i(x_i) = \{\beta[\tfrac{1}{2}, \tfrac{1}{2}(f_1 - i)]\}^{-1} x_i^{\frac{1}{2}-1}(1 - x_i)^{\frac{1}{2}(f_1-i)-1},$$

and $x_1, \cdots, x_{p-1}$ are independent. Further, define $\alpha = 1/(1 - \mathbf{u}'\mathbf{u})$ and $\beta = \text{tr}\,\mathbf{M} + \mathbf{u}'\mathbf{M}\mathbf{u}/(1 - \mathbf{u}'\mathbf{u})$. Then, computing $E(\alpha^i)$, $i = 1, 2, 3, 4$, $E(\alpha^i\beta)$, $i = 1, 2, 3$, $E(\alpha^i\beta^2)$, $i = 1, 2$, $E(\alpha\beta^3)$ and $E(1 - l_{11})^{-i} - E(1 - l_{11,0})^{-i}$, $i = 1, 2, 3, 4$ (where $l_{11,0}$ is a variate whose distribution is the same as that of l_{11} when $\lambda = 0$ and independently distributed of $\mathbf{u}$ and $\mathbf{M}$), we can obtain the first four moments of $U^{(p)}$. It may be pointed out that $E(\alpha^i\beta)$ involves $E(\text{tr}\,\mathbf{M})$, $E(\alpha^i\beta^2)$ involves $E(\text{tr}\,\mathbf{M})^2$ and $E(\text{tr}_2\,\mathbf{M})$, $E(\alpha\beta^3)$, $E(\text{tr}\,\mathbf{M})^3$, $E[(\text{tr}\,\mathbf{M})(\text{tr}_2\,\mathbf{M})]$ and $E(\text{tr}_3\,\mathbf{M})$, where $\text{tr}_i\,\mathbf{M}$ denotes the ith elementary symmetric function in the $(p - 1)$ characteristic roots of $\mathbf{M}$. All these results are available in [8].

Expressions for the first two moments of $U^{(p)}$ have been presented in the previous paper by the authors [7]. For the third and fourth moments we get:

(2.6) $$E(1 + U^{(p)})^3 = E(1 + U_0^{(p)})^3 + A_1(2\lambda^2)^3 + 3A_2(2\lambda^2)^2 + 3A_3(2\lambda^2)$$

where

(2.7) $$A_1 = \eta_3^{(0)} = [(f_1 - p - 1)(f_1 - p - 3)(f_1 - p - 5)]^{-1},$$

(2.8) $$A_2 = (\nu - 2)\eta_3^{(0)} + \eta_2^{(1)},$$

where

(2.9) $$\eta_2^{(1)} = (p - 1)(f_2 - 1)(f_1 - p - 4)A_1/(f_1 - p),$$

(2.10) $$A_3 = (\nu - 2)(\nu - 4)\eta_3^{(0)} + 2(\nu - 2)\eta_2^{(1)} + \eta_1^{(2)},$$

where

(2.11) $$\begin{aligned}\eta_1^{(2)} = {} & [(p - 1)(f_2 - 1)/(f_1 - p - 3)(f_1 - p + 1)(f_1 - p)] \\ & \cdot\{(p - 2)(f_2 - 1) + [(f_2 + 1)(f_1 - 1)/(f_1 - p - 2)] \\ & + [(p + 1)(f_2 + 1)(f_1 - p + 1)/ \\ & (f_1 - p - 1)(f_1 - p - 2)(f_1 - p - 5)]\}.\end{aligned}$$

Similarly

$$(2.12)\quad E(1+U^{(p)})^4 = E(1+U_0^{(p)})^4 + B_1(2\lambda^2)^4 + 4B_2(2\lambda^2)^3 + 6B_3(2\lambda^2)^2 + 4B_4(2\lambda^2),$$

where

$$(2.13)\quad B_1 = \eta_4^{(0)} = A_1/(f_1-p-7)$$

$$(2.14)\quad B_2 = (\nu-2)\eta_4^{(0)} + \eta_3^{(1)}$$

where

$$(2.15)\quad \eta_3^{(1)} = (p-1)(f_2-1)(f_1-p-6)B_1/(f_1-p)$$

$$(2.16)\quad B_3 = (\nu-2)(\nu-4)\eta_4^{(0)} + 2(\nu-2)\eta_3^{(1)} + \eta_2^{(2)}$$

where

$$(2.17)\quad \begin{aligned}\eta_2^{(2)} = \{&[(f_1-p-4)(f_1-p-6)(p-1)(f_2-1)/(f_1-p)^2]\\ &\cdot[[2(f_1-1)(f_1+f_2-p-1)/(f_1-p+1)(f_1-p-2)]\\ &+(p-1)(f_2-1)] - 2(p-1)(p-2)(f_2-1)(f_2-2)/\\ &\{(f_1-p)(f_1-p+1)\}\}B_1\end{aligned}$$

$$(2.18)\quad \begin{aligned}B_4 = {}&(\nu-2)(\nu-4)(\nu-6)\eta_4^{(0)} + 3(\nu-2)(\nu-4)\eta_3^{(1)}\\ &+3(\nu-2)\eta_2^{(2)} + \eta_1^{(3)}\end{aligned}$$

where

$$(2.19)\quad \begin{aligned}\eta_1^{(3)} = \{&[(f_1-p-2)(f_1-p-4)(f_1-p-6)(p-1)(f_2-1)/\\ &(f_1-p)^3]\\ &\cdot\{[2^3(f_1-1)(f_1+f_2-p-1)(f_1+2f_2-p-2)(f_1+p-2)/\\ &(f_1-p-2)(f_1-p-4)(f_1-p+1)(f_1-p+2)]\\ &+[6(f_2-1)(f_1+f_2-p-1)(p-1)(f_1-1)/\\ &(f_1-p-2)(f_1-p+1)] + (p-1)^2(f_2-1)^2\}\\ &-[6(f_1-p-4)(p-1)(p-2)(f_2-1)(f_2-2)/\\ &(f_1-p-2)(f_1-p)(f_1-p+1)(f_1-p+2)]\\ &\cdot[\{(f_1-p)(p-1)+4\}(f_2-p-1)+2(p+1)(p+2)]\\ &+4(p-1)(p-2)(p-3)(f_2-3)(f_2-2)(f_2-1)/\\ &\{(f_1-p)(f_1-p+1)(f_1-p+2)\}\}B_1.\end{aligned}$$

3. Approximations to the distribution of $U^{(p)}$. Pillai [15] has given an approximation to the distribution of $U^{(2)}$ for $f_1 > f_2$ and which is good even for very small values of f_2. The following approximation to the distribution of $U^{(p)}$ for $f_1 > (p - 1)f_2$, based on its moments discussed in the preceding section and [7], generalizes Pillai's results for $U^{(2)}$ [15]:

$$(3.1)\quad g(U^{(p)}) = (U^{(p)})^{p_1-1}/(1 + U^{(p)}/k)^{p_1+q_1+1}k^{p_1}\beta(p_1, q_1 + 1), \quad 0 < U^{(p)} < \infty,$$

where

$$p_1 = 2q_1/\{q_1(h - 1) - 2h\},$$

$$q_1 = 2\{c^2(f_1 - p - 3)h - (c + d)^2(f_1 - p - 1)\}/\{c^2(f_1 - p - 3)(h + 1) - 2(c + d)^2(f_1 - p - 1)\}$$

$$k = c\{q_1(h - 1) - 2h\}/[2(f_1 - p - 1)],$$

$$h = (c + 1.99\, d)^3(f_1 - p - 1)/\{(c + d)^2(f_1 - p - 5)c\},$$

$$c = pf_2 + 2\lambda^2 \quad \text{and} \quad d = (f_1 + (1 - p)f_2 - 1)/(f_1 - p).$$

It may be pointed out that the case $p = 1$ is that of the non-central F [10]. Hence the accuracy of the approximation may be compared in this case with the approximation to the distribution of non-central F obtained by Patnaik and the exact distribution using Table 7 of [10]. However, it should be pointed out that the approximation to the distribution of $U^{(p)}$ in (3.1) has been suggested in this paper using the first three moments and with consideration of accuracy for $p > 1$. From some numerical comparisons made in [8], the respective exact and approximate moments were observed to be closer as p increased. Table 1 gives some idea of the accuracy of the approximation when $p = 1$. It may be observed that the approximation suggested for $U^{(1)}$ is more accurate at the upper tail end than the lower. In this case, the condition $f_1 > (p - 1)f_2$ reduces to $f_1 > 0$.

Again a comparison of the probabilities in Table 1 arouses the natural curiosity

TABLE 1

Values of $\int_0^{U^{(1)}} g(t)\,dt$ from approximate and exact distributions

f_1	f_2	λ^2	$U^{(1)}$	Probability		
				Approximate		Exact
				Eqn. (3.1)	Patnaik	
10	3	2	1.1124	.765	.752	.745
10	3	8	1.1124	.154	.203	.206
10	3	8	1.9656	.503	.520	.517
10	5	3	1.663	.738	.731	.731
10	5	3	2.818	.920	.913	.914
20	3	2	0.4647	.708	.706	.700
20	5	3	0.67775	.671	.665	.664
20	5	12	1.02575	.196	.244	.245

to attempt a generalization of Patnaik's approximation [10]. The following is such a generalization equating the first two respective moments of the exact and approximate distributions:

$$(3.2) \qquad g_1(U^{(p)}) = (U^{(p)})^{\frac{1}{2}\nu_1 - 1}/[(1 + U^{(p)}/k_1)^{\frac{1}{2}(\nu_1+\nu_2)} k_1^{\frac{1}{2}\nu_1} \beta(\tfrac{1}{2}\nu_1, \tfrac{1}{2}\nu_2)], \qquad 0 < U^{(p)} < \infty$$

where

$$k_1 = (pf_2 + 2\lambda^2)/\nu_1,$$
$$\nu_1 = (pf_2 + 2\lambda^2)^2(f_1 - p)/[(4\lambda^2 + pf_2)\{f_1 + f_2(1-p) - 1\}],$$
$$\nu_2 = f_1 - p + 1.$$

4. Further accuracy comparisons. For $p = 2$, Pillai and Jayachandran [16] have given the cdf of $U^{(2)}$ in the following form:

$$(4.1) \qquad F(U^{(2)}) = K'[\textstyle\sum_{j=0}^{6} \sum_{i=0}^{j} (-1)^{i+j} D'_{ij} B_{ij} + \cdots]$$

where $B_{ij} = \int_0^{U^{(2)}} \int_0^{u^2/4} [v^{m+i}/(1 + u + v)^{m+n+j+3}]\, dv\, du$, where $m = (f_2 - 3)/2$, $n = (f_1 - 3)/2$, and K' and D'_{ij} are functions of f_1, f_2 and λ^2 given in [16]. Now define

$$B_x(p', q') = \textstyle\int_0^x z^{p'-1}(1 - z)^{q'-1}\, dz/\beta(p', q').$$

Then the cdf from (3.1) can be written as

$$(4.2) \qquad G(U^{(2)}) = B_{x_1}(p_1, q_1 + 1),$$

where $x_1 = U^{(2)}/(k + U^{(2)})$ and the cdf from (3.2) can be written as

$$(4.3) \qquad G_1(U^{(2)}) = B_{x_2}(\tfrac{1}{2}\nu_1, \tfrac{1}{2}\nu_2),$$

where $x_2 = U^{(2)}/(k_1 + U^{(2)})$. Now $G(U^{(2)}) - F(U^{(2)})$ and $G_1(U^{(2)}) - F(U^{(2)})$ represent respectively the errors of approximations in the cdf from (3.1) and (3.2). Table 2 provides some numerical comparisons in this respect.

The values of $U^{(2)}$ and $F(U^{(2)})$ in Table 2 are taken from [16]. For $p > 2$, the method of comparison assumes the exact cdf to be a Pearson type with the first four moments the same as those of the exact. Thus using the "Table of

TABLE 2

Values of $G(U^{(2)})$, $G_1(U^{(2)})$ and $F(U^{(2)})$

f_1	f_2	λ^2	$U^{(2)}$	$G(U^{(2)})$	$G_1(U^{(2)})$	$F(U^{(2)})$
23	3	1	0.68072	.880	.877	.875
23	3	1.5	0.68072	.843	.833	.829
13	5	0.5	2.17706	.933	.932	.931
23	5	1.5	1.00707	.875	.869	.867
23	7	1	1.31973	.914	.911	.910
23	13	1.5	2.22596	.913	.912	.912

TABLE 3

Upper 5 per cent points using the exact moment quotients and the approximations (3.1) and (3.2)

p	f_1	f_2	λ^2	Percentage points		
				Eqn. (3.1)	Eqn. (3.2)	Exact
3	20	3	12.5	3.873	4.035	4.028
3	50	10	4.5	1.283	1.304	1.300
4	20	4	12.5	4.883	4.971	4.956
4	50	4	12.5	1.409	1.475	1.470
4	50	10	4.5	1.593	1.604	1.598
5	25	5	12.5	4.377	4.407	4.380
5	25	5	32	7.742	7.786	7.768

percentage points of Pearson curves for given $(\beta_1)^{\frac{1}{2}}$ and β_2, expressed in standard measure" [4], upper 5 per cent points are obtained for selected values of f_1, f_2, and λ^2, and similar upper percentage points are obtained for Approximations (3.1) and (3.2). These are presented in Table 3.

Table 2 and 3 show that Approximation (3.1) becomes closer to the exact as p increases. In fact, the moment quotients from (3.1) are closer in general to those of the exact than those from (3.2) even for $p = 1$ as shown by numerical computations in [8]. However, Approximation (3.2) still maintains its accuracy noted for $p = 1$ even for larger values of p considered in the tables above. Further, it should be pointed out that the condition $f_1 > (p - 1)f_2$ applies for both approximations.

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