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Exact Distributional Computations for Roy's Statistic and the Largest Eigenvalue of a Wishart

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Abstract Computational expressions for the exact CDF of Roy's test statistic in MANOVA and the largest eigenvalue of a Wishart matrix are derived based upon their Pfaffian representations given in Gupta and Richards (1985). These expressions allow computations to proceed until a prespecified degree of accuracy is achieved. For both distributions, convergence acceleration methods are used to compute CDF values which achieve reasonable fast run times for dimensions up to 50 and error degrees of freedom as large as 100. Software that implements these computations is described and has been made available on the Web.

Keywords Roy's test · Largest eigenvalue of a Wishart · $_2F_1$ and $_1F_1$ hypergeometric functions · Convergence acceleration

1 Introduction

This paper provides an exact computational expression for the cumulative distribution function (CDF) of the largest eigenvalue of a central matrix beta distribution. The right tail probability from this distribution is the p-value of Roy's (1945) test statistic in MANOVA and is a quantity that has proved to be very difficult to compute. Similar computational expressions are given for the CDF of the largest root of a central Wishart matrix with identity covariance which may be derived by letting the error degrees of freedom in the matrix beta expressions grow to infinity. Software for computing CDF values of both distributions to a prespecified degree of accuracy is described and has been made available on the Web.

Among the four major MANOVA tests, Roy's largest eigenvalue test and the Lawley-Hotelling test still lack p-value approximations that can be accurately computed in all settings and particularly when degrees of freedom are small or matrices have higher dimension. For the other two tests, Wilks' likelihood ratio test and the Bartlett-Nanda-Pillai test have saddlepoint approximations that have been shown to be highly accurate for most all settings; see Butler (2007, §11.1) and the references therein.

For his test, Roy (1945) offered some reduction expressions for exact p-value computation which are tractable in dimensions $k = 2, 3$, and 4. Nanda (1951) and Pillai (1956) extended these procedures up to $k = 8$ while Pillai (1956,

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1965) offered a general approximate expression in the upper tail of the CDF that has limited accuracy for higher dimensional matrices. Kres (1983) provided general tables of 95th and 99th percentiles for the distribution of Roy's test and the largest eigenvalue of a Wishart. For the latter distribution, Johnstone (2001) provided a Tracy-Widom approximation accurate for higher dimensions. It would be useful, however, to be able to compute both distribution functions and maintain high accuracy for all dimensions and degrees of freedom.

Sugiyama (1967) showed that the maximum eigenvalue distributions for the matrix beta and Wishart can be expressed in terms of ${}_2F_1$ and ${}_1F_1$ matrix argument hypergeometric functions. However, until recently, these functions have also proved to be very difficult to compute either exactly or even approximately. Highly accurate Laplace approximations for these functions were developed in Butler and Wood (2002) that have proved useful for many important MANOVA applications, including power function computation in MANOVA for Wilks' test as well as block independence; see Butler and Wood (2005) and Butler (2007, §11.3). These approximations, however, fail to accurately determine p-values for Roy's test and the largest eigenvalue of the Wishart because their relative error accuracy is preserved in the wrong tail of the distribution. The rejection region for Roy's test is in the right tail while it is the CDF that is approximated by Laplace approximation ${}_2\hat{F}_1$. Thus if the true significance of Roy's test is 0.02 and ${}_2\hat{F}_1$ is used to approximate the true CDF value 0.98 with a moderately small relative error of 2.5%, then p-value approximation leads to $1 - {}_2\hat{F}_1 \in (-0.0045, 0.0445)$ or perhaps a negative p-value approximation.

Our computational expressions build upon the theoretical work of Gupta and Richards (1985) who gave exact Pfaffian expressions for matrix argument hypergeometric functions ${}_2F_1$ and ${}_1F_1$ when the matrix arguments are scalar multiples of the identity matrix, as occurs with Roy's test. Thus Gupta and Richards were able to show that the distribution of Roy's test statistic can be expressed as the Pfaffian of a skew-symmetric matrix whose entries are complicated expressions that involve double integration terms as well as hypergeometric functions. Despite their theoretical work, algorithms and software for implementing these computations have been lacking for perhaps two reasons. First, they made an unfortunate error in specifying one of the degrees of freedom for the function ${}_2F_1$ that gives Roy's distribution. Secondly, all entries of the Pfaffian are quite difficult to compute and have been left in complicated forms that require double integration and scalar argument ${}_2F_1$ computation. Numerical stability in computing their expressions is perhaps the most severe problem that we encountered.

Our contributions are algorithmic and computational. We develop expressions for the Pfaffian entries in terms of series expansions that can be computed in Maple. It is necessary to use Maple and retain a sufficiently large number of digits during computation in order to avoid the instability problems of the computations which, for our expressions, concern summing these series expansions. In the case of Roy's test with cutoff $r \in (0,1)$, these summations are shown to be ultimately monotone (decreasing or increasing) which leads to partial sums with a linear convergence rate of r. Thus, far into the right tail of the distribution where $r \approx 1$, this convergence can be very slow. Aitken's (1926) convergence acceleration method is used to improve upon summation efficiency.

For the largest Wishart eigenvalue distribution, terms in the skew-symmetric matrix are alternating sums, whose terms are shown to be ultimately decreasing in magnitude and partial sums are shown to have a superlinear convergence rate. In this case, Wijngaarden's convergence acceleration method is used to improve upon summation efficiency; see Press et al. (1992).

For both distributions, components of the skew-symmetric matrix that specifies the CDF are computed to a prespecified number of significant digits. This allows approximate overall relative error bounds to be determined in our p-value computation for Roy's test and also for the CDF of the largest Wishart eigenvalue.

Our practical contribution is to provide Maple software that may be used to compute both of these CDFs to a prespecified degree of accuracy. This software can be used without knowledge of the Maple programming language; see the readme.txt files zipped with the Maple programs that may be downloaded at *http://www.smu.edu/statistics/faculty/butler.html.*

2 The CDF for Roy's test statistic in MANOVA

In MANOVA, suppose that the error sums of squares matrix W_e is Wishart$_k(n,\Sigma)$ with n degrees of freedom and the hypothesis sums of squares W_h is independently Wishart$_k(m,\Sigma)$. Roy's test is based on the distribution of the largest eigenvalue λ_1 of the random Beta matrix $(W_e+W_h)^{-1}W_h$. It's exact CDF is given in the theorem below.

We assume that $n \geq k$ and, without loss in generality, $m \geq k$. The latter inequality can be assured to hold through the distributional equivalence

$$\lambda_1(k,m,n) \sim \lambda_1(m,k,m+n-k). \qquad (1)$$

We use the following notation:

$$\alpha_i = \tfrac{1}{2}(m+k+1) - i \geq \tfrac{1}{2} \qquad i = 1,...,k$$
$$\beta = \tfrac{1}{2}(n-k+1) \geq \tfrac{1}{2}.$$

Also define the multivariate gamma and beta functions as

$$\Gamma_k(a) = \pi^{k(k-1)/4}\prod_{i=1}^{k}\Gamma\{a-\tfrac{1}{2}(i-1)\} \qquad a > \tfrac{1}{2}(k-1)$$

$$B_k(a,b) = \Gamma_k(a)\Gamma_k(b)/\Gamma_k(a+b)$$

which reduce to univariate versions Γ and B for $k=1$.

Theorem 1 *The exact null distribution function of Roy's statistic $\lambda_1(k,m,n)$ is*

$$F(r) = \Pr(\lambda_1 \leq r) = \frac{1}{B_k(\frac{m}{2},\frac{n}{2})}\frac{\pi^{k^2/2}}{\Gamma_k(k/2)}r^{km/2}\sqrt{|\mathbf{A}_r|} \qquad 0<r<1. \qquad (2)$$

Here, $\mathbf{A}_r = (a_{ij})$ is a skew-symmetric matrix $(a_{ij} = -a_{ji})$ whose structure is determined by whether k is even or odd. For k even, $\mathbf{A}_r$ is $k \times k$ with

$$a_{ij} = r^{-(\alpha_i+\alpha_j)}\left\{2\sum_{l=0}^{L_\beta}(-1)^l\binom{\beta-1}{l}\frac{C_r(\alpha_i+\alpha_j+l,\beta)}{\alpha_i+l} - C_r(\alpha_i,\beta)C_r(\alpha_j,\beta)\right\}, \qquad (3)$$

where

$$C_r(a,b) = B(a,b)I_r(a,b), \qquad (4)$$

$B(a,b)$ is the beta function, and $I_r(\alpha_i,\beta)$ denotes the incomplete beta function as given in (26.5.1) of Abramowitz and Stegun (1972). The range of summation is

$$L_\beta = \begin{cases} \beta-1 & \text{if } n-k \text{ is odd, so } \beta \text{ is an integer} \\ \infty & \text{if } n-k \text{ is even.}\end{cases} \qquad (5)$$

For the case in which k is odd, then $\mathbf{A}_r$ is $(k+1)\times(k+1)$. The upper left $k \times k$ block is the matrix $(a_{ij} : i,j = 1,...,k)$

described above with a_{ij} given in (3). The $(k+1)$st column (row) is determined as

$$a_{i,k+1} = -a_{k+1,i} = r^{-\alpha_i} C_r(\alpha_i, \beta) \qquad i = 1, ..., k. \tag{6}$$

Proof Let $p = \frac{1}{2}(k+1)$. Sugiyama (1967) specified the CDF in terms of a matrix argument ${}_2F_1$ function as

$$\begin{aligned} F(r) &= \frac{\Gamma_k\{(m+n)/2\}\Gamma_k(p)}{\Gamma_k(n/2)\Gamma_k(m/2+p)} r^{km/2} \\ &\quad \times {}_2F_1\left(p-n/2, m/2; m/2+p; rI_k\right) \qquad (7) \\ &= \frac{\Gamma_k\{(m+n)/2\}\Gamma_k(p)}{\Gamma_k(n/2)\Gamma_k(m/2+p)} r^{km/2} \\ &\quad \times {}_2F_1\left(m/2, p-n/2; m/2+p; rI_k\right) \qquad (8) \end{aligned}$$

upon interchanging the first two arguments of ${}_2F_1$. The interchange in (8) is crucial in order that subsequent expressions reduce to their simplest computational form. Gupta and Richards (1985), when using (7), put the second argument of ${}_2F_1$ in (7) as $n/2$ which is incorrect. Despite this error, Gupta and Richards (1985) provide the means by which the simple expressions in Theorem 1 may be determined from (8). According to (3.1) in Gupta and Richards (1985),

$${}_2F_1\left(m/2, p-n/2; m/2+p; rI_k\right) = \frac{\Gamma_k(m/2+p)}{\Gamma_k(m/2)\Gamma_k(p)} \frac{\pi^{k^2/2}}{\Gamma_k(k/2)} \sqrt{|\mathbf{A}_r|}$$

and this leads to the overall expression (2).

The important contribution of our theorem is in reducing the entries of $\mathbf{A}_r$ to the simple forms given in (3) and (6). According to (3.4) of Gupta and Richards (1985), $a_{ij} = 2I_{ij} - J_{ij}$ for $i < j \leq k$ where

$$\begin{aligned} J_{ij} &= B(\alpha_i, 1)B(\alpha_j, 1)\, {}_2F_1(p-n/2, \alpha_i; \alpha_i+1; r) \\ &\quad \times \times\, {}_2F_1(p-n/2, \alpha_j; \alpha_j+1; r) \end{aligned}$$

and the I_{ij} term is evaluated below. The ${}_2F_1$ function is related to the incomplete Beta function $I_r(a,b)$, given in (26.5.23) of Abramowitz and Stegun (1972), according to

$${}_2F_1(1-b, a; a+1; r) = aB(a,b)r^{-a}I_r(a,b). \tag{9}$$

Thus

$$J_{ij} = r^{-(\alpha_i+\alpha_j)} C_r(\alpha_i, \beta) C_r(\alpha_j, \beta)$$

is the latter term in (3).

The expression for I_{ij} in (3.5) of Gupta and Richards (1985) assumes an especially simple form when determined from the matrix argument ${}_2F_1$ function as expressed in (8). In this case

$$I_{ij} = \int_0^1 y^{\alpha_j - 1}(1-ry)^{n/2-p} \left\{ \int_0^y x^{\alpha_i - 1}(1-rx)^{n/2-p} dx \right\} dy \tag{10}$$

and the powers of factors $(1-y)$ and $(1-x)$ in its integrand are zero. Expression (10) can be evaluated by using the generalized Binomial expansion

$$(1-rx)^{n/2-p} = \sum_{l=0}^{L_\beta} \binom{n/2-p}{l} (-rx)^l$$

and termwise integration leads to

$$\begin{aligned} I_{ij} &= \sum_{l=0}^{L_\beta} \binom{\beta-1}{l} \frac{(-r)^l}{\alpha_i + l} \int_0^1 y^{\alpha_i+\alpha_j+l-1}(1-ry)^{n/2-p} dy \\ &= \sum_{l=0}^{L_\beta} u_l \qquad (11) \end{aligned}$$

where

$$\begin{aligned} u_l &= \binom{\beta-1}{l} \frac{(-r)^l}{(\alpha_i+l)(\alpha_i+\alpha_j+l)} \\ &\quad \times {}_2F_1(p-n/2, \alpha_i+\alpha_j+l; \alpha_i+\alpha_j+l+1; r) \qquad (12) \end{aligned}$$

The final form of this term as recorded in (3) results by rewriting ${}_2F_1$ as an incomplete Beta function as expressed in (9).

For k odd, the last column of $\mathbf{A}_r$ is given in (3.7) of Gupta and Richards (1985) and this term reduces to (6) when the ${}_2F_1$ term is reduced by using (9). □

The smallest root λ_k of the matrix beta has a distribution that may be expressed in term of the largest root as described in Johnson and Kotz (1972, §39.2 p. 183). This leads to

$$\lambda_k(k,m,n) \stackrel{\mathscr{D}}{=} 1-\lambda_1(k,n,m). \tag{13}$$

Therefore Theorem 1 also provides the distribution of λ_k upon using the relationship (13).

There are two cases when determining the values $\{I_{ij} : i<j\}$ in skew-symmetric matrix $\mathbf{A}_r = (a_{ij})$ with $a_{ij} = 2I_{ij} - J_{ij}$. When $n-k$ is an odd integer, $L_\beta < \infty$ and the expression for I_{ij} in (11) can be computed exactly as a finite sum. For $n-k$ even, I_{ij} is an infinite sum with the following properties that are shown in the appendix.

Corollary 1 *Suppose $n-k$ is an even integer so (11) is an infinite series. If $(n-k)/2$ is an even integer, the sequence $\{u_l : l \geq (n-k+1)/4-1\}$ is a monotonic decreasing sequence of positive values converging to* 0*; if $(n-k)/2$ is an odd integer, then the sequence is a monotonic increasing sequence of negative values converging to* 0*. The convergence rate for the partial sums of the series is linear with rate r, e.g.*

$$\lim_{l\to\infty} \frac{|u_{l+1}|}{|u_l|} = r \in (0,1).$$

3 Largest eigenvalue of a Wishart$_k(m,I_k)$

The distribution of $\tau_1 = \tau_1(k,m)$, the largest eigenvalue of $W_h \sim \text{Wishart}_k(m,I_k)$ for $m \geq k$, may be determined by taking the appropriate limit of the distribution of $\lambda_1(k,m,n)$ as $n \to \infty$. The weak convergence

$$n\lambda_1(k,m,n) \stackrel{\mathscr{D}}{\to} \tau_1(k,m)$$

as $n \to \infty$, allows two approaches in determining an expansion for the CDF of τ_1. The first approach expresses

$$\Pr\{\lambda_1(k,n,m) \leq r/n\} \tag{14}$$

in terms of $_2F_1$ by using (8), and passes (14) to the limit in n. This leads to the matrix argument confluent $_1F_1$ hypergeometric function expression for the CDF of τ_1 given by Constantine (1963) and conveniently recorded in Muirhead (1982, p. 421). Proceeding as in Theorem 1, and applying the theory of Gupta and Richards (1985) to $_1F_1$ instead of $_2F_1$, then the CDF of τ_1 may be derived as stated in Theorem 2 below.

The second and simpler approach is to take the limit of the right hand side of (2) and (3) directly as $n \to \infty$ but with r replaced by r/n. This approach is used to derive Theorem 3 below.

For cases in which $m<k$, so the Wishart matrix is not full rank, the distributional equivalence

$$\tau_1(k,m) \stackrel{\mathscr{D}}{=} \tau_1(m,k) \tag{15}$$

can be used to reduce the dimension of the Wishart to full rank. This result easily follows by noting that X^TX and XX^T have the same nonzero eigenvalues when X is an $m \times k$ matrix of i.i.d. normal variables.

Theorem 2 *The exact null CDF of $\tau_1(k,m)$ is*

$$F(r) = \Pr(\tau_1 \leq r) = \frac{1}{\Gamma_k(\frac{m}{2})} \frac{\pi^{k^2/2}}{\Gamma_k(k/2)} (r/2)^{km/2} \sqrt{|\mathbf{B}_r|} \qquad 0<r<\infty. \tag{16}$$

Here, $\mathbf{B}_r = (b_{ij})$ is a skew-symmetric matrix ($b_{ij} = -b_{ji}$) whose structure is determined by whether k is even or odd. For k even, $\mathbf{B}_r$ is $k \times k$ with

$$b_{ij} = (r/2)^{-(\alpha_i+\alpha_j)} \left\{ 2\sum_{l=0}^{\infty} \frac{(-1)^l}{l!(\alpha_i+l)} \gamma(\alpha_i+\alpha_j+l, r/2) - \gamma(\alpha_i, r/2)\gamma(\alpha_j, r/2) \right\}, \tag{17}$$

where

$$\gamma(a,r/2)=\Gamma(a)P(a,r/2)=\int_0^{r/2}t^{a-1}e^{-t}dt \quad (18)$$

is the incomplete gamma function given in (6.5.2) of Abramowitz and Stegun (1972). For the case in which k is odd, then $\mathbf{B}_r$ *is* $(k+1)\times(k+1)$. *The upper left* $k\times k$ *block is the matrix* $(b_{ij}: i,j=1,...,k)$ *described above with* b_{ij} *given in (17). The* $(k+1)$*st column (row) is determined as*

$$b_{i,k+1}=-b_{k+1,i}=(r/2)^{-\alpha_i}\gamma(\alpha_i,r/2) \qquad i=1,...,k. \quad (19)$$

Proof For any $r>0$, large n assures that $r/n<1$. Starting with the components of matrix $\mathbf{A}_r$ in Theorem 1,

$$\lim_{n\to\infty} n^a C_{r/n}(a,\beta)=2^a\gamma(a,r/2)$$

so that the term J_{ij} has limit

$$(r/n)^{-(\alpha_i+\alpha_j)}C_{r/n}(\alpha_i,\beta)C_{r/n}(\alpha_j,\beta)\to (r/2)^{-(\alpha_i+\alpha_j)}\gamma(\alpha_i,r/2)\gamma(\alpha_j,r/2)$$

which is the latter term in (17). Likewise for the term I_{ij}, the portion of the lth term in its expansion in (3) that depends on n has the limit

$$n^{\alpha_i+\alpha_j}[\tfrac{1}{2}(n-k-1)]_l\, C_{r/n}(\alpha_i+\alpha_j+l,\beta)\to 2^{\alpha_i+\alpha_j}\gamma(\alpha_i+\alpha_j+l,r/2)$$

which leads to the former term on the right side of (17). The number of terms in the expansion $L_\beta\to\infty$. The remaining limits needed for (16) are easily computed as

$$\lim_{n\to\infty}\frac{1}{B_k(\frac{m}{2},\frac{n}{2})}\frac{\pi^{k^2/2}}{\Gamma_k(k/2)}\left(\frac{r}{n}\right)^{km/2}=\frac{1}{\Gamma_k(\frac{m}{2})}\frac{\pi^{k^2/2}}{\Gamma_k(k/2)}\left(\frac{r}{2}\right)^{km/2}.$$

□

Suppose the infinite series expression for b_{ij} given in (17) is $\mathscr{I}_{ij}=\sum_{l=0}^{\infty}v_l$ where

$$v_l=\frac{(-1)^l}{l!(\alpha_i+l)}\gamma(\alpha_i+\alpha_j+l,r/2).$$

Corollary 2 *The alternating series* $\{v_l: l>r/2\}$ *is monotone decreasing in magnitude, e.g.* $|v_{l+1}|<|v_l|$ *for* $l>r/2$. *The partial sums of the sequence exhibit superlinear convergence to* $\mathscr{I}_{ij}$ *in that*

$$\lim_{l\to\infty}\frac{|v_{l+1}|}{|v_l|}=0$$

for any $r>0$.

A proof is given in the appendix.

4 Computations

4.1 Roy's test

The computation of exact CDF values for Roy's test, to some specified number of digits, requires sufficiently accurate approximations to the I_{ij} terms which contribute to the entries of skew-symmetric matrix $\mathbf{A}_r$. This is not an issue when $n-k$ is odd since the I_{ij} terms are all finite sums which are computed by our supporting software.

For $n-k$ even, the I_{ij} terms are all infinite series that must be approximated. The natural albeit naive estimate for infinite series I_{ij} is the the q-th partial sum

$$s_q=\sum_{l=0}^{q}u_l.$$

A natural measure of how well s_q approximates I_{ij} is the relative error of s_q;

$$E_r(s_q)=\left|(s_q-I_{ij})/I_{ij}\right|. \quad (20)$$

This measure of error is not computable in practice since I_{ij} is unknown and therefore one must consider an approximate relative error of s_q, or

$$\hat{E}_r(s_q)=\left|(s_q-s_{q+1})/s_{q+1}\right|.$$

While there is no guarantee that the approximate relative error will be close to the true relative error, it often is quite close in practice; see for instance Chapra (2004).

Along with a measure of error we require a stopping criterion to identify the numbers of terms to be summed. We take our stopping criterion to be smallest integral q, such that

$$\hat{E}_r(s_q) < 10^{-D} \tag{21}$$

for some specified integer D.

In the appendix we provide a proof that the partial sums of the terms in I_{ij} converge linearly to I_{ij} with rate r. The practical importance of this result is that smaller values of r generally require fewer terms for accurate approximations to I_{ij} than larger values of r and particularly relative to values of r near one. Furthermore, for values of r near one, convergence acceleration methods may provide answers in much less time than the q-th partial sum. Convergence acceleration methods use fewer terms than are used in s_q to accurately approximate I_{ij}. More specifically, a convergence acceleration method transforms a set of $q+1$ terms, $u_0, \ldots, u_q$, in some fashion to produce an approximation which is often much closer to I_{ij} than is s_q.

We found that the convergence acceleration method known as Aitken's δ^2 process, Aitken (1926), provided approximations to I_{ij} in less time than the q-th partial sum. This was to be expected since Aitken's δ^2 process is known to work especially well for partial sums which converge linearly to their limit; see (3.9.7) of Abramowitz and Stegun (1972). Aitken's δ^2 process generates an improved estimate, $\tilde{s}_q$, from three successive partial sums as

$$\tilde{s}_q = s_q - \left(s_q - s_{q+1}\right)^2 / \left(s_q - 2s_{q+1} + s_{q+2}\right). \tag{22}$$

We determine index q for Aitken's method to be smallest integer satisfying (21) when applied to $\{\tilde{s}_q\}$ in (22).

4.2 Largest eigenvalue of a Wishart$_k(m, I_k)$

In this setting, the computation of exact CDF values always involves b_{ij} terms in (17) that must be computed as truncated infinite series. Suppose

$$s_q = \sum_{l=0}^{q} v_l$$

is the q-th partial sum for $\mathscr{I}_{ij}$, the infinite series portion of b_{ij}. The relative error of s_q, or $E_r(s_q)$, is defined as (20) with $\mathscr{I}_{ij}$ replacing I_{ij}. A relative error bound turns out to be

$$E_r(s_q) < \left|v_{q+1}\right| / \min\left\{\left|s_q - v_{q+1}\right|, \left|s_q + v_{q+1}\right|\right\}. \tag{23}$$

To show this, first note that the sequence of partial sums $\{s_q\}$ is a Cauchy sequence and that v_l terms are monotonically decreasing in magnitude for all $l > r/2$, as shown in the appendix. Thus, for $r/2 < q < \tilde{q} = q + Q$,

$$\left|s_q - s_{\tilde{q}}\right| = \begin{cases} \left|v_{q+1}\right| - \sum_{l=1}^{Q/2-1}\left(\left|v_{q+2l}\right| - \left|v_{q+2l+1}\right|\right) - \left|v_{\tilde{q}}\right|, & \text{for } Q \text{ even} \\ \left|v_{q+1}\right| - \sum_{l=1}^{(Q+1)/2-1}\left(\left|v_{q+2l}\right| - \left|v_{q+2l+1}\right|\right), & \text{for } Q \text{ odd} \end{cases}$$

$$< \left|v_{q+1}\right|.$$

Passing to the limit as $\tilde{q} \to \infty$ leads to

$$\left|s_q - \mathscr{I}_{ij}\right| < \left|v_{q+1}\right| \tag{24}$$

for $q > r/2$ so

$$s_q - \left|v_{q+1}\right| < \mathscr{I}_{ij} < s_q + \left|v_{q+1}\right|. \tag{25}$$

From (25), the relative error is bounded by (23) so the stopping criterion for the q-th partial sum is the smallest integer q, greater than $r/2$, such that

$$\left|v_{q+1}\right| / \min\left\{\left|s_q - \left|v_{q+1}\right|\right|, \left|s_q + \left|v_{q+1}\right|\right|\right\} < 10^{-D}. \tag{26}$$

Since $\{s_q\}$ converges superlinearly to b_{ij}, which is like linear convergence but with rate zero, our computational times should not increase very rapidly in r. Nonetheless, we have considered several convergence acceleration methods.

Our preferred method of convergence acceleration in this context is van Wijngaarden's technique which is a highly efficient implementation of Euler's transformation; see Goodwin (1961). Euler's transformation generates a convergent alternating series (from the original series) which converges to $\mathscr{I}_{ij}$ but at a more rapid rate than the original sequence; see Knopp (1990). The q-th partial sum of Euler's transformation for alternating series $\mathscr{I}_{ij}$ is

$$s_q = \frac{1}{2}\sum_{l=0}^{q}\left(-\frac{1}{2}\right)^l \Delta^l v_0,$$

where Δ^l is the l-th forward difference operator defined as

$$\Delta^l v_0 = \sum_{j=0}^{l}\binom{l}{j}\left|v_j\right|.$$

van Winjgaarden's technique is in fact an improved implementation of Euler's transformation. It is well known that Euler's transformation performs best when applied to a partially summed series; see Press et al. (1992). In our application we may write

$$\mathscr{I}_{ij} = \sum_{l=0}^{\infty}\tilde{v}_l,$$

where $\tilde{v}_0 = s_{\breve{q}}$ and $\tilde{v}_l = (-1)^{\breve{q}+l}\left|v_{\breve{q}+l}\right|$ for $l \geq 1$. van Winjgaarden's technique first determines $\breve{q}$ and then applies Euler's transformation to partially summed terms $\{\tilde{v}_l\}$; see Press et al. (1992).

Since there is no guarantee that the terms generated by van Winjgaarden's technique will eventually be monotonically decreasing, we can no longer use (26) as the basis for a stopping criterion. Instead, we take as our stopping criterion the smallest value of q satisfying (21).

We also considered algorithm 1 from Cohen et al. (2000), another convergence acceleration method, but found it to yield inaccurate answers. This came as no surprise since the v_l terms do not satisfy the requisite condition which guarantees the accuracy of the algorithm.

4.3 Error bounds on probabilities

Error bounds can be specified for probabilities of these largest eigenvalue distributions using the error bounds on the elements of matrices $\mathbf{A}_r$ or $\mathbf{B}_r$ that have been computed to a certain degree of accuracy. The basic idea is to determine the relative error in probability computation when the components of $\mathbf{A}_r$ are computed to a relative error of 10^{-D}.

For Roy's test, let p denote the probability computation from matrix $\mathbf{A}_r$ when components of $\mathbf{A}_r$ are subject to error. The differential of $\ln p$ is

$$dp/p = d\left(\ln|\mathbf{A}_r|\right)/2 = \operatorname{tr}\left(\mathbf{A}_r^{-1}d\mathbf{A}_r\right)/2. \qquad (27)$$

Entries of $\mathbf{A}_r = (a_{ij})$ are of the form $a_{ij} = 2I_{ij} - J_{ij}$ where only $\{I_{ij} : i \neq j\}$ are subject to computational error due to truncation of their infinite series expressions; diagonal entries $\{a_{ii}\}$ are zero and not subject to error so $da_{ii} \equiv 0$ for all i. If the stopping criterion (21)

$$|(\hat{I}_{ij} - I_{ij})/I_{ij}| < 10^{-D} \qquad (28)$$

holds, as it often does in practice, then

$$\left|dI_{ij}/I_{ij}\right| < 10^{-D} \qquad i \neq j.$$

Additional entries besides the diagonal of $\mathbf{A}_r$ that do not need to be estimated, and whose differentials can therefore be taken as 0, include the $(k+1)$st column and row when k is odd. Thus,

$$|da_{ij}| = 2|dI_{ij}| \leq 2\times 10^{-D}\left|I_{ij}\right| \qquad i \neq j$$

which leads to a relative error bound for p as

$$
\begin{aligned}
|dp|/p &= 1/2\left|\sum_{i=1}^{k}\sum_{i\neq j=1}^{k} a^{ij} da_{ij}\right| \\
&\leq 10^{-D}\sum_{i=1}^{k}\sum_{i\neq j=1}^{k} |a^{ij}|\left|I_{ij}\right| \\
&= 10^{-D}\,\mathrm{tr}\{[\mathbf{A}_r^{-1}]\,[I]\} \qquad (29)
\end{aligned}
$$

where $[\mathbf{A}_r^{-1}] = (|a^{ij}|)$, and $[I] = (\left|I_{ij}\right|)$ with $I_{ii} = 0$. The inequality in (29) is potentially quite conservative.

A similar bound on the relative error of a probability for the largest eigenvalue of a Wishart is

$$|dp|/p < 10^{-D}\,\mathrm{tr}\{[\mathbf{B}_r^{-1}]\,[\mathscr{I}]\}, \qquad (30)$$

where $[\mathscr{I}] = (\left|\mathscr{I}_{ij}\right|)$ with $\mathscr{I}_{ii} = 0$.

5 Numerical results

The performance of these numerical methods for computing p-values for Roy's test and the distribution of the largest eigenvalue of a Wishart are considered. In both instances, the computations are for exact CDF values, obtained by using partial sums and convergence acceleration methods for estimated 95th and 99th percentiles. These estimated percentiles were simulated by using 95th and 99th empirical percentiles from 10 million simulated values of the eigenvalues. Our goal in the exact computations was to produce answers accurate to at least three digits, after rounding.

Our computations were performed using Maple 11 programs that are available for general use at *http://www.smu.edu/statistics/faculty/butler.html.* Instructions are provided to run the programs which assume no knowledge of either Maple programming or of running such software (although the user must have the software). Maple was used primarily because a very high number of significant digits can be carried when calculating with floating point numbers. This is crucial in implementing such computations which often involve small numbers obtained as differences of much larger numbers due to the alternating nature of the series under approximation. This differencing causes a loss in the number of significant digits in the final answer; see Scheid (1989) for further elaboration on this phenomenon.

In the case of Roy's test with $n-k$ an odd integer, elements of $\mathbf{A}_r$ are finite sums and our program performs exact summation with run times typically less than a second.

In all other cases in which infinite series expansions must be truncated, extensive numerical experimentation was used to determine program settings that would yield accurate answers with the least amount of time. These settings involve SF, the number of digits that Maple uses in its computations and D, a bound on the true or approximate relative error when approximating elements of $\mathbf{A}_r$ or $\mathbf{B}_r$. Run times were recorded in an hour:minute: second (h:mm:ss) format and all computations were performed on an Intel dual-core 2.66GHz processor with 2.96GB of RAM.

5.1 Exact computations for Roy's test for $n-k$ even

Numerical experimentation showed that the time required to produce sufficiently accurate CDF values (at least three digits as measured by the conservative upper "Bound") increased quickly with k and only moderately with m. Our study therefore only considered the speed of CDF computations for Roy's test with $k=m$. Our settings include computations for dimensions k ranging from 4 to 54 and use error degrees of freedom $n = 30$, 50, and 100.

Tables 1 and 2 record run times needed to accurately determine CDF values for the estimated 95th and 99th percentiles respectively. These estimated percentiles (Perc.) are the listed values of r determined from 10^7 eigenvalue simulations. For target value $\phi = 0.95$ or 0.99, the exact computation of $F(r)$ will differ from ϕ by a relative error of about $10^{-7/2}\sqrt{\phi(1-\phi)}$, which is $0.0^4 7$ or $0.0^4 3$ respectively, where 0^4 indicates four zeros. These errors follow from the delta method which, by weak convergence laws, assumes $F(r) = (F \circ \hat{F}^{-1})(\phi) \sim N(\phi, \phi(1-\phi)/10^7)$. From a practical perspective, this means that only the first four digits of $F(r)$ should be expected to agree with ϕ due to error in the simulated values of r.

Tables 1 and 2 are also meant to provide some guidance on how to choose good values of D and SF for the programs. In general, for problems where there is a big difference between k and m, values of D and SF that give the best run times may need to be found by trial and error. We suggest using our table entries as starting values and increasing D and SF in increments of 5 and 10 respectively, until there is no change in the first three digits of the CDF value, after rounding.

Tables 1 and 2 show that Aitken's δ^2 process consistently outperforms the partial sums in terms of run times. Furthermore, its advantage over partial sums becomes more substantial in the last few cases considered that have larger values for both $k = m$ as well as r. Probability computations should be accurate to three significant digits, after rounding, if the conservative relative error bound is less that $0.0^3 5$. In every case considered this bound is smaller thus indicating at least three significant digits after rounding.

To summarize, our software provides "exact" computation of p-values for Roy's test in a wide range of settings. For odd $n-k$, the computation is exact, while for even $n-k$ the relative error bound (29) can be used to determine a conservative bound on the relative error. Due to the linear convergence rate in r, quite fast run times result for values for n as large as 100 when r is not much greater than 0.9. Reasonable run times result with r as large as 0.99. Aitken's δ^2 process is programmed into the publicly available Maple programs and should always be used in place of the q-th partial sum. The greatest gains in efficiency over partial sums can be expected farther out into the right tail of the distribution.

5.2 Exact computations for the largest eigenvalue of a $\text{Wishart}_k(m, I_k)$

In the case of Wishart eigenvalues, numerical experimentation showed that computation times were sensitive to the value of k but were only moderately so to the value of m. Thus, computational speed was again studied with $k = m$ as listed under column "Dim." in Tables 3 and 4. These tables present CDF computations for estimated 95th and 99th percentiles that use van Wijngaarden's convergence acceleration method as well as the q-th partial sum. The relative error bounds for the partial sum method have been left out because they agree with those of van Wijngaarden's method to three significant digits.

We see that in every case considered, van Winjgaarden's technique outperformed partial sums in terms of run times. Furthermore, its advantage over partial sums becomes more pronounced in the most computationally intensive cases with larger k. Finally, relative error bound (30) guaranteed accuracy in every case considered.

In summary, our software can be used to compute, in reasonable time, Wishart CDF values for values of k and m as large as 50. Furthermore, van Wijngaarden's convergence acceleration technique is generally recommended instead of partial sums and is programmed into the publicly available Maple program.

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Table 1 *Computational run times (h:mm:ss) for p-values of Roy's test where r is an estimated 95th percentile from the distribution of* $\lambda_1(k,m,n)$ *determined by simulating* 10^7 λ_1*-values.* [a]*For all settings,* $m = k$*.* [b]*The conservative relative error bound (29) reported using* 0^3 *to indicate 3 zeros.* [c]*Denotes a run time that was less than* 0.5 *second.*

95th Percentile										
Setting[a]	Perc.	Aitken's δ^2					Partial Sums			
k,n	r	D	SF	$F(r)$	Bound[b]	h:mm:ss	D	SF	$F(r)$	h:mm:ss
4,30	0.44938	6	8	0.949929	$.0^3113$	0:00:00[b]	6	8	0.949929	0:00:00[c]
14,30	0.88908	17	23	0.950097	$.0^3403$	0:00:02	17	23	0.950081	0:00:03
24,30	0.99161	33	40	0.949759	$.0^3146$	1:53:21	33	40	0.949748	2:14:13
4,50	0.29847	6	16	0.949953	$.0^3101$	0:00:00[c]	6	8	0.949821	0:00:00[c]
14,50	0.71061	16	24	0.950218	$.0^3373$	0:00:01	16	23	0.949766	0:00:01
24,50	0.89227	29	37	0.950409	$.0^3131$	0:00:41	29	37	0.950412	0:00:47
34,50	0.97050	44	54	0.949961	$.0^4910$	1:29:18	44	52	0.949967	1:39:22
4,100	0.16150	5	40	0.949974	$.0^4926$	0:00:00[c]	6	10	0.949927	0:00:00[c]
14,100	0.45340	16	26	0.950284	$.0^4733$	0:00:01	16	26	0.950284	0:00:01
24,100	0.64476	26	40	0.949572	$.0^3554$	0:00:06	26	40	0.949580	0:00:06
34,100	0.77376	38	55	0.950070	$.0^3345$	0:01:12	38	55	0.950071	0:01:16
44,100	0.86102	51	69	0.950025	$.0^3199$	0:06:01	51	69	0.950021	0:06:25
54,100	0.91941	65	83	0.950020	$.0^3132$	1:22:00	65	84	0.949994	1:34:39

Table 2 *Similar runs times as in Table 1 but with r as an estimated 99th percentile.* [a]*For all settings,* $m = k$*.*

99th Percentile										
Setting[a]	Perc.	Aitken's δ^2					Partial Sums			
k,n	r	D	SF	$F(r)$	Bound	h:mm:ss	D	SF	$F(r)$	h:mm:ss
4,30	0.52711	6	8	0.990384	$.0^3110$	0:00:00[c]	6	8	0.990384	0:00:00[c]
14,30	0.91481	17	23	0.990045	$.0^3395$	0:00:11	17	22	0.989511	0:00:13
24,30	0.99511	33	40	0.989566	$.0^3145$	2:47:14	33	40	0.989531	3:22:37
4,50	0.35901	6	13	0.990016	$.0^4978$	0:00:00[c]	6	9	0.989767	0:00:00[c]
14,50	0.74849	16	24	0.989970	$.0^3365$	0:00:01	16	24	0.989969	0:00:01
24,50	0.91077	29	38	0.989919	$.0^3129$	0:01:25	29	38	0.989921	0:01:37
34,50	0.97752	43	53	0.990410	$.0^3898$	1:35:00	43	53	0.990383	1:50:54
4,100	0.19816	6	37	0.989993	$.0^4900$	0:00:00[c]	1	10	0.989901	0:00:00[c]
14,100	0.48886	16	26	0.990284	$.0^4715$	0:00:01	16	26	0.990284	0:00:01
24,100	0.67268	26	41	0.989700	$.0^3542$	0:00:06	26	41	0.989698	0:00:06
34,100	0.79436	38	55	0.989961	$.0^3339$	0:01:16	38	55	0.989965	0:01:19
44,100	0.87555	51	69	0.989976	$.0^3196$	0:06:26	51	69	0.989972	0:06:53
54,100	0.92915	65	84	0.989960	$.0^3131$	1:25:51	65	84	0.989960	1:38:57

Table 3 *Computational run times for CDF values of $\tau_1 = \tau_1(k,m)$, the largest eigenvalue of a Wishart$_k(m, I_k)$ matrix. The percentile r is an estimated 95th percentile from the distribution of τ_1 determined by simulating 10^7 τ_1-values.* [a]*For all settings, $m = k$.*

95th Percentile										
Dim.[a]	Perc.	van Wijngaarden					Partial Sums			
k	r	D	SF	$F(r)$	Bound	h:mm:ss	D	SF	$F(r)$	h:mm:ss
10	43.04154	11	29	.950007	$.0^3287$	0:00:03	11	32	.949974	0:00:04
15	63.85394	16	46	.950101	$.0^3138$	0:00:13	16	48	.949641	0:00:17
20	84.49639	21	63	.950060	$.0^4701$	0:00:48	21	64	.949737	0:01:05
25	105.02812	25	77	.950049	$.0^3370$	0:01:52	25	82	.949829	0:02:41
30	125.49347	30	96	.950144	$.0^3199$	0:04:06	30	99	.949969	0:06:09
35	145.90589	35	109	.950011	$.0^3109$	0:08:18	35	119	.950017	0:14:52
40	166.28269	40	132	.950023	$.0^4599$	0:17:17	40	132	.949835	0:47:15
45	186.62608	44	148	.950026	$.0^3333$	0:40:57	44	150	.949617	2:09:30
50	206.94297	49	165	.949984	$.0^3187$	1:38:58	49	167	.949708	4:29:11

Table 4 *Similar run times as in Table 3 but using r as an estimated 99th percentile.* [a]*For all settings, $m = k$.*

99th Percentile										
Dim.[a]	Perc.	van Wijngaarden					Partial Sums			
k	r	D	SF	$F(r)$	Bound	h:mm:ss	D	SF	$F(r)$	h:mm:ss
10	48.95275	11	29	.990145	$.0^3279$	0:00:03	11	32	.989996	0:00:05
15	70.58583	16	47	.990067	$.0^3134$	0:00:14	14	49	.989952	0:00:20
20	91.83661	21	63	.989968	$.0^4685$	0:00:50	20	65	.990347	0:01:13
25	112.92604	25	79	.989945	$.0^3361$	0:01:58	25	83	.990287	0:02:57
30	133.90197	30	96	.990057	0^3195	0:04:15	30	100	.990112	0:06:49
35	154.73310	35	114	.990072	$.0^3106$	0:08:44	35	117	.990081	0:17:14
40	175.45746	39	132	.989983	$.0^3587$	0:17:07	39	135	.990017	0:59:05
45	196.17872	44	149	.990084	$.0^3327$	0:43:51	44	151	.989765	2:27:32
50	216.80902	49	168	.990006	$.0^3183$	1:47:56	49	168	.990114	4:58:49

7 Appendix

7.1 Proof of Corollary 1

Term $|u_l|$ is given as

$$\binom{\beta-1}{l}\frac{r^l}{\alpha_i+l}\int_0^1 y^{\alpha_i+\alpha_j+l-1}(1-ry)^{n/2-p}dy$$

It is immediately obvious that all the terms in the above expression, except for the generalized binomial coefficient, are monotonically decreasing in l. Note that

$$\left|\frac{\binom{\beta-1}{l+1}}{\binom{\beta-1}{l}}\right| = \left|\frac{\beta-l-1}{l+1}\right| < 1$$

for all $l \geq \beta/2-1$ and therefore $\{|u_l| : l \geq (n-k+1)/4-1\}$ is monotonically decreasing. in l. It easy to verify that if $(n-k)/2$ is an even integer, the sequence $\{u_l : l \geq (n-k+1)/4-1\}$ is a sequence of positive values and if $(n-k)/2$ is an odd integer, it is a sequence of negative values.

The eventual monotonicity of the $|u_l|$ terms and results from Clark et al. (1969) allow us to study the convergence of partial sums to I_{ij} by simply considering the limit

$$\lim_{l\to\infty}\frac{|u_{l+1}|}{|u_l|}.$$

In particular, the convergence of partial sum s_q is linear if this limit is in the unit interval but not zero or one, superlinear if the limit is zero and logarithmic if the limit is one. The substitution $du = rdy$ in each integral below yields

$$\begin{aligned}\frac{|u_{l+1}|}{|u_l|} &= \frac{\left|\binom{\beta-1}{l+1}\frac{r^{l+1}}{\alpha_i+l+1}\int_0^1 y^{\alpha_i+\alpha_j+l}(1-ry)^{n/2-p}dy\right|}{\left|\binom{\beta-1}{l}\frac{r^l}{\alpha_i+l}\int_0^1 y^{\alpha_i+\alpha_j+l-1}(1-ry)^{n/2-p}dy\right|} \\ &= \left|\frac{\binom{\beta-1}{l+1}}{\binom{\beta-1}{l}}\right|\left|\frac{\alpha_i+l+1}{\alpha_i+l}\right| \\ &\quad\times\frac{B(\alpha_i+\alpha_j+l+1,\beta)I_r(\alpha_i+\alpha_j+l+1,\beta)}{B(\alpha_i+\alpha_j+l,\beta)I_r(\alpha_i+\alpha_j+l,\beta)}\end{aligned}$$

so that clearly

$$\lim_{l\to\infty}\frac{|u_{l+1}|}{|u_l|} = \lim_{l\to\infty}\frac{B(\alpha_i+\alpha_j+l+1,\beta)I_r(\alpha_i+\alpha_j+l+1,\beta)}{B(\alpha_i+\alpha_j+l,\beta)I_r(\alpha_i+\alpha_j+l,\beta)}$$

To show that this limit is r it suffices, from equation (3), to prove, for $a = \alpha_i+\alpha_j+l$ and $b = \beta$, that

$$\frac{B(a+1,b)I_r(a+1,b)}{B(a,b)I_r(a,b)} \to r$$

as $a \to \infty$ or equivalently, as $l \to \infty$.

From (26.5.4) of Abramowitz and Stegun (1972) we have

$$B(a,b)I_r(a,b) = \frac{r^a(1-r)^b}{a}\left(1+\sum_{q=0}^{\infty}B(a,b)\frac{B(a+1,q+1)}{B(a+b,q+1)}r^{q+1}\right).$$

As $a \to \infty$, it is easily shown using Stirling's approximation that

$$B(a,b)\frac{B(a+1,q+1)}{B(a+b,q+1)} = O(a^{-b})$$

for every $q \geq 0$. Thus

$$\begin{aligned}\frac{B(a+1,b)I_r(a+1,b)}{B(a,b)I_r(a,b)} &= \frac{r^{a+1}(1-r)^b/(a+1)\left(1+O(a^{-b})\right)}{r^a(1-r)^b/a\left(1+O(a^{-b})\right)} \\ &\to r.\end{aligned}$$

7.2 Proof of Corollary 2

Consider the ratio

$$\frac{|v_{l+1}|}{|v_l|} = \frac{l!(\alpha_i+l)}{(l+1)!(\alpha_i+l+1)}\frac{\gamma(\alpha_i+\alpha_j+l+1,r/2)}{\gamma(\alpha_i+\alpha_j+l,r/2)}.$$

Incomplete gamma function $\gamma(a,x)$ can be expressed in terms of the confluent hypergeometric function ${}_1F_1$ by using equation (6.5.12) of Abramowitz and Stegun (1972)

$$\gamma(a,x) = a^{-1}x^a e^{-x}\ {}_1F_1\ (1,a+1,x) \tag{31}$$

where

$$\begin{aligned}{}_1F_1(1,a+1,x) = 1 &+ \frac{1}{a+1}x + \frac{x^2}{(a+1)(a+2)} \\ &+ \cdots + \frac{x^q}{\prod_{k=1}^{q-1}(a+k)} + \cdots\end{aligned} \tag{32}$$

as described in equation (13.1.2) of Abramowitz and Stegun (1972). Note that each term in this expansion is decreasing in $a > 0$ so that ${}_1F_1(1,a+1,x)$ is a decreasing function in

$a > 0$ for $x > 0$ fixed. Substituting for the gamma function as in (31) and simplifying, the ratio is

$$\frac{1}{l+1}\frac{\alpha_i+l}{\alpha_i+l+1}\frac{\alpha_i+\alpha_j+l}{\alpha_i+\alpha_j+l+1}\frac{r}{2}\frac{{}_1F_1(1,\alpha_i+\alpha_j+l+2,r/2)}{{}_1F_1(1,\alpha_i+\alpha_j+l+1,r/2)} < \frac{1}{l+1}\frac{r}{2} \tag{33}$$

upon using the monotonic decreasing property of ${}_1F_1(1,a+1,x)$ in a. For $l > r/2$, this ratio of absolute terms will be less than one.

Results from Clark et al. (1969) allow us to study the convergence of partial sum s_q again by simply considering the limit

$$\lim_{l\to\infty}\frac{|v_{l+1}|}{|v_l|}.$$

Using bound (33) it is easily established that this limit is zero and as such the partial sums converge superlinearly to $\mathscr{I}_{ij}$.