SERIES REPRESENTATIONS OF DISTRIBUTIONS OF QUADRATIC FORMS IN NORMAL VARIABLES. I. CENTRAL CASE

By Samuel Kotz[1], N. L. Johnson[2] and D. W. Boyd[3]

University of Toronto, University of North Carolina and University of Alberta

1. Introduction. Suppose that $X' = (X_1, X_2, \cdots, X_n)$ is a random vector with a multivariate normal distribution with expected value vector $(\xi_1, \xi_2, \cdots, \xi_n)$ and variance-covariance matrix V.

The object of this paper is to give unified derivations of a number of series representations of the distributions of quadratic forms

$$Q(X) = Q(X_1, \cdots, X_n) = X'AX = \sum_{i=1}^n \sum_{j=1}^n a_{ij}X_iX_j$$

where A is a real symmetric matrix.

The representations are all known, but the method of derivation presented here differs from earlier methods, sometimes slightly, sometimes substantially. We also give recurrence relationships for calculating coefficients of the series which are, in some cases, simpler than those heretofore available. Further we obtain a number of new bounds for errors committed in truncating the various series.

The cumulative distribution function of $Q(X)$ is

$$\Pr[Q(X) \leqq y]. \tag{1}$$

By performing suitable linear transformations, (see, e.g. [9]), (1) can be shown to be equal to

$$\Pr\left[\sum_{i=1}^n \alpha_i(Z_i + \delta_i)^2 \leqq y\right] \tag{2}$$

where Z_i's are independent unit normal variables, and $\alpha_1 \geqq \alpha_2 \geqq \alpha_3 \geqq \cdots \geqq \alpha_n$ are the eigenvalues of VA. The δ_i's are the same functions of the ξ_i's as the Z_i's are of the X_i's.

In the special (central or homogeneous) case when $\xi_1 = \xi_2 = \cdots = \xi_n = 0$, all δ_i's are also equal to zero and (2) becomes:

$$\Pr\left[\sum_{i=1}^n \alpha_i Z_i^2 \leqq y\right]. \tag{3}$$

We will denote the cumulative distribution functions (2) and (3) by

$$F_n(\alpha_1, \alpha_2, \cdots, \alpha_n; \delta_1, \delta_2, \cdots, \delta_n; y) \equiv F_n(\boldsymbol{\alpha}; \boldsymbol{\delta}; y)$$

and $G_n(\boldsymbol{\alpha}, y)$ respectively. The corresponding densities will be denoted by lower case letters. Thus $g_n(1, 1, \cdots, 1; y) = g_n(\mathbf{1}; y)$ is the probability density of a central χ^2 with n degrees of freedom; while $f_n(\mathbf{1}; \boldsymbol{\alpha}; y)$ corresponds to a noncentral

Received 8 July 1966; revised 2 December 1966.

[1] Supported by the Air Force Office of Scientific Research, Grant AF-AFOSR-1009-66.

[2] Supported by the Air Force Office of Scientific Research, Grant AF-AFOSR-760-65.

[3] Supported by the Air Force Office of Scientific Research, Grant AF-AFOSR-1009-66.

χ^2 with n degrees of freedom and noncentrality parameter $\sum_{i=1}^{n} \delta_i^2$. (We shall also use the notation $G(n; y)$ and $g(n; y)$ for $G_n(\mathbf{1}; y)$ and $g_n(\mathbf{1}; y)$ respectively.)

We will restrict our discussion to *positive definite forms*. For these forms, $\alpha_n > 0$.

Various methods have been used to derive expansions of $G_n(\boldsymbol{\alpha}; y)$ and $F_n(\boldsymbol{\alpha}; \boldsymbol{\delta}; y)$. Ruben [9] gives a very complete derivation of representations of these functions as series in χ^2 and noncentral χ^2 distribution functions. He gives convenient methods for obtaining the coefficients in the expansion, good estimates for the truncation error and a proof of the uniform convergence of the expansion, as well as a discussion of the best choice of the disposable parameters to improve convergence. Another form of expansion is the power series expansion given by Pachares [6] for the central case ($\boldsymbol{\delta} = \mathbf{0}$), and Shah and Khatri [12] for the noncentral case ($\boldsymbol{\delta} \neq \mathbf{0}$), using the method of Pachares. The derivation is quite complicated, and in the noncentral case leads to a double series. A proof of uniform convergence is given in each case, and error estimates are presented, of which the one given in [6] is particularly useful.

Gurland [2], [3] gives a simple derivation of an expansion of $G_n(\boldsymbol{\alpha}; y)$ in Laguerre polynomials. The expression for the coefficients is not very convenient for computation, however. The paper [3] contains an estimate of the truncation error which proves uniform convergence of the expansion in case $\alpha_1 \leqq 3\alpha_n$. For the noncentral case, Shah [11], using Gurland's method, obtains an expansion for $F_n(\boldsymbol{\alpha}; \boldsymbol{\delta}; y)$, as a double series of Laguerre polynomials. No discussion of truncation error or uniform convergence is given, and the expression for the coefficients is rather complicated.

We shall show that it is possible to derive all the above expansions by a uniform method which is in essence the same as that of Gurland [2], but which also leads to a simple and direct proof of uniform convergence and provides error estimates in all cases. The method of computing the coefficients is by a recurrence relationship, used by Ruben in his χ^2 expansions [9]. In the noncentral case, this method gives single series expansions in the power series and Laguerre series cases, more useful for computation than the double series of [11] and [12].

Because of the special nature of the central case more precise bounds on the coefficients can be obtained than in the noncentral case. For this reason, we present the two cases separately, although the second contains the first as a particular case.

The present Part I of the paper is restricted to the central case.

The general method used will now be outlined. We seek a series expansion for $g_n(\boldsymbol{\alpha}; y)$ of the form

$$g_n(\boldsymbol{\alpha}; y) = \sum_{k=0}^{\infty} c_k h_k(y) \tag{4}$$

where the sequence $\{h_k\}$ is a sequence of known functions (e.g., $h_k(y) = y^k$ for the power series expansion).

In this connection the following lemma will be used. (We will denote by $\hat{f}$ the Laplace transform of the function f defined on $[0, \infty]$.)

LEMMA 1. *Let* $\{h_k\}_0^\infty$ *be a sequence of measurable complex valued functions on* $[0, \infty]$; *let* $\{c_k\}_0^\infty$ *be a sequence of complex numbers such that*

$$\sum_{k=0}^\infty |c_k||h_k(y)| \leqq Ae^{by} \quad \textit{for almost all} \quad y \,\varepsilon\, [0, \infty], \tag{5}$$

where A, b *are real constants.*

Define

$$f(y) = \sum_{k=0}^\infty c_k h_k(y) \qquad (\textit{well defined } \text{a.e. } \textit{by } (5)).$$

Then $\hat{h}_k$ *and* $\hat{f}$ *exist for* $\operatorname{Re} s > b$, *and*

$$\hat{f}(s) = \sum_{k=0}^\infty c_k \hat{h}_k(s), \qquad \operatorname{Re} s > b.$$

The proof is an immediate consequence of Lebesgue's dominated convergence theorem.

In all types of expansions considered in the sequel we shall apply Lemma 1 with $\hat{h}_k$ of the following special form:

$$\hat{h}_k(s) = \xi(s)\eta^k(s) \tag{6}$$

where $\xi(s)$ is a non-vanishing, analytic for $\operatorname{Re} s > b$, function and η is analytic for $\operatorname{Re} s > b$ and has an inverse function ζ (i.e. $\eta(\zeta(\theta)) = \theta$). For example, in the case of the power series expansion $\xi(s) = 1/s, \eta(s) = 1/s$, if $h_k(y) = y^k/\Gamma(k+1)$.

Define

$$M(\theta) = (L_n \circ \zeta / \xi \circ \zeta)(\theta) = L_n(\zeta(\theta))/\xi(\zeta(\theta)), \tag{7}$$

where $L_n(\alpha; s)$ is the Laplace transform of $g_n(\alpha; y)$ which is known to be

$$L_n(\alpha; s) = \int_0^\infty e^{-sy} g_n(\alpha; y)\, dy = \prod_{j=1}^n (1 + 2s\alpha_j)^{-\frac{1}{2}}.$$

Assuming that $\{c_k\}_0^\infty$ and $\{h_k\}_0^\infty$ are data as in Lemma 1 and defining the function f to be

$$f(y) = \sum_{k=0}^\infty c_k h_k(y),$$

we obtain from the lemma that

$$(\hat{f} \circ \zeta / \xi \circ \zeta)(\theta) = \sum_{k=0}^\infty c_k \theta^k \tag{8}$$

for θ such that $\operatorname{Re} \zeta(\theta) > b$.

We now *choose* the coefficients c_k so that

$$M(\theta) = (\hat{f} \circ \zeta / \xi \circ \zeta)(\theta) = \sum_{k=0}^\infty c_k \theta^k. \tag{9}$$

Since M is known, we use Cauchy's inequality to obtain

$$|c_k| \leqq m(\rho)/\rho^k \tag{10}$$

where

$$m(\rho) = \max_{|\theta|=\rho} |M(\theta)| \tag{11}$$

and ρ is less than the radius of convergence of the series (9).

Using these estimates and estimates of the functions $h_k(y)$ which are derived in various ways depending on the particular functions involved, we verify that the chosen sequence $\{c_k\}$ and the given $\{h_k\}$ satisfy condition (5) of the lemma.

Therefore, by Lemma 1, the steps leading to (8) are justified, i.e.

$$\hat{f}(s) = \sum_{k=0}^{\infty} c_k \hat{h}_k(s), \qquad \text{Re } s > b.$$

On both sides of (9) replace θ by $\eta(s)$, multiply by $\xi(s)$ and use $\zeta \circ \eta(s) = s$ to obtain:

$$L_n(\alpha; s) = \hat{f}(s), \qquad \text{Re } s > b.$$

Finally, by the uniqueness of the Laplace transform we obtain

$$g_n(\alpha; y) = f(y) = \sum_{k=0}^{\infty} c_k h_k(y).$$

It also follows from (5) that $\sum_{k=0}^{\infty} c_k h_k(y)$ converges uniformly on every finite y-interval (or if $b < 0$ for all y).

On account of the uniform convergence, we may integrate term-by-term to obtain,

$$G_n(\alpha; y) = \sum_{k=0}^{\infty} c_k \int_0^y h_k(x)\, dx, \tag{12}$$

where the series is uniformly convergent on every bounded y-interval.

In the application of the above method to particular cases, we shall not distinguish between $M(\theta)$ and $f \circ \zeta / \xi \circ \zeta$ (cf. (9)) and, similarly, we shall write formally $g_n(\alpha; y) = \sum_{k=0}^{\infty} c_k h_k(y)$, subject to later justification as explained above.

The estimate (10), (or a better one if possible), is used to obtain a bound for the truncation error for the series expansion. This estimate will not always be the best possible, since direct methods, if available, usually yield improvements. This is the case in Pachares' expansion [6], so we will indicate his bounds for the error term.

2. Determination of the coefficients c_k and notation for truncation errors. Although the expression (9) defines the numbers c_k uniquely, it may not yield a particularly convenient expression for them. In the cases we are considering, the coefficients d_k of θ^k in the expansion

$$N(\theta) = \log M(\theta) = \sum_{k=1}^{\infty} d_k \theta^k / k \tag{13}$$

will be obtained in a rather simple form.

It is easy to see by differentiating (13), multiplying through by $M(\theta)$ and equating the coefficients of θ^{k-1} that:

$$\begin{aligned} c_0 &= M(0), \\ c_k &= (1/k) \sum_{r=0}^{k-1} d_{k-r} c_r, \qquad k \geqq 1, \end{aligned} \tag{14}$$

where the d_k are determined by (13).

In computations using (4), it is important to have an estimate of the truncation error. We write

$$e_N(y) = \left|\textstyle\sum_{k=N+1}^{\infty} c_k h_k(y)\right|, \tag{15}$$

and

$$E_N(y) = \left|\textstyle\sum_{k=N+1}^{\infty} c_k \int_0^y h_k(x)\,dx\right|, \tag{16}$$

with superscripts to indicate the particular series used.

Obtaining upper bounds for e_N and E_N will usually involve using (10), but other methods are possible and sometimes better.

3. Series expansions for central positive-definite forms. We seek expansions for $g_n(\alpha; y)$ in each of the following forms:

$$g_n(\alpha; y) = \textstyle\sum_{k=0}^{\infty} c_k^P(-1)^k (y/2)^{n/2+k-1}[2\Gamma(n/2+k)]^{-1} \quad (\textit{Power series}), \tag{17}$$

$$g_n(\alpha; y) = \textstyle\sum_{k=0}^{\infty} c_k^L g(n; y/\beta) k!\,\Gamma(n/2)[\beta\Gamma(n/2+k)]^{-1} L_k^{(n/2-1)}(y/2\beta) \quad (\textit{Laguerre series}) \tag{18}$$

where $\beta > 0$ is to be chosen later, $g(n; y)$ is the central χ^2 density with n degrees of freedom, and $L_k^{(a)}(x)$ is the generalized Laguerre polynomial defined by Rodrigues' formula.

$$L_k^{(a)}(x) = (1/k!)\,e^x x^{-a}(d^k/dx^k)(e^{-x}x^{k+a}), \qquad a > 1, \tag{19}$$

or by

$$\textstyle\sum_{k=0}^{\infty} L_k^{(a)}(x)t^k = (1-t)^{-a-1}\exp(-xt/(1-t)), \qquad |t| < 1. \tag{20}$$

(see Szego [13].)

Also, we seek an expansion of the form

$$g_n(\alpha; y) = \textstyle\sum_{k=0}^{\infty} c_k^C(1/\beta)g(n+2k; y/\beta) \quad (\textit{Chi-squared expansion}). \tag{21}$$

The coefficients c_k^P, c_k^L, c_k^C are required, as well as conditions for the convergence of the indicated series (if these should exist).

In connection with the estimates of the coefficients c_k for various particular cases the following formula is found to be useful:

LEMMA 2. *If $q(\theta) = -k_1\theta(1-k_2\theta)^{-1}$ where θ is complex, k_1 and k_2 are real and $k_1 > 0$, $0 < k_2 < \rho^{-1}$, then*

$$\max_{|\theta|=\rho} \exp[q(\theta)] = \exp[k_1\rho/(1+k_2\rho)].$$

PROOF:

$$\begin{aligned}
\max_{|\theta|=\rho}\exp[q(\theta)] &= \exp[\max_{|\theta|=\rho}\operatorname{Re} q(\theta)] \\
&= \exp[-k_1 \min_{|\theta|=\rho}\operatorname{Re}(1-k_2\theta)^{-1}\theta] \\
&= \exp[-(k_1/k_2)\min_{|\theta|=\rho}\operatorname{Re}\{(1-k_2\theta)^{-1}-1\}] \\
&= \exp[(k_1/k_2) - (k_1/k_2)\min_{|\theta|=\rho}\operatorname{Re}(1-k_2\theta)^{-1}] \\
&= \exp[(k_1/k_2)\{1-(1+k_2\rho)^{-1}\}] \\
&= \exp[k_1\rho/(1+k_2\rho)].
\end{aligned}$$

4. Power Series. In what follows the same notation is used as in the general method outlined in equations (4) to (12).

We first need the relationship:

$$\int_0^\infty e^{-sy}(y/2)^{n/2+k-1}[(-1)^k/2\Gamma(n/2+k)]\cdot dy = (-1)^k/(2s)^{\frac{1}{2}n+k}. \tag{22}$$

Then, comparing (6) with (22), we have

$$\xi(s) = (2s)^{-n/2}, \qquad \eta(s) = -1/2s. \tag{23}$$

Thus, putting $\theta = \eta(s)$,

$$s = -1/2\theta = \xi(\theta). \tag{24}$$

Finally

$$\begin{aligned} L_n(\alpha; \xi(\theta))/\xi[\zeta(\theta)] &= M(\theta) \\ &= (-1/\theta)^{n/2}\prod_{j=1}^n (1-\alpha_j/\theta)^{-\frac{1}{2}} \\ &= C\prod_{j=1}^n (1-\theta/\alpha_j)^{-\frac{1}{2}}, \end{aligned} \tag{25}$$

where

$$C = \prod_{j=1}^n \alpha_j^{-\frac{1}{2}}. \tag{26}$$

We may expand (25) in powers of θ provided

$$|\theta/\alpha_j| < 1, \qquad j = 1, 2, \cdots, n, \tag{27}$$

so

$$|\theta| < \min \alpha_j = \alpha_n. \tag{28}$$

By (26), (28) is equivalent to

$$|s| > 1/2\alpha_n \tag{29}$$

and this is true if

$$\operatorname{Re} s > 1/(2\alpha_n). \tag{30}$$

The coefficients c_k^P may be obtained from (25) by noticing that the factor

$$\prod_{j=1}^n (1-\theta/\alpha_j)^{-\frac{1}{2}} \tag{31}$$

is the moment generating function for the quadratic form

$$\sum_{j=1}^n (1/2\alpha_j)X_j^2. \tag{32}$$

Hence, if $\mu_k'(\alpha)$ denotes the kth moment about the origin of $g_n(\alpha; y)$, and if $\alpha^* = (1/2\alpha_n, \cdots, 1/2\alpha_1)$, then

$$\sum_{k=0}^\infty \mu_k'(\alpha^*)\theta^k/k! = \int_0^\infty e^{\theta y}g_n(\alpha^*; y)\, dy = \prod_{j=1}^n (1-\theta/\alpha_j)^{-\frac{1}{2}}. \tag{33}$$

Thus, from (25), and (33)

$$c_k^P = C\mu_k'(\alpha^*)/k!. \tag{34}$$

Since

$$\sum_{j=1}^{n} (1/2\alpha_j)X_j^2 \leqq (2\alpha_n)^{-1} \sum_{j=1}^{n} X_j^2, \tag{35}$$

so

$$\begin{aligned} \mu_k'(\boldsymbol{\alpha}^*) &= E[(\textstyle\sum_{j=1}^{n} (1/2\alpha_j)X_j^2)^k] \leqq (2\alpha_n)^{-k} E[(\textstyle\sum_{j=1}^{n} X_j^2)^k] \\ &= (2\alpha_n)^{-k} 2^k \Gamma(n/2 + k)/\Gamma(n/2), \end{aligned} \tag{36}$$

since $E[(\sum_{j=1}^{n} X_j^2)^k]$ is the kth moment of χ_n^2. Thus, from (34),

$$|c_k^P| \leqq (C/\alpha_n^k)\Gamma(n/2 + k)/k!\,\Gamma(n/2). \tag{37}$$

Thus, in the series (17),

$$\begin{aligned} &\textstyle\sum_{k=0}^{\infty} |c_k^P|(y/2)^{n/2+k-1}/2\Gamma(n/2 + k) \\ &\quad \leqq (C/2\Gamma(n/2))(y/2)^{n/2-1} \textstyle\sum_{k=0}^{\infty} (y/2\alpha_n)^k/k! \\ &\quad = (C/2\Gamma(n/2))(y/n)^{n/2-1} \exp (y/2\alpha_n), \qquad y > 0. \end{aligned} \tag{38}$$

This proves the uniform absolute convergence of the series (17) for bounded y-intervals, and also justifies taking the Laplace transform of the series term-by-term if Re $s > 1/2\alpha_n$. Hence, using Lemma 1, and the uniqueness theorem for the Laplace transform,

$$g_n(\boldsymbol{\alpha}; y) = (y/2)^{n/2-1} \sum_{k=0}^{\infty} c_k^P(-1)^k(y/2)^k/2\Gamma(n/2 + k). \tag{39}$$

Integrating (39) term-by-term,

$$G_n(\boldsymbol{\alpha}; y) = (y/2)^{n/2} \sum_{k=0}^{\infty} c_k^P(-1)^k(y/2)^k/\Gamma(n/2 + k + 1). \tag{40}$$

The coefficients c_k^P are determined by equations (14) with $M(0) = C$, $d_k^P = \frac{1}{2}\sum_{j=1}^{n} \alpha_j^{-k}$ $(k \geqq 1)$.

The error terms e_N^P and E_N^P may be estimated, using (37). We have

$$\begin{aligned} e_N^P(y) &= |\textstyle\sum_{k=N+1}^{\infty} c_k^P(y/2)^{n/2-1}(-y/2)^k/2\Gamma(n/2 + k)| \\ &\leqq C(y/2)^{n/2-1} \textstyle\sum_{k=N+1}^{\infty} (y/2\alpha_n)^k/2\Gamma(n/2)k! \\ &\leqq (1/2\Gamma(n/2))(y/2\alpha_n)^{n/2+N} e^{y/2\alpha_n}/\alpha_n(N + 1)!, \quad \text{since } C \leqq \alpha_n^{-n/2}. \end{aligned} \tag{41}$$

In fact, a better estimate of $e_N^P(y)$ may be obtained by the method of Pachares, as we shall indicate later.

For $E_N^P(y)$, we could use the method indicated in (41) to obtain a similar estimate. However, we may proceed as follows: (cf. Pachares [6]). By definition, if $X = (X_1, X_2, \cdots X_n)'$, and putting $Z_j = X_j(\alpha_j/y)^{\frac{1}{2}}$,

$$\begin{aligned} G_n(\boldsymbol{\alpha}; y) &= (2\pi)^{-n/2} \textstyle\int_{\Sigma\alpha_j x_j^2 \leqq y} \exp(-\frac{1}{2}|X|^2)\, d\mathbf{x} \\ &= (2\pi)^{-n/2} C y^{n/2} \textstyle\int_{\Sigma Z_j^2 \leqq 1} \exp(-\frac{1}{2}y \sum_{j=1}^{n} Z_j^2/\alpha_j)\, d\mathbf{Z} \\ &= (2\pi)^{-n/2} C_y^{n/2} \textstyle\sum_{k=0}^{\infty} (-y/2)^k(1/k!) \int_{\Sigma Z_j^2 \leqq 1} (\sum_{j=1}^{n} Z_j^2/\alpha_j)^k\, d\mathbf{Z}. \end{aligned} \tag{42}$$

By the uniqueness of the power series expansion, comparing (40) and (42), we have

(43) $$c_k^P = (C\Gamma(n/2 + k + 1)/k!\,\pi^{n/2}) \int_{\Sigma Z_j^2 \leqq 1} (\textstyle\sum_{j=1}^n Z_j^2/\alpha_j)^k \, d\mathbf{Z}.$$

For the exponential series, for $t \geqq 0$, and integer r,

(44) $$\textstyle\sum_{k=0}^{2r} (-t)^k/k! \geqq e^{-t} \geqq \sum_{k=0}^{2r+1} (-t)^k/k!\,.$$

Thus,

$$\begin{aligned} E_N^P(y) &= |\textstyle\sum_{k=N+1}^\infty c_k^P(-1)^k(y/2)^{n/2+k}/\Gamma(n/2 + k + 1)| \\ &= C(y/2)^{n/2}|\pi^{-n/2} \int_{\Sigma Z_j^2 \leqq 1} \textstyle\sum_{k=N+1}^\infty (1/k!)(-\tfrac{1}{2}y \sum_{j=1}^n Z_j^2/\alpha_j)^k \, d\mathbf{Z}| \\ &\leqq C(y/2)^{n/2}\pi^{-n/2} \int_{\Sigma Z_j^2 \leqq 1} (1/(N + 1)!)(\tfrac{1}{2}y \textstyle\sum_{j=1}^n Z_j^2/\alpha_j)^{N+L} \, d\mathbf{Z} \\ &\qquad\qquad\qquad\qquad (\text{using } (44), \text{ to estimate } \textstyle\sum_{N+1}^\infty) \\ &= (y/2)^{n/2+N+1}c_{N+1}^P/\Gamma(n/2 + N + 2), \quad \text{using } (43) \text{ with } k = N + 1 \end{aligned}$$

Now, using (37) to estimate c_{N+1}^P, one obtains

(45) $$\begin{aligned} E_N^P(y) &\leqq (y/2)^{n/2+N+1}C\Gamma(n/2 + N + 1) \\ &\qquad \cdot[\alpha_n^{N+1}(N + 1)!\,\Gamma(n/2)\Gamma(n/2 + N + 2)]^{-1} \\ &\leqq (y/2\alpha_n)^{n/2+N+1}/(N + 1)!\,(n/2 + N + 1)\Gamma(n/2). \end{aligned}$$

To estimate $e_N^P(y)$ by this method, note that, using (43)

(46) $$\begin{aligned} e_N^P(y) &= (y/2)^{n/2-1}C/\pi^{-n/2} \\ &\quad \cdot|\int_{\Sigma Z_j^2 \leqq 1} (n/2)\{\textstyle\sum_{k=N+1}^\infty (1/k!\,2)(-\tfrac{1}{2}y \sum_{j=1}^n Z_j^2/\alpha_j)^k\} \, d\mathbf{Z} \\ &\quad + \int_{\Sigma Z_j^2 \leqq 1} \{\textstyle\sum_{k=N+1}^\infty (1/(k - 1)!\,2)(-\tfrac{1}{2}y \sum_{j=1}^n Z_j^2/\alpha_j)^k\} \, d\mathbf{Z} \\ &\leqq (y/2)^{n/2-1}C\pi^{-n/2} \\ &\quad \cdot\{|\int_{\Sigma Z_j^2 \leqq 1} (n/2)\cdot\tfrac{1}{2}(-\tfrac{1}{2}y\textstyle\sum_{j=1}^n Z_j^2/\alpha_j)^{N+1} \, d\mathbf{Z}|\cdot 1/(N + 1)! \\ &\quad + (1/N!)|\int_{\Sigma Z_j^2 \leqq 1} \tfrac{1}{2}(-\tfrac{1}{2}y\textstyle\sum_{j=1}^n Z_j^2/\alpha_j)^{N+1} \, d\mathbf{Z}|\} \\ &\leqq (y/2)^{n/2+N}c_{N+1}^P/2\Gamma(n/2 + N + 1) \\ &\leqq (y/2\alpha_n)^{n/2+N}(n/2 + N + 1)/2(N + 1)!\,\Gamma(n/2)\alpha_n\,. \end{aligned}$$

This estimate is generally better than (41) except for quite small y.

Formulas (40) and (45) were obtained by Pachares [6] by a different method and by Robbins [7], who gave a more complicated expression for the c_k^P.

5. Laguerre Expansion. We now seek an expansion of the form (18). From Szego ([13], p. 370) we have

(47) $$\int_0^\infty e^{-sy}k!\,[2\beta\Gamma(n/2 + k)]^{-1}(y/2\beta)^{n/2-1}e^{-y/2}L_k^{(n/2-1)}(y/2\beta) \, dy = (1 + 2s\beta)^{-n/2-k}(2s\beta)^k.$$

Comparing with (6), we have

(48) $$\xi(s) = (1 + 2s\beta)^{-n/2}; \qquad \eta(s) = 2s\beta/(1 + 2s\beta).$$

Thus, with $\theta = \eta(s)$, we have

(49) $$s = \theta/2\beta(1 - \theta) = \zeta(\theta), \quad \text{and} \quad 1 + 2s\beta = (1 - \theta)^{-1}.$$

Then

(50) $$\begin{aligned} M(\theta) &= (1 - \theta)^{-n/2} \textstyle\prod_{j=1}^{n} (1 + (\alpha_j/\beta)\cdot\theta/(1 - \theta))^{-\frac{1}{2}} \\ &= \textstyle\prod_{j=1}^{n} (1 - \gamma_j\theta)^{-\frac{1}{2}}, \end{aligned}$$

where

(51) $$\gamma_j = 1 - \alpha_j/\beta, \qquad j = 1, 2, \cdots, n.$$

Note that $M(\theta)$ is the moment generating function of $g_n(\gamma/2; y)$, where $\gamma = (\gamma_1, \cdots, \gamma_n)'$, hence

(52) $$c_k^{\,L} = \mu_k'(\gamma)/2^k k!, \qquad k = 0, 1, \cdots.$$

The conditions under which

(53) $$M(\theta) = \textstyle\sum_{k=0}^{\infty} c_k^{\,L}\theta^k,$$

are

(54) $$|\gamma_j\theta| < 1, \quad \text{for all} \quad j = 1, \cdots, n.$$

Hence, if

(55) $$\epsilon = \max_{1 \leq j \leq n} |\gamma_j|,$$

we must have

(56) $$|\theta| < 1/\epsilon.$$

In order to be able to apply the Laplace transform to (18), the expansion (53) must hold for Re $s > b$, where $s = \zeta(\theta)$ and b is some positive number.

Since ζ is a bilinear mapping, the image of $|\theta| = \rho$ (where ρ is some positive number) is a circle c_ρ (or straight line) in the s-plane with center

(57) $$s_0 = \sigma_0 + i\tau_0 = -\rho^2/2\beta(\rho^2 - 1),$$

and radius

(58) $$r_0 = \rho/2\beta(\rho^2 - 1).$$

(Note that C_1 is the imaginary axis.) Figure 1 shows the circle c_ρ.

Since $r_0 > 0$,

(59) $$1 < \rho.$$

Thus, if the image of $|\theta| < 1/\epsilon$ is to contain a half-plane Re $s > b$, we must have

(60) $$\epsilon < 1.$$

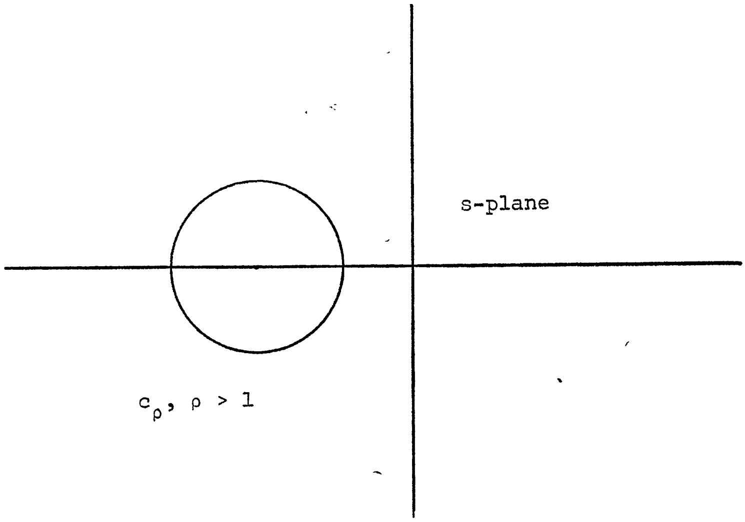

FIG. 1

Equivalently,

$$\max_j |1 - \alpha_j/\beta| < 1 \tag{61}$$

or

$$\beta > \tfrac{1}{2} \max \alpha_j = \tfrac{1}{2}\alpha_1 , \tag{62}$$

and, in this case, the image of $|\theta| < 1/\epsilon$ in the s-plane contains

$$\operatorname{Re} s > -1/2\beta(\epsilon + 1). \tag{63}$$

Bounds for the coefficients c_k^L from (59) may be obtained using exactly the same method as in finding (39). They are:

$$| c_k^L | \leqq \epsilon^k \Gamma(n/2 + k)/k!\, \Gamma(n/2). \tag{64}$$

In order to obtain a bound of the form (5), we use the generating function (see (20)):

$$\sum_{k=0}^{\infty} L_k^{(n/2-1)}(x)t^k = (1 - t)^{-n/2} \exp(-xt/(1 - t)), \quad \text{for} \quad |t| < 1. \tag{65}$$

Using Lemma 2, we obtain:

$$\begin{aligned} \eta(R; x) &= \max_{|t|=R} |(1 - t)^{-n/2} \exp(-xt/(1 - t))| \\ &\leqq (1 - R)^{-n/2} \exp(xR/(1 + R)), \quad \text{for} \quad x \geqq 0. \end{aligned} \tag{66}$$

Moreover, by Cauchy's inequality

$$\begin{aligned} |L_k^{(n/2-1)}(x)| &\leqq \eta(R; x)/R^k, \qquad \text{for any } R \text{ with } 0 < R < 1, \\ &\leqq (1 - R)^{-n/2}R^{-k} \exp(xR/(1 + R)) \\ &\leqq e^{x/2}/(1 - R)^{n/2}R^k. \end{aligned} \tag{67}$$

Inserting these bounds in (18), we have

$$(68)\quad \sum_{k=0}^{\infty} |c_k^L| [g(n; y/\beta) k!\, \Gamma(n/2)/\beta\Gamma(n/2 + k)] |L_k^{(n/2-1)}(y/2\beta)| \\ \leqq (1/\beta) g(n; y/\beta)(1 - R)^{-n/2} e^{y/4\beta}(1 - \epsilon/R)^{-1},$$

provided we choose R to satisfy $\epsilon < R < 1$. This establishes uniform convergence of (18) for all bounded intervals of $y > 0$, so that the Laplace transform of the series may be taken term-by-term for Re $s \geqq 0$. Hence the series converges uniformly for all $y > 0$; provided $\beta > \frac{1}{2}\alpha_1$.

The c_k^L are determined by the equations (14) with $M(0) = 1$, $d_k = \frac{1}{2}\sum_{j=1}^{n} \gamma_j^k$.

To obtain the series for $G_n(\alpha; y)$, we use Rodrigues formula (19) to derive

$$(69)\quad \int_0^y (1/2\beta) e^{-x/2\beta}(x/2\beta)^{n/2-1} L_k^{(n/2-1)}(x/2\beta)\, dx \\ = (1/k) e^{-y/2\beta}(y/2\beta)^{n/2} L_{k-1}^{(n/2)}(y/2\beta), \quad \text{for} \quad k \geqq 1.$$

For $k = 0$, we have instead, by definition

$$(70)\quad \int_0^y (1/2\beta)(e^{-x/2\beta}/(n/2))(x/2\beta)^{n/2-1} L_k^{(n/2-1)}(x/2\beta)\, dx \\ = (1/2^{n/2}\Gamma(n/2)) \int_0^{y/\beta} x^{n/2-1} e^{-x/2}\, dx = G(n; y/\beta)$$

where $G(n; y)$ is the cumulative distribution function of χ^2 with ν d.f.

Then, from (18), since that series converges uniformly for all $y \geqq 0$, we may integrate term-by-term to obtain

$$(71)\quad G_n(\boldsymbol{\alpha}; y) = G(n; y/\beta) + \sum_{k=1}^{\infty} (c_k^L (k - 1)!/\Gamma(n/2 + k)) \\ \cdot (y/2\beta)^{n/2} e^{-y/2} L_{k-1}^{(n/2)}(y/2\beta).$$

Or, using the definition of $g(n + 2; y/2\beta)$,

$$(72)\quad G_n(\boldsymbol{\alpha}; y) = G(n; y/\beta) + \sum_{k=1}^{\infty} c_k^L (2(k - 1)!\Gamma(n/2 + 1)/\Gamma(n/2 + k)) \\ \cdot g(n + 2; y/\beta)\, L_{k-1}^{(n/2)}(y/2\beta)$$

where the series converges uniformly and absolutely for all $y \geqq 0$, provided $\beta > \frac{1}{2}\alpha_1$.

Formulae (18) and (71) are being used as bases for constructing computer routines for calculation of $g_n(\boldsymbol{\alpha}; y)$ and $G_n(\boldsymbol{\alpha}; y)$.

An estimate for $e_N^L(y)$ using (64) and (67) is

$$(73)\quad e_N^L(y) \leqq (1/\beta) g(n; y/\beta) \inf_{\epsilon<R<1} \{(\epsilon/R)^{N+1}(1 - \epsilon/R)^{-1}(1 - R)^{-n/2} \\ \cdot \exp((y/2\beta)\cdot R/(1 + R))\}.$$

A choice of R which makes the formula take a simple form (but which may not be best from other points of view) is $R = \epsilon^{\frac{1}{2}}$. Since $R/(1 + R) < \frac{1}{2}$ for $R < 1$, we have for this choice

$$(74)\quad e_N^L(y) \leqq (1/\beta) g(n; y/\beta) e^{y/4\beta}(1 - \epsilon^{\frac{1}{2}})^{-n/2-1} \epsilon^{\frac{1}{2}(N+1)}.$$

Similarly,

$$(75)\quad E_N^L(y) \leqq (n/(N+1))g(n+2;\, y/\beta) \cdot \min_{\epsilon<R<1}\{R(1-R)^{-(n/2+1)}[\exp(yR/2(1+R))](\epsilon/R)^{N+1}/(1-\epsilon/R)\}.$$

Again taking the special case $R = \epsilon^{\frac{1}{2}}$, since $\exp(yR/2\beta(1+R)) < e^{y/4\beta}$,

$$(76)\quad E_N^L(y) \leqq (n/(N+1))g(n+2;\, y/\beta)e^{y/4\beta}\epsilon^{\frac{1}{2}(N+2)}/(1-\epsilon^{\frac{1}{2}})^{n/2+2}.$$

Formulae (74) and (76) are being used in control of accuracy in the computer routines referred to earlier.

In [2], Gurland derived formula (71) by inverting the characteristic function. Pointwise convergence only was proved. In [3] Gurland investigated the error term $E_N(y)$ by use of the characteristic function. He showed then that the series expansion for $M(\theta)$ is uniformly convergent for all y, provided β satisfies

$$(77)\qquad \tfrac{2}{3}\alpha_1 < \beta < 2\alpha_n\,,$$

so that the α_j must satisfy

$$(78)\qquad \alpha_n > \tfrac{1}{3}\alpha_1\,.$$

There is no such restriction in the bounds (75) and (76).

The error estimate in [3] does not involve y, and hence does not tend to zero with increasing y as do (75) and (76).

Since the rates of convergence of (18) and (71) depend essentially on the size of $\epsilon = \max|1-\alpha_j/\beta|$, it would seem wise to choose β so that ϵ is as small as possible. Hence, we consider taking β to make ϵ equal to

$$(79)\qquad \epsilon_0 = \inf_{\beta>0}\max_{1\leqq j\leqq n}|1-\alpha_j/\beta| = (\alpha_1-\alpha_n)/(\alpha_1+\alpha_n).$$

Straightforward algebraic calculations show that this requires $\beta = \frac{1}{2}(\alpha_1+\alpha_n)$. (It should be noted that, for given β, the bounds (73) and (75) for e_N^L and E_N^L are increasing functions of ϵ.)

In an abstract [4], Hotelling indicated that he had obtained a Laguerre expansion for $g_n(\boldsymbol{\alpha}; y)$. Grad and Solomon [1] gave a few more details of Hotelling's method, though neither [1] nor [4] gave an explicit formula for the coefficients c_k^L, and conditions for convergence of the expansion were not indicated. Essentially, in Hotelling's method, β is not mentioned explicitly but is taken at the outset to be $(1/n)\sum_{j=1}^n \alpha_j$, making $c_1^L = 0$. The first five coefficients c_k^L are given in Grad and Solomon [1], when $\beta = (1/n)\sum_{j=1}^n \alpha_j$, and were used by them to compute $G_n(\boldsymbol{\alpha}; y)$ for various $\boldsymbol{\alpha}$. For $\boldsymbol{\alpha} = (1.2, 0.9, 0.9)$, the approximation is accurate to 4 decimal places. For $\boldsymbol{\alpha} = (2.1, 0.6, 0.3)$, $\beta = 1$, for which $\beta > \frac{1}{2}\alpha_1$ is not satisfied, the approximation was quite poor, as would be expected, since then the series (18) and (71) are not convergent.

It should be mentioned here that the numbers d_k^L, by which the coefficients c_k^L are determined using (14), may be obtained without explicitly determining the eigenvalues of the matrix VA. For, the numbers $1-(\alpha_j/\beta) = \gamma_j$ are the eigenvalues of $I-(1/\beta)VA$, and hence

(80) $$d_k^L = \tfrac{1}{2}\textstyle\sum_{j=1}^n \gamma_j^k = \tfrac{1}{2}\operatorname{tr}(I - (1/\beta)VA)^k.$$

6. Representation in series of χ^2's. We now seek the coefficients c_k^C in the expansion of $g_n(\alpha; y)$ in χ^2 density functions, as in (21). By our general formulation of the method of obtaining such expansions, we shall need

(81) $$\textstyle\int_0^\infty e^{-sy}(1/\beta)g(n + 2k; y/\beta)\, dy = (1 + 2s\beta)^{-n/2-k}.$$

Comparing with (6), we have

(82) $$\xi(s) = (1 + 2s\beta)^{-n/2}, \qquad \eta(s) = (1 + 2s\beta)^{-1}.$$

Hence, if $\theta = \eta(s)$, then

(83) $$s = (1 - \theta)/2\beta\theta = \zeta(\theta); \qquad \xi[\zeta(\theta)] = \theta^{n/2}.$$

As described in the introduction (equation (7)), we expand $M(\theta)$ in powers of θ, where in this case

(84) $$\begin{aligned} M(\theta) &= \textstyle\prod_{j=1}^n (\beta/\alpha_j)^{\frac{1}{2}}\{1 - (1 - \beta/\alpha_j)\theta\}^{-\frac{1}{2}} \\ &= \textstyle\sum_{k=0}^\infty c_k^C\theta^k, \end{aligned}$$

provided

(85) $$|\theta| < \min |1 - \beta/\alpha_j|^{-1} = 1/\epsilon,$$

with $\epsilon = \max |1 - \beta/\alpha_j|$. From (82) this means

(86) $$|1 + 2s\beta| > \max |1 - \beta/\alpha_j|$$

and hence (84) holds at least for

(87) $$\operatorname{Re} s > (1/2\beta)\{\max |1 - \beta/\alpha_j| - 1\}.$$

As in the previous two cases, we can recognize $M(\theta)$ as a constant multiple of the moment generating function of $g_n(\gamma/2; y)$, where in this case

(88) $$\gamma_j = 1 - \beta/\alpha_j, \qquad \gamma = (\gamma_1, \gamma_2, \cdots, \gamma_n)'.$$

(There should be no confusion with the values of γ given in the Laguerre expansion.) Thus, from (84) and (85)

(89) $$c_k^C = A\mu_k'(\gamma)/2^k k!,$$

where $A = \prod_{j=1}^n (\beta/\alpha_j)^{\frac{1}{2}}$. Then, just as in deriving (37) and (64), since $\epsilon = \max |\gamma_j|$,

(90) $$\mu_k'(\gamma) \leqq \epsilon^k 2^k \Gamma(n/2 + k)/\Gamma(n/2),$$

so that

(91) $$|c_k^C| \leqq A\epsilon^k\Gamma(n/2 + k)/k!\, \Gamma(n/2)$$

hence

(92) $$\textstyle\sum_{k=0}^\infty |c_k^C| \cdot |(1/\beta)g(n + 2k; y/\beta)| \leqq A(1/\beta)g(n; y/\beta)e^{\epsilon y/2\beta},$$

which establishes the uniform convergence of the series on the right of (21) for any bounded interval of y (and for *all* y if $\epsilon < 1$). Thus we can take the Laplace transform of each side of (21) for Re $s > 1/2\beta(\epsilon - 1)$, and by (84) (and (87)) the transforms will be equal, so equality actually holds in (21), and the series is uniformly convergent in any bounded y-interval of $y > 0$, for any β, and uniformly convergent for all $y > 0$ if β is chosen so that $\epsilon = \max |1 - \beta/\alpha_j| < 1$.

Integrating term-by-term, we obtain the following series, uniformly convergent on any bounded y-interval of $y > 0$.

$$G_n(\boldsymbol{\alpha}; y) = \sum_{k=0}^{\infty} c_k^C G(n + 2k; y/\beta). \tag{93}$$

The c_k^C are determined by (14) with $M(0) = A$; $d_k^C = \frac{1}{2}\sum_{j=1}^{n} (1 - \beta\alpha_j^{-1})^k$, $(k \geqq 1)$.

To estimate the error terms $e_N^C(y)$ and $E_N^C(y)$, we again use (91) (compare (92)), and obtain

$$\begin{aligned} e_N^C &\leqq A(1/\beta)[\epsilon^{N+1}/(N + 1)!](y/2\beta)^{n/2+N} \exp[-\tfrac{1}{2}y(1 - \epsilon)/\beta]2\Gamma(n/2) \\ &= (\Gamma(n/2 + N + 1)/\Gamma(n/2))A(1/\beta)(\epsilon^{N+1}/(N + 1)!) \\ &\quad \cdot g(n + 2N + 2; (1 - \epsilon)y/\beta)(1 - \epsilon)^{n/2-N}, \qquad 0 < \epsilon < 1. \end{aligned} \tag{94}$$

The choice of the bound to be used (i.e. value of ϵ) will depend on circumstances. The estimate for $E_N^C(y)$ is most simply obtained by integrating $e_N^C(y)$, giving, for $0 < \epsilon < 1$,

$$\begin{aligned} E_N^C(y) \leqq{} & A[\Gamma(n/2 + N + 1)/\Gamma(n/2)][\epsilon^{N+1}/(N + 1)!](1 - \epsilon)^{-n/2-N-1} \\ & \cdot G(n + 2N + 2; (1 - \epsilon)y/\beta) \end{aligned} \tag{95}$$

and, for $\epsilon > 1$,

$$\begin{aligned} E_N^C(y) \leqq{} & [A/\Gamma(n/2)]\Gamma(n/2 + N + 1)(\epsilon^{N+1}/(N + 1)!)\,(y/2\beta)^{n/2+N+1} \\ & \cdot \exp[(\epsilon - 1)y/2\beta]. \end{aligned} \tag{96}$$

(A is defined in (89).)

Formula (93) was derived by Ruben in [9]. Recursion formulae for the coefficients and the error bound (96) were also derived by Ruben [9]. Particular cases of (93) had been obtained in various ways by Robbins [7], when $\beta^n = \prod_{j=1}^{n} \alpha_j$, and by Robbins and Pitman [8], when $\beta = \alpha_n$.

For some choices of β, (21) and (93) are mixture representations. In this case the coefficients c_k^C satisfy (see Robbins and Pitman [8]):

$$c_k^C \geqq 0, \quad \text{and} \quad \sum_{k=0}^{\infty} c_k^C = 1. \tag{97}$$

Ruben [9] considered the question of determining the values of β for which (93) is a mixture representation. Some results are as follows: For $0 < \beta \leqq \alpha_n$, (93) is a mixture. If α_H is the harmonic mean of the α_j, then for $\beta > \alpha_H$, (93) is not a mixture. For $\alpha_n < \beta < \alpha_H$ the answer depends on the distribution of the values of the α_j, and examples are given in [9] of distribution of the α_j, for which $\beta = \alpha_H$ does give a mixture representation.

Ruben [9] also discusses the best choice of β for computational purposes and suggests that the choice $\beta = 2\alpha_1\alpha_n(\alpha_1 + \alpha_n)^{-1}$ may be close to the optimal choice, and is certainly better than $\beta = \alpha_1$ or $\beta = \alpha_n$.

A justification for the choice $\beta = 2\alpha_1\alpha_n(\alpha_1 + \alpha_n)^{-1}$ can be given here, in much the same way as it was done for the Laguerre expansion, if we observe that from (94) it would seem that the best choice of ϵ, independent of y is one in which ϵ/β is as small as possible.

Ruben [9] points out that the fact that the series (93) converges uniformly for all y if $\epsilon < 1$ implies that, for such ϵ, we make $y = \infty$ in (93) to obtain

$$\sum_{k=0}^{\infty} c_k^{\,C} = 1, \qquad \text{if } \epsilon < 1. \tag{98}$$

The condition $\epsilon < 1$ means

$$\max |1 - \beta/\alpha_j| < 1 \quad \text{or} \quad \beta < 2\alpha_n . \tag{99}$$

Ruben [9] shows that $\beta < 2\alpha_n$ is necessary and sufficient in order that $\Sigma c_k^{\,C} = 1$.

We note that the numbers $d_k^{\,C}$ which are given by

$$d_k^{\,C} = \tfrac{1}{2} \operatorname{tr} (I - \beta A^{-1}V^{-1})^k \tag{100}$$

may be computed without calculating the eigenvalues of VA. The matrix VA must be inverted, but this is usually simpler than calculating the eigenvalues.

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