

ASYMPTOTIC EXPANSIONS FOR THE JOINT AND MARGINAL DISTRIBUTIONS OF THE LATENT ROOTS OF THE COVARIANCE MATRIX

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Let nS be an $m \times m$ matrix having the Wishart distribution $W_m(n, \Sigma)$. For large n and simple latent roots of Σ , it is known that the latent roots of S are asymptotically independently normal. In this paper an expansion, up to and including the term of order n^{-1} , is given for the joint density function of the roots of S in terms of normal density functions. Expansions for the marginal distributions of the roots are also given, valid when the corresponding roots of Σ are simple.

1. Introduction and summary. Let S be the covariance matrix formed from a sample of size $n + 1$ drawn from an m -variate normal distribution with population covariance matrix Σ (assumed to be positive definite); then nS has the Wishart distribution (see e.g. T. W. Anderson [2], page 157). Let $l_1 > l_2 > \dots > l_m > 0$ and $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_m > 0$ denote the latent roots of S and Σ respectively. It is known (Girshick [6], T. W. Anderson [3]) that if λ_i is a simple root then, for large n , l_i is asymptotically independent of the other sample roots and the limiting distribution of $(n/2)^{1/2}(l_i/\lambda_i - 1)$ is standard normal $N(0, 1)$. We will assume throughout this paper that all the roots of Σ are simple. The extreme roots l_1 and l_m are first considered in Section 2. Sugiyama [15] has shown that the distribution function of l_1 can be expressed in a form involving a confluent hypergeometric function ${}_1F_1$ of matrix argument. It is shown that the distribution function of l_m can be expressed in terms of another confluent hypergeometric function defined earlier by Muirhead [13]. Then a system of partial differential equations (pde's) is used to expand the two distribution functions up to and including terms of order n^{-1} .

In Section 3 an expansion is given, up to and including the term of order n^{-1} , for the joint density function of l_1, \dots, l_m in terms of normal density functions. This expansion then yields an expansion for the marginal density function of l_i which has also been obtained by Sugiura [14] using another method.

2. Expansions of the extreme root distributions. We consider first the largest root l_1 . Sugiyama [15], [16] has shown that the distribution function of l_1 can

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be expressed in the form

$$(2.1) \quad P(l_1 < y) = \left[\frac{\Gamma_m(p)(\frac{1}{2}ny)^{\frac{1}{2}mn}}{\Gamma_m(\frac{1}{2}n + p)} \right] (\det \Sigma)^{-\frac{1}{2}n} {}_1F_1(\frac{1}{2}n; \frac{1}{2}n + p; -\frac{1}{2}ny\Sigma^{-1}),$$

where $p = (m + 1)/2$, $\Gamma_m(a) = \pi^{m(m-1)/4} \prod_{i=1}^m \Gamma(a - (i - 1)/2)$ and ${}_1F_1$ is a confluent hypergeometric function of matrix argument (see Herz [7], Constantine [5]). Since (2.1) depends on Σ only via its latent roots we can regard Σ as being diagonal, i.e. $\Sigma = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)$. An expansion for large n has been obtained for the ${}_1F_1$ function in (2.1) by Muirhead [12]; however this expansion is of limited interest since it is valid only over the range $0 \leq y < \lambda_m$ and one would usually be interested in the upper tail of the distribution. Using (2.1) Sugiyama [16] has obtained an approximation to $P(l_1 < y)$ in terms of a product of χ^2 probabilities.

Now assume that $\lambda_1, \dots, \lambda_m$ are all distinct; from (2.1) the distribution function of $x_1 = (n/2)^{\frac{1}{2}}(l_1/\lambda_1 - 1)$ can be written as

$$(2.2) \quad P(x_1 < x) = [\Gamma_m(p)/\Gamma_m(\frac{1}{2}n + p)](\det R)^{n/2} {}_1F_1(\frac{1}{2}n; \frac{1}{2}n + p; -R),$$

where $R = \text{diag}(r_1, r_2, \dots, r_m)$ with $r_i = [n/2 + (n/2)^{\frac{1}{2}}x]z_i$, $z_i = \lambda_i/\lambda_1$ ($i = 1, 2, \dots, m$). (Note that $z_1 = 1$ is a dummy variable and the R.H.S. of (2.2) is a function of x, z_2, \dots, z_m .) A system of pde's satisfied by the ${}_1F_1$ function has been given by Muirhead [12]. Starting with this system it can be readily verified that $P \equiv P(x_1 < y)$ satisfies each of the m pde's

$$(2.3) \quad \begin{aligned} & \frac{\partial^2 P}{\partial x^2} + x \frac{\partial P}{\partial x} + \left(\frac{2}{n}\right)^{\frac{1}{2}} \left[2x \frac{\partial^2 P}{\partial x^2} + (1 + x^2 - \frac{1}{2}A_1) \frac{\partial P}{\partial x} - x \sum_{k=2}^m z_k \frac{\partial P}{\partial z_k} \right. \\ & - 2 \sum_{k=2}^m z_k \frac{\partial^2 P}{\partial x \partial z_k} \left. \right] + \frac{2}{n} \left[x^2 \frac{\partial^2 P}{\partial x^2} + x(1 - \frac{1}{2}A_1) \frac{\partial P}{\partial x} \right. \\ & + \sum_{k=2}^m z_k \left(1 + \frac{1}{2}A_1 - \frac{1}{2(1 - z_k)} \right) \frac{\partial P}{\partial z_k} - 2x \sum_{k=2}^m z_k \frac{\partial^2 P}{\partial x \partial z_k} \\ & \left. + \sum_{k=2}^m \sum_{j=2}^m z_j z_k \frac{\partial^2 P}{\partial z_k \partial z_j} \right] = 0 \end{aligned}$$

and

$$(2.4) \quad \begin{aligned} & (z_i - 1) \frac{\partial P}{\partial z_i} + \left(\frac{2}{n}\right)^{\frac{1}{2}} \left[\frac{1}{2(1 - z_i)} \frac{\partial P}{\partial x} + xz_i \frac{\partial P}{\partial z_i} \right] \\ & + \frac{2}{n} \left[z_i \frac{\partial^2 P}{\partial z_i^2} + \frac{x}{2(1 - z_i)} \frac{\partial P}{\partial x} + (1 - \frac{1}{2}A_i) \frac{\partial P}{\partial z_i} \right. \\ & \left. - \frac{1}{2(1 - z_i)} \sum_{k=2}^m z_k \frac{\partial P}{\partial z_k} - \frac{1}{2} \sum_{j=2, j \neq i}^m \frac{z_j}{z_i - z_j} \frac{\partial P}{\partial z_j} \right] = 0 \end{aligned} \quad (i = 2, 3, \dots, m),$$

where

$$(2.5) \quad A_i = \sum_{j=1, j \neq i}^m \frac{z_j}{z_j - z_i} \quad (i = 1, 2, \dots, m).$$

We now look for a solution of these m pde's (2.3) and (2.4) of the form

$$(2.6) \quad P = \Phi(x) + \sum_{k=1}^{\infty} (2/n)^{k/2} Q_k,$$

where $\Phi(\cdot)$ denotes the standard normal distribution function and the Q_k are functions of x, z_2, \dots, z_m . (That P possesses such an expansion follows from results in the next section.) We substitute the series (2.6) into (2.3) and (2.4) and equate coefficients of powers of $(2/n)^{1/2}$ on the L.H.S.'s to zero. Equating the constant term in (2.3) to zero gives

$$d^2\Phi(x)/dx^2 + x d\Phi(x)/dx = 0,$$

verifying that $\Phi(x) = (2\pi)^{-1/2} \int_{-\infty}^x \exp(-t^2/2) dt$ is indeed the correct limiting distribution function. Now equate the coefficient of $(2/n)^{1/2}$ in (2.4) to zero. We obtain

$$(z_i - 1)\partial Q_1/\partial z_i + (1 - z_i)^{-1}\varphi(x)/2 = 0, \quad (i = 2, 3, \dots, m)$$

where $\varphi(\cdot)$ denotes the standard normal density function. This may be solved to give Q_1 in the form

$$(2.7) \quad Q_1 = -A_1\varphi(x)/2 + f(x),$$

where A_1 is given by (2.5) and $f(x)$ is a function of x alone, which has yet to be determined. Equating the coefficient of $(2/n)^{1/2}$ in (2.3) to zero gives

$$(2.8) \quad \partial^2 Q_1/\partial x^2 + x \partial Q_1/\partial x + [1 - x^2 - \frac{1}{2}A_1]\varphi(x) = 0.$$

Substituting (2.7) in (2.8) gives

$$d^2f/dx^2 + x df/dx + (1 - x^2)\varphi(x) = 0,$$

the complete solution of which is

$$f(x) = (1 - x^2)\varphi(x)/3 + k_1\Phi(x) + k_2,$$

where k_1 and k_2 are arbitrary constants. The boundary conditions $P(x_1 < \infty) = 1$ and $P(x_1 < -\infty) = 0$ may be used to show that $k_1 = k_2 = 0$. Hence we have

$$(2.9) \quad Q_1 = -\frac{1}{6}\varphi(x)[2H_2(x) + 3A_1H_0(x)],$$

where $H_j(x)$ denotes the Hermite polynomial of degree j (tabulated to $j = 10$ in Kendall and Stuart [9], page 155). Similarly, equating the coefficient of $2/n$ in the L.H.S.'s of (2.3) and (2.4) to zero and solving the resulting equations gives

$$(2.10) \quad Q_2 = -\frac{1}{72}\varphi(x)[4H_5(x) + 18H_3(x) + 12A_1H_3(x) - 18B_1H_1(x) + 9A_1^2H_1(x)],$$

where

$$A_1 = \sum_{j=2}^m (z_j - 1)^{-1}, \quad B_1 = \sum_{j=2}^m (z_j - 1)^{-2}.$$

Coefficients of higher powers of $(2/n)^{1/2}$ in (2.6) may be obtained in a similar manner if required. The expansion is summarized in the following:

THEOREM 2.1. *The distribution function of $x_1 = (n/2)^{1/2}(l_1/\lambda_1 - 1)$, when the latent*

roots of Σ are simple, can be expanded for large n as

$$(2.11) \quad P(x_1 < x) = \Phi(x) + (2/n)^{\frac{1}{2}}Q_1 + (2/n)Q_2 + O(n^{-\frac{3}{2}}),$$

where $\Phi(\cdot)$ denotes the standard normal distribution function and Q_1, Q_2 are given by (2.9), (2.10) respectively.

Consider now the distribution of the smallest root l_m . We first derive an exact expression for its distribution function. Since nS is $W_m(n, \Sigma)$ we have

$$(2.12) \quad P(l_m > y) = [(\frac{1}{2}n)^{\frac{1}{2}mn}(\det \Sigma)^{-\frac{1}{2}n}/\Gamma_m(\frac{1}{2}n)] \times \int_{S>yI} \exp(-\frac{1}{2}n \operatorname{tr}(\Sigma^{-1}S)) \det S^{\frac{1}{2}n-p} dS,$$

where $p = (m + 1)/2$. Making the transformation $T = y^{-1}S - I$ it is easily seen that (2.12) becomes

$$(2.13) \quad P(l_m > y) = [\Gamma_m(p)/\Gamma_m(\frac{1}{2}n)](\frac{1}{2}ny)^{\frac{1}{2}mn}(\det \Sigma)^{-\frac{1}{2}n} \exp(-\frac{1}{2}ny \operatorname{tr} \Sigma^{-1}) \times \Psi(p, \frac{1}{2}n + p; \frac{1}{2}ny\Sigma^{-1}),$$

where

$$\Psi(a, c; R) \equiv_{\text{def.}} [1/\Gamma_m(a)] \int_{S>0} \exp(-\operatorname{tr}(RS))(\det S)^{a-p} \det(I + S)^{c-a-p} dS.$$

The function Ψ is another confluent hypergeometric function of matrix argument (see Muirhead [13]).

Another expression for $P(l_m > y)$ has been obtained by Khatri [10], in the case when $n/2 - p$ is a nonnegative integer, as a finite series of zonal polynomials.

Now put $x_m = (n/2)^{\frac{1}{2}}(l_m/\lambda_m - 1)$. From (2.13) we have

$$P(x_m > x) = [\Gamma_m(p)/\Gamma_m(\frac{1}{2}n)](\det R)^{\frac{1}{2}n} \exp(-\operatorname{tr} R)\Psi(p, \frac{1}{2}n + p; R),$$

where $R = \operatorname{diag}(r_1, r_2, \dots, r_m)$ with $r_i = (n^{\frac{1}{2}}z + (n/2)^{\frac{1}{2}}x)z_i, z_i = \lambda_m/\lambda_{m-i+1}$ ($i = 1, 2, \dots, m$). (Again, $z_1 = 1$ is a dummy variable.) Using the system of pde's satisfied by the Ψ function given by Muirhead [13] it can readily be shown that the distribution function of $x_m, P \equiv P(x_m < x)$, satisfies each of the m pde's (2.3) and (2.4). The only difference here is that now $z_i = \lambda_m/\lambda_{m-i+1}$ instead of λ_1/λ_i as it was in the largest root distribution. Hence

THEOREM 2.2. *The distribution function of $x_m(n/2)^{\frac{1}{2}}(l_m/\lambda_m - 1)$, when the latent roots of Σ are simple, can be expanded for large n as*

$$P(x_m < x) = \Phi(x) + (2/n)^{\frac{1}{2}}Q_1 + (2/n)Q_2 + O(n^{-\frac{3}{2}}),$$

where $z_i = \lambda_m/\lambda_{m-i+1}$ in Q_1 and Q_2 given by (2.9) and (2.10) respectively.

From the general form of the expansion for the marginal distribution of l_i obtained in the next section, it may be conjectured that the distribution functions of each of the variables $(n/2)^{\frac{1}{2}}(l_i/\lambda_i - 1)$ ($i = 1, 2, \dots, m$) satisfy the system of pde's (2.3) and (2.4), with appropriate changes in the definitions of the z_i . The authors have not been able to show this.

3. Expansion of the joint distribution. In this section we derive an expansion

for the joint density function of l_1, \dots, l_m when each of the roots $\lambda_1, \dots, \lambda_m$ is assumed to be simple. The joint density function of l_1, \dots, l_m can be expressed in the form (see James [8])

$$(3.1) \quad \pi^{\frac{1}{2}m^2} (\frac{1}{2}n)^{\frac{1}{2}m^2} [\Gamma_m(\frac{1}{2}n)\Gamma_m(\frac{1}{2}m)]^{-1} \prod_{i=1}^m l_i^{n/2-p} \lambda_i^{-n/2} \prod_{i<j}^m (l_i - l_j) \times {}_0F_0(-\frac{1}{2}nL, \Sigma^{-1}),$$

where $p = (m + 1)/2$, $L = \text{diag}(l_1, \dots, l_m)$, $\Sigma = \text{diag}(\lambda_1, \dots, \lambda_m)$ and ${}_0F_0$ is a hypergeometric function with two argument matrices. The ${}_0F_0$ function in (3.1) has been expanded for large n by G. Anderson [1] by expressing it as an integral over the orthogonal group. After making the transformation from l_1, \dots, l_m to x_1, \dots, x_m where $x_i = (n/2)^{\frac{1}{2}}(l_i/\lambda_i - 1)$ ($i = 1, 2, \dots, m$), Anderson's method can be adapted to expand the resulting ${}_0F_0$ function for large n . However it is simpler, and equivalent, to transform Anderson's expansion directly. In [1] it is shown that the joint density function can be expressed as

$$(3.2) \quad k_1 \prod_{i=1}^m [\lambda_i^{(m-n-1)/2} l_i^{n/2-p} \exp(-nl_i/2\lambda_i)] \prod_{i<j}^m [(l_i - l_j)/(\lambda_i - \lambda_j)]^{\frac{1}{2}} \cdot G,$$

where

$$k_1 = (n/2)^{mn/2-m(m-1)/4} / \prod_{i=1}^m \Gamma((n - i + 1)/2)$$

and

$$(3.3) \quad G = 1 + (2n)^{-1} \sum_{i<j}^m \lambda_i \lambda_j (\lambda_i - \lambda_j)^{-1} (l_i - l_j)^{-1} + O(n^{-2}).$$

(Anderson did not show in general that the remainder term in (3.3) is of order n^{-2} ; this has been shown by Chikuse (unpublished).) Now put $x_i = (n/2)^{\frac{1}{2}}(l_i/\lambda_i - 1)$ ($i = 1, 2, \dots, m$). From (3.2) the joint density function of x_1, \dots, x_m can be expressed as

$$(3.4) \quad k_2 F_1 F_2 [1 + (2n)^{-1} \sum_{i<j}^m \lambda_i \lambda_j / (\lambda_i - \lambda_j)^2 + O(n^{-\frac{3}{2}})],$$

where

$$k_2 = (n/2)^{mn/2-m(m+1)/4} \exp(-mn/2) / \prod_{i=1}^m \Gamma((n - i + 1)/2),$$

$$F_1 = \prod_{i=1}^m [(1 + (2/n)^{\frac{1}{2}} x_i)^{n/2-p} \exp(-(n/2)^{\frac{1}{2}} x_i)]$$

and

$$F_2 = \prod_{i<j}^m [1 + (2/n)^{\frac{1}{2}} (x_i \lambda_i - x_j \lambda_j) / (\lambda_i - \lambda_j)]^{\frac{1}{2}}.$$

It remains to expand k_2 , F_1 and F_2 in (3.4) for large n . For example, by expanding the gamma functions for large n it follows that

$$k_2 = (2\pi)^{-m/2} [1 - (24n)^{-1} m(2m^2 + 3m - 1) + O(n^{-2})].$$

The functions F_1 and F_2 can be easily expanded in terms of powers of $n^{-\frac{1}{2}}$; however these expansions, up to and including the terms of order n^{-1} , are quite lengthy and are omitted here. Substituting these expansions in (3.4) gives an expansion of the joint density function of x_1, \dots, x_m . This final result is summarized in the following

THEOREM 3.1. *The joint density function of $x_i = (n/2)^{\frac{1}{2}}(l_i/\lambda_i - 1)$ ($i = 1, 2, \dots$,*

m), where $\lambda_1, \dots, \lambda_m$ are simple roots of Σ , may be expanded for large n as

$$(3.5) \quad \prod_{i=1}^m \varphi(x_i) \cdot \left\{ 1 + (2/n)^{\frac{1}{2}} \sum_{i=1}^m P_{1i}(x_i) + (2/n) \left(\sum_{i=1}^m P_{2i}(x_i) + \sum_{i < j}^m P_{1i}(x_i)P_{1j}(x_j) + \frac{1}{2} \sum_{i < j}^m \frac{x_i x_j \lambda_i \lambda_j}{(\lambda_i - \lambda_j)^2} \right) + O(n^{-\frac{3}{2}}) \right\},$$

where $\varphi(\cdot)$ denotes the standard normal density function,

$$(3.6) \quad P_{1i}(x) = \frac{1}{6}[2H_3(x) + 3A_i H_1(x)],$$

$$(3.7) \quad P_{2i}(x) = \frac{1}{72}[4H_6(x) + 18H_4(x) + 12A_i H_4(x) - 18B_i H_2(x) + 9A_i^2 H_2(x)],$$

$H_j(x)$ is the Hermite polynomial of degree j , and

$$(3.8) \quad A_i = \sum_{j=1, j \neq i}^m \lambda_j / (\lambda_i - \lambda_j), \quad B_i = \sum_{j=1, j \neq i}^m \lambda_j^2 / (\lambda_i - \lambda_j)^2.$$

Note that A_i is the same as in (2.5).

By integrating out the other variables in (3.5) an expansion of the marginal density function of x_i can be obtained.

COROLLARY. *The marginal density function of $x_i = (n/2)^{\frac{1}{2}}(l_i/\lambda_i - 1)$, where λ_i is a simple root of Σ , may be expanded for large n as*

$$(3.9) \quad \varphi(x_i) \{ 1 + (2/n)^{\frac{1}{2}} P_{1i}(x_i) + (2/n) P_{2i}(x_i) + O(n^{-\frac{3}{2}}) \}.$$

where $P_{1i}(x_i)$ and $P_{2i}(x_i)$ are given by (3.6) and (3.7) respectively.

The expansion (3.9), in the cases $i = 1$ and m , agrees with the expansions for the extreme root distributions given in the previous section. Sugiura [14] has also obtained (3.9) using another method.

Asymptotic moments of l_i can be obtained from (3.9); we obtain

$$(3.10) \quad \begin{aligned} E(l_i) &= \lambda_i + A_i \lambda_i / n + O(n^{-2}), \\ \text{Var}(l_i) &= 2\lambda_i^2 / n - 2\lambda_i^2 B_i / n^2 + O(n^{-3}), \\ \kappa_3(l_i) &= 8\lambda_i^3 / n^2 + O(n^{-3}), \quad \kappa_4(l_i) = 48\lambda_i^4 / n^3 + O(n^{-4}), \end{aligned}$$

where $\kappa_3(l_i)$ and $\kappa_4(l_i)$ denote the third and fourth cumulants of l_i and A_i, B_i are given by (3.8). From (3.5) we obtain

$$(3.11) \quad \text{Cov}(l_i, l_j) = 2[\lambda_i \lambda_j / (\lambda_i - \lambda_j)]^2 / n^2 + O(n^{-3}).$$

These expressions agree with results obtained by Lawley [11] without using the asymptotic normality. In fact, it can be readily verified that the expansion (3.9) for the marginal density function of x_i can also be obtained by substituting the expressions (3.10) for the first four moments of l_i in the general Edgeworth expansion given in Kendall and Stuart [9], page 164. Similarly, the expansion (3.5) of the joint density function of x_1, \dots, x_m could also have been obtained using (3.10) and (3.11) in a multivariate Edgeworth expansion (see Chambers [4]).

In [1], Anderson showed that, if λ_i is a simple root of Σ , then for large n ,

nl_i/λ_i is approximately distributed as χ^2 with n degrees of freedom. It was pointed out by the referee that if, instead of $x_i = (n/2)^{\frac{1}{2}}(l_i/\lambda_i - 1)$ we consider $\bar{x}_i = (n/2)^{\frac{1}{2}}(l_i - \lambda_i - A_i \lambda_i/n)/\lambda_i(1 - B_i/n)^{\frac{1}{2}}$, so that $E(\bar{x}_i) = O(n^{-\frac{3}{2}})$ and $\text{Var}(\bar{x}_i) = 1 + O(n^{-2})$, then the series obtained agrees, through terms of order n^{-1} , with the Edgeworth series for $(\chi_n^2 - n)/(2n)^{\frac{1}{2}}$. This suggests that a χ^2 approximation might be a little sharper than the normal approximation.

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