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Asymptotic Expansions for the Joint and Marginal Distributions of the Latent Roots of the Covariance Matrix

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1. Introduction.

Let $\Sigma$ be an $m \times m$ matrix having the Wishart distribution $W_m (\eta, \Sigma)$. Let $\lambda_1 > \lambda_2 > \cdots > \lambda_m > 0$ and $\lambda_1 > \lambda_2 > \cdots > \lambda_m > 0$ denote the latent roots of $\Sigma$ and $\Sigma$ respectively. For large $n$ and simple latent roots of $\Sigma$, it is known that the latent roots of $\Sigma$ are asymptotically independently normal. We assume throughout this paper that all the roots of $\Sigma$ are simple. In this paper an expansion, up to and including the term of order $n^{-1}$, is given for the joint density function of $\lambda_1, \ldots, \lambda_m$ in terms of normal density functions. Expansions for the marginal distributions of the roots are also given, valid when the corresponding roots of $\Sigma$ are simple.

2. Expansions for the extreme root distributions.

We consider first the largest root $\lambda$. From the exact
expression for the distribution function of $L$ by Sugiyama [15], [16], the distribution function of $X = (n/2)^{1/2} (L/\Lambda, -1)$ can be written as

\[ P(x_1 < x) = \left[ \Pi_{m} (p) / \Pi_{m} (r) \right] (\det R)^{m/2} \eta \Gamma_i \left( \frac{\alpha}{2} - \frac{r}{2} + \frac{p}{2} ; -R \right), \]

where \( p = \frac{1}{2} (m+1) \), \( \Pi_{m} (a) = \pi^{m(m+1)/4} \Pi_{i=1}^{m} \Gamma (a - (i-1)/2) \), \( R = \text{diag} (r_1, r_2, \ldots, r_m) \) with \( r_i = \left[ n/2 + (n/2)^{1/2} x \right] / z_i - z_i = \lambda_1 / \lambda_2 \)

\((i=1, \ldots, m)\) and \( \eta \) is a confluent hypergeometric function of matrix argument (see Herz [9], Constantine [5]). A system of partial differential equations (pde's) satisfied by the \( \eta \) function has been given by Muirhead [12]. Starting with this system it can be readily verified that \( P = P(x_1 < x) \) satisfies each of the \( m \) pde's

\[
\begin{align*}
(2.2) \quad \frac{2^p}{2x^2} + \frac{2^p}{3x} + \left( \frac{2}{n} \right)^{1/2} \left[ 2x \frac{2^p}{2x^2} + (1 + x^2 - \frac{1}{2} A_1) \right] \frac{2^p}{2x} - \sum_{k=2}^{m} z_k \frac{2^p}{2z_k} \\
+ \frac{2}{n} \left[ x^2 \frac{2^p}{2x^2} + x \left( 1 - \frac{1}{2} A_1 \right) \frac{2^p}{2x} \\
+ \sum_{k=2}^{m} z_k \left( 1 + \frac{1}{2} A_1 - \frac{1}{2 (1 - 2k)} \right) \frac{2^p}{2z_k} - 2x \sum_{k=2}^{m} z_k \frac{2^p}{2z_k} \\
+ \sum_{k=2}^{m} \frac{2^p}{2z_k} \left( 1 - \frac{1}{2} A_1 - \frac{1}{2 (1 - 2k)} \right) \frac{2^p}{2z_k} \right] = 0
\end{align*}
\]

and

\[
(2.3) \quad \frac{2^p}{2z_i} + \left( \frac{2}{n} \right)^{1/2} \left[ \frac{1}{2 (1 - z_i)} \frac{2^p}{2x} + x z_i \frac{2^p}{2z_i} \right] + \frac{2}{n} \left[ z_i \frac{2^p}{2z_i} \right]
\]
\[
\frac{x}{2(1 - z_i)} \frac{\partial P}{\partial x} + (1 - \frac{1}{2} A_i) \frac{\partial P}{\partial z_i} - \frac{1}{2(1 - z_i)} \sum_{k=2}^{m} z_k \frac{\partial P}{\partial z_k} \\
- \frac{1}{2} \sum_{j \neq i}^{m} \frac{z_j}{z_i - z_j} \frac{\partial P}{\partial z_j} \bigg] = 0 \quad (i = 2, 3, \ldots, m),
\]

where

\[(2.4) \quad A_i = \frac{\sum_{j \neq i}^{m} z_j}{z_i - z_j} \quad (i = 1, 2, \ldots, m).\]

We now look for a solution of these m pde's (2.2) and (2.3) of the form

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

where the \(Q_k\) are functions of \(x, z_2, \ldots, z_m\). (That \(P\) possesses such an expansion follows from results in the next section.)

We substitute the series (2.5) into (2.2) and (2.3) and equate coefficients of powers of \((2/n)^{1/2}\) on the L.H.S. is to zero. Equating the coefficient of \((2/n)^{1/2}\) in (2.2) and (2.3) to zero and using the boundary conditions \(P(x, < \infty) = 1\) and \(P(x, < -\infty) = 0\), we have

\[
(2.6) \quad Q = -(1/6) \Phi(x) [2 H_0(x) + 3 A_1 H_0(x)],
\]

where \(H_j(x)\) denotes the Hermite polynomial of degree \(j\) (see Kendall and Stuart [9], p. 155). Similarly, equating the coefficient of \(1/n^2\) in (2.2) and (2.3) to zero and solving
the resulting equations gives

\[(2.7)\quad Q_2 = -(1/2)g(x)[4H_1(x) + 10H_2(x) + 12A_1H_1(x) - 10B_1H_1(x) + 6A_1^2H_2(x)],\]

where \[A_i = \sum_{j=2}^{m} (z_j - 1), \quad B_i = \sum_{j=2}^{m} (z_j - 1)^2.\]

Coefficients of higher powers of \((2/n)^{1/2}\) in (2.5) may be obtained in a similar manner if required. The expansion is summarized in the following

**Theorem 2.1.** The distribution function of \(X = (2/n)^{1/2}(y, 1, -1)\), when the latent roots of \(\Sigma\) are simple, can be expanded for large \(n\) as

\[(2.8)\quad P(x < x) = F(x) + (2/n)^{1/2}Q_1 + (2/n)^2Q_2 + O(n^{-3/2}),\]

where \(Q_1\) and \(Q_2\) are given by (2.6) and (2.7) respectively.

Consider now the distribution of the smallest root \(l_{\text{min}}\).

Since \(nS \approx W_n(n, \Sigma)\) we have

\[(2.9)\quad P(l_{\text{min}} > y) = \left(\frac{1}{2^m n^{m/2}}\right) \left(\frac{1}{(2/m)}\right) \left(\frac{\Gamma (m/2)}{\Gamma (m)}\right) \left(\sum_{S \geq y^2} \exp \left(-\frac{1}{2} \text{tr}(S^{-1/2})\right) \det S^{-1/2} dS\right).

Making the transformation \(T = y^2S - I\) it is easily seen that

\[(2.10)\quad P(l_{\text{min}} > y) = \left(\frac{1}{2^m n^{m/2}}\right) \left(\frac{\Gamma (m/2)}{\Gamma (m)}\right) \left(\frac{1}{(2/m)}\right) \left(\frac{1}{(2/m)}\right) \exp \left(-\frac{1}{2} \text{tr}(\Sigma^{-1})\right)\]

\[\times \Psi (\frac{1}{2} n + p; \frac{1}{2} n y \Sigma^{-1}),\]

\(-4-\)
where \( \Psi(a, c; R) \equiv \Gamma(1/2, a) \Gamma(1/2) \exp(-a(RS)) \left( \det(I+R) \right)^{a-p} \left( \det(I+S) \right)^{c-a-p} \). 

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

Putting \( x_m = (n/2)^{1/2} (l_m / \lambda_m - 1) \) and using the system of pde's satisfied by the \( \Psi \) function given by Muirhead [13] it can readily be shown that the distribution function of \( x_m, P(x_m < x) \), satisfies each of the \( m \) pde's (2.2) and (2.3). The only difference here is that now \( z_i = \lambda_m / \lambda_{m-i+1} \) instead of \( \lambda_1 / \lambda_i \) as it was in the largest root distribution. Hence

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

\[
P(x_m < x) = \varphi(x) + (2/n)^{1/2} \theta_i + (2/n) \eta_i + O(n^{-3/2}),
\]

where \( z_i = \lambda_m / \lambda_{m-i+1} \) in \( Q_i \) and \( Q_2 \) given by (2.6) and (2.7) respectively.

3. Expansion for the joint distribution.

The joint density function of \( l_1, \ldots, l_m \) can be
expressed in the form (see James [8])

\[ (3.1) \quad \pi^m (2^n)^{m} \pi_{m}^{p \left( \frac{1}{2} \right) n} \left( \frac{1}{2} \right)^m \prod_{i=1}^{m} \left( l_{i} - l_{i} \right)^{\left( \frac{1}{2} \right) n} \prod_{i<j}^{m} \left( \lambda_{i} - \lambda_{j} \right) \right] \int_{0}^{1} \left( - \frac{1}{2} n \cdot L \cdot \Sigma^{-1} \right) \]

where \( p = \frac{1}{2} (m+1) \), \( L = \text{diag} \left( l_{1}, \cdots, l_{m} \right) \), \( \Sigma = \text{diag} \left( \lambda_{1}, \cdots, \lambda_{m} \right) \) and \( \int_{0}^{1} \) is a hypergeometric function with two argument matrices. The \( \int_{0}^{1} \) function in (3.1) has been expanded for large \( n \) by G. Anderson [1] by expressing it as an integral over the orthogonal group. In [1] it is shown that the joint density function can be expressed as

\[ (3.2) \quad \pi_{l_{1}}^{m} \prod_{i=1}^{m} \left( \lambda_{i}^{-1} - \lambda_{i}^{-1} \right)^{\left( \frac{1}{2} \right) n} \prod_{i<j}^{m} \left( \lambda_{i} - \lambda_{j} \right) \int_{0}^{1} \left( - \frac{1}{2} n \cdot L \cdot \Sigma^{-1} \right) \]

where \( \pi_{l_{1}} = (n/2)^{m(n-1)/2} \prod_{i=1}^{m} \left( \lambda_{i}^{m/2} - \lambda_{i}^{m/2} \right) \)

and

\[ (3.3) \quad G = 1 + 2 (2n)^{-1} \sum_{i<j}^{m} \lambda_{i} \lambda_{j} \left( \lambda_{i} - \lambda_{j} \right)^{\left( \frac{1}{2} \right) n} \left( l_{i} - l_{j} \right) + O \left( n^{-2} \right) \]

(Anderson did not show in general that the remainder term in (3.3) is of order \( n^{-2} \); this has been shown by the author in her Ph.D. thesis at Yale University in the more general case.) Now putting \( \lambda_{i} = (n/2)^{1/2} \lambda_{i} \), (3.2) the joint density function of \( \lambda_{1}, \cdots, \lambda_{m} \) can be expressed as
\[(3.4) \quad k_2 \frac{F_1}{F_2} \left[ 1 + \frac{(2\pi)^{-1}}{\sqrt{m}} \sum_{i<j} \frac{\lambda_i \lambda_j}{(\lambda_i - \lambda_j)^2} + O \left( n^{-2} \right) \right], \]

where
\[k_2 = \left( \frac{n}{2} \right)^{m/2 - m(m+1)/4} \exp \left( -\frac{m^2}{2} \right) \prod_{i<j} \left( \frac{1}{(m+1)} \right)^{m(m+1)/2},\]
\[F_1 = \prod_{i<j} \left[ \left( 1 + \frac{\lambda_i}{\lambda_j} \right)^{m/2 - 1} - \exp \left( -\frac{m^2}{2} \lambda_i^2 \right) \right].\]

and
\[F_2 = \prod_{i<j} \left[ 1 + \frac{\lambda_i}{\lambda_j} \left( \frac{\lambda_i}{\lambda_j} - \frac{\lambda_i}{\lambda_j} \right) / (\lambda_i - \lambda_j) \right]^{1/2}.\]

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

The functions \(F_1\) and \(F_2\) can be easily expanded in terms of powers of \(n^{-1/2}\); 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 \(X_1, \ldots, X_m\). The final result is summarized in the following

**Theorem 3.1.** The joint density function of \(X_i = (n/2)^{1/2} (i; \lambda_i - 1)\)
\((i = 1, \ldots, m)\), where \(\lambda_1, \ldots, \lambda_m\) are simple roots of \(\Sigma_i\), may be expanded for large \(n\) as
\[(3.5) \quad \prod_{i=1}^{m} P_i(x_i) \cdot \{ 1 + (2/n)^{1/2} \sum_{i=1}^{m} P_{i^2}(x_i) + (2/n) \left( \sum_{i=1}^{m} P_{2i}(x_i) \right) \\
+ \sum_{i,j} P_i(x_i) P_j(x_j) + \frac{1}{n} \sum_{i,j} \frac{\alpha_i \alpha_j}{(\lambda_i - \lambda_j)^2} \} + O(n^{-3/2}), \]

where

\[(3.6) \quad P_{1^2}(x) = \left( 1/n \right) \left\{ 2H_2(x) + 3A_i H_1(x) \right\}, \]

\[(3.7) \quad P_{2^1}(x) = \left( 1/n \right) \left\{ 4H_4(x) + 10H_2(x) + 12A_i H_2(x) - 18A_i H_1(x) + 9A_i^2 H_1(x) \right\}, \]

\[H_j(x) \text{ is the Hermite polynomial of degree } j, \text{ and} \]

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

Note that \(A_i\) is the same as in (2.4).

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 \(X_i = (n/2) (1; U_i - 1)\), where \(U_i\) is a simple root of \(Z_i\), may be expanded for large \(n\) as

\[(3.9) \quad f(x_i) \sim 1 + (2/n)^{1/2} P_{1^2}(x_i) + (2/n) P_{2^1}(x_i) + O(n^{-3/2}), \]

where \(P_{1^2}(x_i)\) and \(P_{2^1}(x_i)\) 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. Sugiyama [14] has also obtained (3.9) using another method.

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

\[
E(l_i) = \lambda_i + A_i \lambda_i / n + O(n^{-2}),
\]

(3.10) \[
\Var(l_i) = 2 \lambda_i^2 / n - 2 A_i^2 B_i / n^2 + O(n^{-3}),
\]

\[
\kappa_3(l_i) = 8 \lambda_i^3 / n^2 + O(n^{-3}), \quad \kappa_4(l_i) = 48 \lambda_i^4 / n^3 + O(n^{-4}),
\]

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) \[
\Cov(l_i, l_j) = 2 \left( \lambda_i \lambda_j / (A_i - A_j) \right)^2 / n^2 + O(n^{-3}).
\]

These expansions agree with results obtained by Lawley [11] without using the asymptotic normality.

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REFERENCES


