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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 $nS$ be an $m \times m$ matrix having the Wishart distribution $W_m(n, \Sigma)$. Let $\ell_1 > \ell_2 > \cdots > \ell_m > 0$ and $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_m > 0$ denote the latent roots of $S$ and $\Sigma$ respectively. For large $n$ and simple latent roots of $\Sigma$, it is known that the latent roots of $S$ 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 $\ell_1, \cdots, \ell_m$ 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 $\ell_1$. From the exact expression for the distribution function of $\ell_1$ by Sugiyama [15], [16], the distribution function of $x_1 = (n/2)^{1/2}(\ell_1/\lambda_1 - 1)$ can be written as

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

where $p = \frac{1}{2}(m+1)$, $\Gamma_m(a) = \pi^{m(m-1)/4}\prod_{i=1}^{m}\Gamma(a-(i-1)/2)$, $R =$ diag $(r_1, r_2, \cdots, r_m)$ with $r_i = [n/2 + (n/2)^{1/2}x]z_i$, $z_i = \lambda_1/\lambda_i$ $(i = 1, \cdots, m)$ and ${}_1F_1$ is a confluent hypergeometric function of matrix argument (see Herz [7], Constantine [5]). A system of partial differential equations (pde's) satisfied by the ${}_1F_1$ function has been given by Muirhead [12]. Starting with this system it can be readily verified that $P \equiv P(x_1 < x)$ satisfies each of the $m$ pde's

$$(2.2)\quad \frac{\partial^2 P}{\partial x^2} + x\frac{\partial P}{\partial x} + \left(\frac{2}{n}\right)^{\frac{1}{2}}\Big[2x\frac{\partial^2 P}{\partial x^2} + (1 + x^2 - \tfrac{1}{2}A_1)\frac{\partial P}{\partial x} - x\sum_{k=2}^{m} z_k\frac{\partial P}{\partial z_k}$$
$$-2\sum_{k=2}^{m} z_k\frac{\partial^2 P}{\partial x\,\partial z_k}\Big] + \frac{2}{n}\Big[x^2\frac{\partial^2 P}{\partial x^2} + x(1 - \tfrac{1}{2}A_1)\frac{\partial P}{\partial x}$$
$$+\sum_{k=2}^{m} z_k\left(1 + \tfrac{1}{2}A_1 - \frac{1}{2(1-z_k)}\right)\frac{\partial P}{\partial z_k} - 2x\sum_{k=2}^{m} z_k\frac{\partial^2 P}{\partial x\,\partial z_k}$$
$$+\sum_{k=2}^{m}\sum_{j=2}^{m} z_j z_k\frac{\partial^2 P}{\partial z_k\,\partial z_j}\Big] = 0$$

and

$$(2.3)\quad (z_i - 1)\frac{\partial P}{\partial z_i} + \left(\frac{2}{n}\right)^{\frac{1}{2}}\Big[\frac{1}{2(1-z_i)}\frac{\partial P}{\partial x} + xz_i\frac{\partial P}{\partial z_i}\Big] + \frac{2}{n}\Big[z_i\frac{\partial^2 P}{\partial z_i^2}$$

$$+\frac{x}{2(1-z_i)}\frac{\partial P}{\partial x}+(1-\tfrac{1}{2}A_i)\frac{\partial P}{\partial z_i}-\frac{1}{2(1-z_i)}\sum_{k=2}^{m} z_k\frac{\partial P}{\partial z_k}$$
$$-\frac{1}{2}\sum_{\substack{j=2\\ j\neq i}}^{m}\frac{z_j}{z_i-z_j}\frac{\partial P}{\partial z_j}\;]=0 \qquad (i=2,3,\cdots,m),$$

where

$$(2.4)\qquad A_i=\sum_{\substack{j=1\\ j\neq i}}^{m}\frac{z_i}{z_j-z_i}\qquad (i=1,2,\cdots,m).$$

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

$$(2.5)\qquad P=\Phi(x)+\sum_{k=1}^{\infty}(2/n)^{k/2}Q_k,$$

where the $Q_k$ are functions of $x, z_2, \cdots, z_m$. (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.'s 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

$$(2.6)\qquad Q_1=-(1/6)\varphi(x)\,[2H_2(x)+3A_1H_0(x)],$$

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

(2.7) $Q_2 = -(1/72)\varphi(x)[4H_5(x)+18H_3(x)+12A_1H_3(x)-18B_1H_1(x)+9A_1^2H_1(x)]$,

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 (2.5) may be obtained in a similar manner if required. The expansion is summarized in the following

<u>Theorem 2.1.</u> The distribution function of $x_1 = (n/2)^{1/2}(l_1/\lambda_1 - 1)$, when the latent roots of $\Sigma$ are simple, can be expanded for large $n$ as

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

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

Consider now the distribution of the smallest root $l_m$. Since $nS$ is $W_m(n, \Sigma)$ we have

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

Making the transformation $T = y^{-1}S - I$ it is easily seen that (2.9) becomes

(2.10) $P(l_m > y) = [\Gamma_m(p)/\Gamma_m(\frac{1}{2}n)]\det(\frac{1}{2}ny\Sigma^{-1})^{\frac{1}{2}n}\exp(-\frac{1}{2}ny\,tr\,\Sigma^{-1})$

$\cdot\Psi(p, \frac{1}{2}n+p; \frac{1}{2}ny\Sigma^{-1})$,

where $\Psi(a,c;R) \overset{def.}{\equiv} [1/\Gamma_m(a)] \int_{S>0} \exp(-tr(RS))(\det)^{a-p} \det(I+S)^{c-a-p} dS.$
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 $x_m$, $P \equiv P(x_m < x)$, 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

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

where $z_i = \lambda_m/\lambda_{m-i+1}$ in $Q_1$ and $Q_2$ given by (2.6) and (2.7) respectively.

## 3. Expansion for the joint distribution.

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

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

where $p=\frac{1}{2}(m+1)$, $L=\mathrm{diag}(l_1,\cdots,l_m)$, $\Sigma=\mathrm{diag}(\lambda_1,\cdots,\lambda_m)$ 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. In [1] it is shown that the joint density function can be expressed as

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

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 the author in her Ph.D. thesis at Yale University in the more general case.) Now putting $x_i=(n/2)^{1/2}(l_i/\lambda_i-1)$ $(i=1,\cdots,m)$, from (3.2) the joint density function of $x_1,\cdots,x_m$ can be expressed as

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

where
$$k_2 = (n/2)^{mn/2-m(m+1)/4} \exp(-mn/2)/\prod_{i=1}^{m}\Gamma((n-i+1)/2),$$
$$F_1 = \prod_{i=1}^{m} \{(1+(\tfrac{2}{n})^{1/2}x_i)^{n/2-p}\exp(-(n/2)^{1/2}x_i)\}$$

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

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 $n^{-1/2}$; 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 $x_1,\cdots,x_m$. The final result is summarized in the following

Theorem 3.1. The joint density function of $x_i=(n/2)^{1/2}(l_i/\lambda_i-1)$ $(i=1,\cdots,m)$, where $\lambda_1,\cdots,\lambda_m$ are simple roots of $\Sigma$, may be expanded for large $n$ as

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

where

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

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

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

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

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.

<u>Corollary</u> The marginal density function of $x_i=(n/2)^{1/2}(l_i/\lambda_i-1)$, where $\lambda_i$ is a simple root of $\Sigma$, may be expanded for large $n$ as

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

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

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

$$\text{(3.10)} \qquad \mathrm{Var}(l_i) = 2\lambda_i^2/n - 2\lambda_i^2 B_i/n^2 + O(n^{-3}),$$

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

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

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

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

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