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IMPROVED APPROXIMATIONS TO DISTRIBUTIONS OF THE LARGEST AND THE SMALLEST LATENT ROOTS OF A WISHART MATRIX

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Summary

Normalizing transformations of the largest and the smallest latent roots of a sample covariance matrix in a normal sample are obtained, when the corresponding population roots are simple. Using our results, confidence intervals for population roots may easily be constructed. Some numerical comparisons of the resulting approximations are made in a bivariate case, based on exact values of the probability integral of latent roots.

1. Introduction

Distributions of latent roots of a sample covariance matrix in a normal sample have been studied by many authors. Some works have been done on the derivation of asymptotic distributions, and others on that of exact distributions. A survey of the area of asymptotic distributions is found in Muirhead [8] and Siotani [10], [11], and that of the area of exact distributions in Krishnaiah [6].

From a practical point of view, it is desirable to obtain simple and accurate approximations to the distributions of latent roots which it may be possible to get the confidence intervals for the population roots. It is well known that a limiting normal approximation to the distribution of a sample correlation coefficient in a normal sample can remarkably be improved by Fisher's z-transformation in the tail areas of the distribution curve. So normalizing transformations of some variates appear to be interesting on the grounds of simplicity and accuracy. A theoretical approach for Fisher's z-transformation was made by Konishi [5].

The purpose of this paper is to investigate transformations of this sort for the largest and the smallest latent roots of the sample covariance

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matrix, when the corresponding population roots are simple. Using our results, confidence intervals and percentile points can easily be obtained. In view of principal component analysis, it is of interest to construct a confidence interval for the largest population root and to test the hypothesis that the smallest population root is equal to a small positive value. Accuracies of approximations to be suggested here are checked in a bivariate case, based on exact values of the probability integrals of latent roots.

2. Normalizing transformations of latent roots

Let $l_1, l_2, \cdots, l_p$ be the latent roots with the descending order $l_1 > l_2 > \cdots > l_p > 0$ of the sample covariance matrix S based on a sample of size $N=n+1$ from a p-variate normal distribution with population covariance matrix Σ, and let $\lambda_1, \lambda_2, \cdots, \lambda_p$ $(\lambda_1 \geqq \cdots \geqq \lambda_p > 0)$ be the latent roots of Σ. In order to find simple and accurate approximations to the distributions of l_1 and l_p in the tail areas of the distribution curves, we use the following lemma.

LEMMA. *Let $f(l_\alpha)$ be an analytic function in a neighborhood of $l_\alpha = \lambda_\alpha$. Assume that λ_α is simple root and that $f'(\lambda_\alpha) \neq 0$. Then an asymptotic expansion for the distribution of $f(l_\alpha)$ is, neglecting the term of order $1/n$, given by*

$$
\text{(2.1)} \quad \Pr\left[\frac{\sqrt{n}\{f(l_\alpha)-f(\lambda_\alpha)\}}{\sqrt{2}\,\lambda_\alpha f'(\lambda_\alpha)} < x\right] = \Phi(x) - \frac{1}{\sqrt{2n}}\left[\sum_{\beta\neq\alpha}^{p} \frac{\lambda_\beta}{\lambda_\alpha-\lambda_\beta} - \frac{2}{3} + \left\{\frac{2}{3} + \lambda_\alpha f''(\lambda_\alpha) f'(\lambda_\alpha)^{-1}\right\} x^2\right]\phi(x) + O(n^{-1}),
$$

where $\phi(x)$ is the first derivative of the standard normal distribution function $\Phi(x)$ and $f'(\lambda_\alpha)$, $f''(\lambda_\alpha)$ are the derivatives of $f(l_\alpha)$ at $l_\alpha = \lambda_\alpha$.

This is straightforward from Theorem 2.1 in Konishi [4]. From Lemma it follows that the limiting distribution of

$$
\text{(2.2)} \quad \sqrt{n}\,(l_\alpha - \lambda_\alpha)/\sqrt{2}\,\lambda_\alpha
$$

is normal with mean 0 and variance 1. Although (2.2) does not contain the latent roots other than λ_α, this approximation is poor on the whole domain of l_α.

In approximating the values of the probability integral $\Pr(l_\alpha < l_0)$ by using (2.1), the function f is restricted to strictly monotone function in $(0, +\infty)$ and the value of x is taken as $x = \sqrt{n}\{f(l_0) - f(\lambda_\alpha)\}/\{\sqrt{2}\,\lambda_\alpha f'(\lambda_\alpha)\}$. Hence the absolute value of x is zero at $l_0 = \lambda_\alpha$ and becomes larger as l_0 moves away from λ_α. This implies that the absolute value of x is fairly large in the tail areas. In considering a transformation of the largest latent root l_1, the value of $\sum_{\beta=2}^{p} \lambda_\beta/(\lambda_1-\lambda_\beta)$ in (2.1) is always positive. In order to improve the normal approximation (2.2) to the distribution of l_1 in the tail areas, it seems reasonable to find a function which reduces the coefficient of x^2 in the term of order $1/\sqrt{n}$ in (2.1) to zero, that is,

$$\frac{2}{3}+\lambda_1 f''(\lambda_1)f'(\lambda_1)^{-1}=0 .$$

Solving this differential equation and choosing a constant suitably leads to $f(l_1)=l_1^{1/3}$. It follows from (2.1) that the limiting distribution of

$$\sqrt{n}\,(l_1^{1/3}-\lambda_1^{1/3})\Big/\left(\frac{\sqrt{2}}{3}\lambda_1^{1/3}\right) \tag{2.3}$$

is normal with mean 0 and variance 1. An approximate confidence interval for λ_1 is easily constructed in the following:

$$l_1\Big/\left(1+\frac{1}{3}\sqrt{\frac{2}{n}}z_{\alpha/2}\right)^3<\lambda_1<l_1\Big/\left(1-\frac{1}{3}\sqrt{\frac{2}{n}}z_{\alpha/2}\right)^3 ,$$

where $z_{\alpha/2}$ denotes the upper 50α percentile point of the standard normal distribution.

We now consider a transformation for the smallest latent root l_p, based on the asymptotic formula (2.1). In the case of l_p, the value of $\sum_{\beta=1}^{p-1} \lambda_\beta/(\lambda_p-\lambda_\beta)$ in (2.1) is always negative and is, in many practical situations, smaller than $-p$. Hence we first search for a function such that

$$-p-\frac{2}{3}+\left\{\frac{2}{3}+\lambda_p f''(\lambda_p)f'(\lambda_p)^{-1}\right\}a=0$$

for a fixed number $x^2=a$. A solution of this differential equation may be found to be

$$f(l_p)=l_p^{\{(p+2/3)/a+1/3\}} . \tag{2.4}$$

To obtain an accurate approximation in the tail areas, we set $a=x^2=(2\sigma)^2=4$ in (2.4), which yields $l_p^{(p+2)/4}$. From (2.1), the limiting distribution of

$$\sqrt{n}\,\{l_p^{(p+2)/4}-\lambda_p^{(p+2)/4}\}\Big/\left\{\frac{\sqrt{2}\,(p+2)}{4}\lambda_p^{(p+2)/4}\right\} \tag{2.5}$$

is normal with mean 0 and variance 1. It is easy from (2.5) to obtain the lower 100α percentile point for l_p and to construct a confidence interval for λ_p.

For the αth largest latent root l_α ($\alpha \neq 1, p$), we can not know whether the value of $\sum_{\beta \neq \alpha}^{p} \lambda_\beta/(\lambda_\alpha - \lambda_\beta)$ is positive or negative. So it is difficult to find a transformation which improves the normal approximation (2.2). Girshick [3] suggested an asymptotic variance stabilizing transformation $(1/\sqrt{2}) \log l_\alpha$, which may be obtained by solving the differential equation $\sqrt{2}\,\lambda_\alpha f'(\lambda_\alpha) = 1$ in (2.1). The limiting distribution of

$$\sqrt{n}\left(\frac{1}{\sqrt{2}} \log l_\alpha - \frac{1}{\sqrt{2}} \log \lambda_\alpha\right) \tag{2.6}$$

is normal with mean 0 and variance 1. This approximation is however not accurate, as we may see later. An asymptotic expansion for the distribution of l_α has been individually obtained by Anderson [1], Muirhead and Chikuse [9] and Sugiura [12]. A confidence interval for λ_α based on an asymptotic expansion formula has been considered by Fujikoshi [2]. The result is however of intractable form in a practical application.

3. Numerical comparisons

In the case of $p=2$, some numerical comparisons of approximate distributions discussed in Section 2 are made in Tables 3.1 and 3.2, based on exact values of the probability integral $\Pr(l_\alpha < l_0)$.

Sugiyama [13], [14] has derived the exact distribution function of l_1 in a form involving a hypergeometric function of matrix argument. A hypergeometric function can be represented as power series in terms of zonal polynomials. We calculate exact values of $\Pr(l_1 < l_0)$, using tables for zonal polynomials of order two given by Sugiyama [15]. In the case $p=2$ Muirhead [7] has presented various expressions for the distributions of l_α, which do not contain zonal polynomials.

It can be seen from (2.5) that in the case where $p=2$, l_2 need not be transformed, and so an accuracy of the limiting normal distribution for l_2 is checked in Table 3.2. In the accompanying tables, the notations L_α, $L_\alpha^{1/3}$ and $\log L_\alpha$ ($\alpha=1, 2$) stand for the cases that the values of $\Pr(l_\alpha < l_0)$ are approximated by (2.2), (2.3) and (2.6), respectively, and AL_α the case that the values of $\Pr(l_\alpha < l_0)$ are approximated by using the asymptotic expansion formula of Sugiura [12].

Table 3.1 shows that the normal approximation (2.2) based on the limiting distribution of l_1 can remarkably be improved by the transformation $l_1^{1/3}$ in the tail areas, especially in the upper tail area. For some values of population roots $L_1^{1/3}$ is more accurate than AL_1. The asymp-

Table 3.1. Comparison of exact and approximate values of $\Pr(l_1 < l_0)$ for $N=21$

l_0	exact	$L_1^{1/3}$	L_1	AL_1	$\log L_1$
		$\lambda_1=2.0,\ \lambda_2=1.0$			
3.2	.9465	.9462	.9711	.9466	.9314
3.3	.9582	.9575	.9800	.9574	.9433
3.4	.9675	.9667	.9865	.9661	.9533
3.5	.9749	.9741	.9911	.9732	.9616
3.6	.9807	.9799	.9942	.9789	.9684
3.7	.9853	.9845	.9964	.9837	.9741
		$\lambda_1=3.0,\ \lambda_2=1.0$			
4.7	.9430	.9371	.9634	.9432	.9221
4.9	.9588	.9540	.9774	.9582	.9396
5.1	.9706	.9667	.9865	.9693	.9533
5.3	.9792	.9762	.9923	.9776	.9640
5.5	.9854	.9831	.9958	.9839	.9723
5.7	.9899	.9881	.9977	.9887	.9788
		$\lambda_1=4.0,\ \lambda_2=1.0$			
2.1	.0334	.0333	.0665	.0353	.0207
2.2	.0440	.0432	.0773	.0463	.0293
2.3	.0566	.0550	.0894	.0592	.0400
6.5	.9586	.9522	.9759	.9581	.9376
6.7	.9678	.9624	.9836	.9668	.9485
6.9	.9751	.9706	.9890	.9738	.9576
7.1	.9808	.9772	.9928	.9794	.9652
7.3	.9853	.9824	.9954	.9839	.9714

Table 3.2. Comparison of exact and approximate values of $\Pr(l_2 < l_0)$ for $N=42$

l_0	exact	L_2	AL_2	$\log L_2$
		$\lambda_1=3.0,\ \lambda_2=1.0$		
0.60	.0295	.0350	.0303	.0103
0.65	.0574	.0565	.0583	.0255
1.35	.9538	.9434	.9539	.9128
1.40	.9691	.9649	.9693	.9361
1.45	.9797	.9792	.9798	.9537
		$\lambda_1=4.0,\ \lambda_2=1.0$		
0.60	.0285	.0350	.0293	.0103
0.65	.0557	.0565	.0566	.0255
1.40	.9670	.9649	.9674	.9361
1.45	.9782	.9792	.9784	.9537
1.50	.9858	.9882	.9858	.9668

totic variance stabilizing transformation $\log L_\alpha$ leads to a less accurate approximation. It may be seen from these tables that AL_α provides high accuracy in both tails. We note however that AL_α is cumbersome to use in a practical situation.

Remark. It must be remarked that all approximations for l_α discussed here become extremely less accurate, provided that the ratios of the population root λ_α to the adjacent roots $\lambda_{\alpha+1}$, $\lambda_{\alpha-1}$ near the unity. Table 3.3 compares the maximum error between exact and approximate distributions in the case $p=2$:

$$\text{Error}=\text{Max}\,|\Pr(l_1<l_0;\ n, \lambda_1, \lambda_2)-A(l_0)|\times 10^5$$

where $A(l_0)$ is obtained by using an asymptotic expansion for the distribution of l_1 due to Sugiura [12] and exact values are calculated to five decimal places at intervals of 0.1 between 1 and 99 percentile points for $n=20$, 40, 100 and $\lambda_1=1.5$, 2.0, 3.0, 4.0 ($\lambda_2=1.0$).

Table 3.3. Comparison of the maximum errors

λ_1	λ_2	$n=20$	$n=40$	$n=100$
1.5	1.0	1901	1546	599
2.0	1.0	1399	525	88
3.0	1.0	489	129	28
4.0	1.0	288	86	—

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