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A Note on the Asymptotic Distributions of Dimensionality Estimators in Discriminant Analysis

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Abstract

The purpose of this paper is to simplify and study the asymptotic distribution of the dimensionality estimators in discriminant analysis based on Akaike's and Mallows' methods for samples from a multivariate distribution with finite fourth moments.

1. Introduction

In multiple discriminant analysis the number of discriminant functions useful for discrimina-ting among several groups is called the dimensionality. The purpose of this paper is to simplify and study the asymptotic distribution of the dimensionality estimators based on Akaike's and Mallows' methods for samples from a multivariate distribution with finite fourth moments. We also investigate via simulation studies how robust the asymptotic distribution of the dimensionality estimator is to the departure from normality.

Let $\mathrm{y}_{i1},\cdots,\mathrm{y}_{iq_i}$ $(i=1,\cdots,p)$ be i.i.d. $m\times 1$ absolutely continuous random vectors with mean μ_i, covariance matrix Σ and finite fourth moments. Suppose that the samples are independent across populations. Let $\overline{\mathrm{y}}_i$ be the sample mean of the q_i observations in the i the sample $(i=1,\cdots,p)$ and $\overline{\mathrm{y}}$ be the sample mean of all n observations, $(n=\Sigma_{i=1}^{p} q_i)$. Then matrices A and B are defined as

$$A=\sum_{i=1}^{p} q_i(\overline{\mathrm{y}}_i-\overline{\mathrm{y}})(\overline{\mathrm{y}}_i-\overline{\mathrm{y}})' \text{ and } B=\sum_{i=1}^{p}\sum_{j=1}^{q_i}(y_{ij}-\overline{\mathrm{y}}_i)(y_{ij}-\overline{\mathrm{y}}_i)'.$$

The matrix Ω is defined as $\Omega=\Sigma^{-1}\Sigma_{i=1}^{p} q_i(\mu_i-\overline{\mu})(\mu_i-\overline{\mu})'$ where $\overline{\mu}=\frac{1}{n}\Sigma_{i=1}^{p} q_i\mu_i$.

From now on, we will assume that $p\geq m+1$ so that AB^{-1} has m nonzero eigenvalues $f_1>\cdots>f_m>0$. In particular, if $\mathrm{y}_{i1},\cdots,\mathrm{y}_{iq_i}$ are independent $N_m(\mu_i,\Sigma)$ random vectors

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$(i = 1,\dots,p)$, then we have that the distributions of A and B are

$$A \sim W_m(p-1, \Sigma, \Omega) \quad \text{and} \quad B \sim W_m(n-p, \Sigma)\ .$$

Ω is called the noncentrality matrix.

For the asymptotic theory there is no loss of generality in assuming that Ω is the diagonal matrix defined by $\Omega = diag\{w_1,\dots,w_m\}$, $\Omega = n_2\boldsymbol{\theta}$, and $\Sigma = I_m$ where $n_2 = n - p$ and $\boldsymbol{\theta}$ is the fixed matrix defined by $\boldsymbol{\theta} = diag\{\theta_1,\dots,\theta_m\}$. This means that we consider the case where A, B, Ω, and Σ are already transformed to canonical form. Thus the dimensionality is, in fact, the rank of Ω. We can regard this estimation problem as one of deciding which of the m hypotheses is true:

$$H_k : \theta_{k+1} = \dots = \theta_m = 0\ (\theta_k > 0),\ k = 0,1,\dots,m-1.$$

The likelihood ratio test statistic for H_k is given by

$$T_k = n_2 \sum_{i=k+1}^{m} \log(1 + f_i)$$

where $f_1 > \dots > f_m > 0$ are the eigenvalues of AB^{-1}. The asymptotic distribution of T_k is $\chi^2_{(m-k)(n_1-k)}$ when H_k is true.

We need an asymptotic expansion of f_i for the purpose of deriving the asymptotic expansion of test statistic T_k. Suppose θ_i is simple. Then, using the result for perturbation expansion given in Problem 4.6.3 in Siotani *et al* (1985), *pg*. 186, we can obtain the asymptotic expansion of f_i given by

$$f_i = \theta_i + \frac{1}{\sqrt{n_2}}(E_{ii}(n) - \theta_i U_{ii}(n)) + \frac{1}{n_2}[-(E_{ii}(n) - \theta_i U_{ii}(n)) + \sum_{j\neq i}^{m} \frac{1}{\theta_i - \theta_j}\{E_{ii}(n) - \theta_i U_{ii}(n)\}^2 + F_{ii}(n)] + O_p(n_2^{-\frac{3}{2}}), \tag{1}$$

where $E_{ij}(n)$, $F_{ij}(n)$, and $U_{ij}(n)$ are the ij^{th} element of matrices $E(n), F(n)$, and $U(n)$ defined as follows:

$$E(n) = \frac{1}{\sqrt{n_2}} \sum_{i=1}^{p} q_i[(\bar{\varepsilon}_i - \bar{\varepsilon})(\mu_i - \bar{\mu})' + (\mu_i - \bar{\mu})(\bar{\varepsilon}_i - \bar{\varepsilon})'],$$

$$F(n) = \sum_{i=1}^{p} q_i(\bar{\varepsilon}_i - \bar{\varepsilon})(\bar{\varepsilon}_i - \bar{\varepsilon})',$$

$$U(n) = \frac{1}{\sqrt{n_2}} \sum_{i=1}^{p} \sum_{j=1}^{q_i} [(\varepsilon_{ij} - \bar{\varepsilon}_i)(\varepsilon_{ij} - \bar{\varepsilon}_i)' - I_m],$$

where $\bar{y}_i = \mu_i + \bar{\varepsilon}_i$, $\bar{y} = \bar{\mu} + \bar{\varepsilon}$, $\bar{\varepsilon}_i = \frac{1}{q_i} \Sigma_{j=1}^{q_i} \varepsilon_{ij}$, and $\bar{\varepsilon} = \frac{1}{n} \Sigma_{i=1}^{p} q_i \bar{\varepsilon}_i$.

We can rewrite $\frac{1}{n_2}$ A and $\frac{1}{n_2}$ B as

$$\frac{1}{n_2} A = \theta + \frac{1}{\sqrt{n_2}} E(n) + \frac{1}{n_2} F(n), \quad \frac{1}{n_2} B = I_m + \frac{1}{\sqrt{n_2}} U(n). \tag{2}$$

For our purpose we derive an asymptotic expansion for T_k in the following way using the idea given in Muirhead and Waternaux (1980). The test criterion T_k is rewritten as

$$T_k = n_2 \left[\log |I + AB^{-1}| - \sum_{i=1}^{k} \log(1 + f_i) \right]. \tag{3}$$

Substituting (1) and (2) into the expression (3) for T_k we can show, after straightforward but lengthy algebraic manipulation, that T_k has the following expansion:

$$T_k = n_2 \sum_{i=k+1}^{m} \log(1 + \theta_i) + \sqrt{n_2} C + D + O_p(n_2^{-\frac{1}{2}}),$$

where

$$C = \sum_{i=k+1}^{m} \frac{E_{ii}(n) - \theta_i U_{ii}(n)}{1 + \theta_i},$$

$$D = \sum_{i=k+1}^{m} \frac{F_{ii}(n)}{(1 + \theta_i)} - \sum_{i=1}^{k} \sum_{j=k+1}^{m} \frac{E_{ij}(n)^2}{(1 + \theta_j)(\theta_i - \theta_j)}$$

$$+ \sum_{i=1}^{k} \sum_{j=k+1}^{m} \frac{4\theta_j E_{ij}(n) U_{ij}(n)}{(1 + \theta_i)(1 + \theta_j)(\theta_i - \theta_j)} - \sum_{i=k+1}^{m} \sum_{j=k+1}^{m} \frac{E_{ij}(n) U_{ij}(n)}{(1 + \theta_i)(1 + \theta_j)}$$

$$+ \sum_{i=1}^{k} \sum_{j=k+1}^{m} \frac{\theta_j(\theta_j - 2\theta_i - \theta_i^2) U_{ij}(n)^2}{(1 + \theta_i)(1 + \theta_j)(\theta_i - \theta_j)} + \sum_{i=k+1}^{m} \sum_{j=k+1}^{m} \frac{\theta_i(\theta_j + 2) U_{ij}(n)^2}{2(1 + \theta_i)(1 + \theta_j)}$$

$$- \sum_{i=k+1}^{m} \sum_{j=k+1}^{m} \frac{E_{ij}(n)^2}{2(1 + \theta_i)(1 + \theta_j)}$$

2. Akaike's and Mallows' Methods

Applying Akaike's and Mallows' methods under normal sampling, Fujikoshi and Veitch(1979) worked on estimating the dimensionality in the MANOVA model that is applied directly to discriminant analysis. Akaike's criterion for discriminant analysis is equivalent to choosing k to minimize

$$A_k = n \sum_{i=k+1}^{m} \log(1 + f_i) - 2(m - k)(n_1 - k),$$

where $A_m = 0$ and $n_1 = p - 1$. And Mallows' criterion is equivalent to choosing k to minimize

$$C_k = n_2 \sum_{i=k+1}^{m} f_i - 2(m - k)(n_1 - k),$$

where $C_m = 0$ and $n_2 = n - p$.

Let K be the dimensionality, the number of nonzero population eigenvalues. Hence our estimate of the dimensionality based on Akaike's and Mallows' methods are defined by

$$\widehat{K}_A = k \quad \text{when} \quad A_k = \min(A_0, \cdots, A_m)$$

$$\widehat{K}_C = k \quad \text{when} \quad C_k = \min(C_0, \cdots, C_m).$$

Backhouse and McKay(1982) evaluated the performance of various methods for estimatingthe dimensionality in discriminant analysis under normal sampling. And Fujikoshi(1985) studied the statistical properties of these methods under normal sampling. In particular, he derived the asymptotic distribution of the dimensionality estimators based on these two methods for the MANOVA model. In this section we derive the asymptotic distribution of the dimensionality estimators which are much simpler than the asymptotic distribution given by Fujikoshi(1985). In addition, this asymptotic distribution is obtained for samples from a multivariate distribution with finite fourth moments.

First we consider the asymptotic distribution of $\widehat{K}_A$ when $K = k_0$($i.e.\ \theta_1 > \cdots > \theta_{k_0} > \theta_{k_0+1} = \cdots = \theta_m = 0$). Using the fact that f_i converges to $\theta_i\ (1 \le i \le m)$ in probability, we have that

$$\frac{1}{n} A_k \to^p \log \prod_{i=k+1}^{k_0} (1 + \theta_i), \qquad (0 \le k < k_0),$$

$$\frac{1}{n} A_k \to^p 0, \qquad (k_0 \le k \le m).$$

This implies that

$$\lim_{n\to\infty} P(\hat{K}_A = k) = 0, \qquad (0 \le k < k_0), \qquad (4)$$

$$\lim_{n\to\infty} P(\hat{K}_A = k) = \lim_{n\to\infty} P(A_k \le A_s,\ s = k_0,\dots,m), \qquad (k_0 \le k \le m), \qquad (5)$$

provided that the limit exists.
We rewrite

$$A_k = \frac{n}{n_2} T_k - 2(m-k)(n_1-k), \qquad (6)$$

where

$$T_k = n_2 \log \prod_{i=k+1}^{m} (1 + f_i).$$

We recall the following expansion for T_k :

$$T_k = n_2 \sum_{i=k+1}^{m} \log(1+\theta_i) + \sqrt{n_2}C + D + O_p(n_2^{-\frac{1}{2}}).$$

When $K = k$, the expansion for T_k reduces to

$$T_k = \sum_{i=k+1}^{m} [F_{ii}(n) - \sum_{j=1}^{k} \frac{1}{\theta_j} E_{ij}(n)^2] + O_p(n_2^{-\frac{1}{2}}).$$

Thus when $K = k$, A_k reduces to

$$A_k = \frac{n}{n_2} \sum_{i=k+1}^{m} [F_{ii}(n) - \sum_{j=1}^{k} \frac{1}{\theta_j} E_{ij}(n)^2] - 2(m-k)(n_1-k) + O_p(n_2^{-\frac{1}{2}}).$$

We can show easily the followings. For details see Hwang(1994).

$$\frac{n}{n_2} \Big[\sum_{i=s+1}^{k} [F_{ii}(n) - \sum_{j=1}^{s} \frac{1}{\theta_j} E_{ij}(n)^2] + \sum_{i=k+1}^{m} \sum_{j=s+1}^{k} \frac{1}{\theta_j} E_{ij}(n)^2 \Big] \to^L \chi_1(s,k),$$

$$\frac{n}{n_2} \Big[\sum_{i=k+1}^{s} [F_{ii}(n) - \sum_{j=1}^{k} \frac{1}{\theta_j} E_{ij}(n)^2] + \sum_{i=s+1}^{m} \sum_{j=k+1}^{s} \frac{1}{\theta_j} E_{ij}(n)^2 \Big] \to^L \chi_2(k,s).$$

Furthermore, the joint distributions as s varies also converge. Substituting (6) into (4) and (5), we obtain the following theorem.

Theorem 1 Let $f_i\ (i = 1,\dots,m)$ be the eigenvalues of AB^{-1} obtained based on samples drawn from a multivariate distribution with finite fourth moments and suppose that $K = k_0$.

Then

$$\lim_{n\to\infty} P(\hat{K}_A = k) = P(k \mid k_0),$$

where

$$P(k \mid k_0) = \begin{cases} 0, & 0 \le k < k_0 \\ P(\chi_1(s,k) > 2m_{sk},\ s = k_0, \cdots, k-1) & \\ \cdot P(\chi_2(k,s) \le 2m_{ks},\ s = k+1, \cdots, m), & k_0 \le k \le m \end{cases}$$

If we take $k_0 = m - 2$, then the asymptotic probability of overestimating the dimensionality by one is

$$P(m-1 \mid m-2) = P(\chi^2_{(n_1-m+3)} > 2(n_1 - m + 3)) \cdot P(\chi^2_{(n_1-m+1)} \le 2(n_1 - m + 1)).$$

We obtain from Theorem 1 that the asymptotic probability of correctly assessing the dimensionality reduces to

$$P(k_0 \mid k_0) = P(\chi_2(k_0,s) \le 2m_{k_0 s},\ s = k_0 + 1, \cdots, m).$$

For some special cases $P(k_0 \mid k_0)$ can be simplied. For the case when $k_0 = m - 1$ we have

$$P(m-1 \mid m-1) = P(\chi^2_{(n_1-m+1)} \le 2(n_1 - m + 1)).$$

We now consider the asymptotic distribution of K_c when $K = k_0$. Since f_i converges to $\theta_i\ (1 \le i \le m)$ in probability, we have that

$$\frac{1}{n} C_k \to^p \sum_{i=k+1}^{k_0} \theta_i, \qquad (0 \le k < k_0),$$

$$\frac{1}{n} C_k \to^p 0, \qquad (k_0 \le k \le m).$$

This implies that

$$\lim_{n\to\infty} P(\hat{K}_C = k) = 0, \qquad (0 \le k < k_0),$$

$$\lim_{n\to\infty} P(\hat{K}_C = k) = P(C_k \le C_s,\ s = k_0, \ldots, m), \qquad (k_0 \le k \le m),$$

provided that the limits exist. We write

$$C_k = \tilde{T}_k - 2(m-k)(n_1-k),$$

where

$$\tilde{T}_k = n_2 \sum_{i=k+1}^{m} f_i = n_2\left[\operatorname{tr}(AB^{-\frac{1}{2}}) - \sum_{i=1}^{k} f_i \right].$$

Then, using the same arguments as before, we obtain the following expansion:

$$C_k = n_2 \sum_{i=k+1}^{m} \theta_i + \sqrt{n_2}\,\tilde{C} + \tilde{D} + O_p(n_2^{-\frac{1}{2}}),$$

where

$$\tilde{C} = \sum_{i=k+1}^{m} (E_{ii}(n) - \theta_i U_{ii}(n)),$$

$$\tilde{D} = \sum_{i=k+1}^{m} F_{ii}(n) - \sum_{i=1}^{k} \sum_{j=k+1}^{m} \frac{E_{ij}(n)^2}{\theta_i - \theta_j}$$

$$- \sum_{i=1}^{k} \sum_{j=k+1}^{m} \frac{2\theta_j}{\theta_i - \theta_j} E_{ij}(n) U_{ij}(n) - \sum_{i=k+1}^{m} \sum_{j=k+1}^{m} E_{ij}(n) U_{ij}(n)$$

$$+ \sum_{i=k+1}^{m} \sum_{j=1}^{m} \theta_i\, U_{ij}(n)^2 - \sum_{i=1}^{k} \sum_{j=k+1}^{m} \frac{\theta_i \theta_j}{\theta_i - \theta_j} U_{ij}(n)^2$$

When the null hypothesis H_k is true the expansion for C_k reduces to

$$C_k = \sum_{i=k+1}^{m} [F_{ii}(n) - \sum_{j=1}^{k} \frac{1}{\theta_j} E_{ij}(n)^2] - 2(m-k)(n_1-k) + O_p(n_2^{-\frac{1}{2}}).$$

Recall that for

$$A_k = \frac{n}{n_2} \sum_{i=k+1}^{m} [F_{ii}(n) - \sum_{j=1}^{k} \frac{1}{\theta_j} E_{ij}(n)^2] - 2(m-k)(n_1-k) + O_p(n_2^{-\frac{1}{2}}).$$

Thus we see for any multivariate distribution the asymptotic distribution of the dimensionality estimators based on the two methods are same.

3. Monte Carlo Studies

First we study the performance of Akaike's method and Mallows' method in estimating the dimensionality for normal sampling. The Monte Carlo study consisted of generating 500 values of a noncentral *Wishart* matrix A and a central *Wishart* matrix B.

Second we study the sampling distributions of the dimensionalities estimated by Akaike's method and Mallows' method for sampling from an elliptical t-distribution on 5 degrees of freedom. Sampling distributions using the normal based criterion A_k and Mallows' criterion S_k were obtained. The study consisted of generating 500 samples of size n = 56, 106, 206 of an 4-variate elliptical t-distribution on 5 degrees of freedom for 6 populations with parameters $\mu_i (i = 1, \cdots, 6)$ and $V = (\frac{3}{5}) I_4$. These samples can be generated using the following relationship :

$$y_{ij} = \mu_i + Z^{-\frac{1}{2}}(4V)x,$$

where $x \sim N_4(0, I_m)$ and Z *is* χ^2_5.

Generation of the samples, computation of the sample eigenvalue and the analysis were conducted using SAS/BASICS and SAS/IML. Table 1 presents the results or the probability of the estimate taking value 3 when the true dimensionality is 2 using Akaike's and Mallows' methods. From the asymptotic theory we have

$$\lim_{n\to\infty} P(\hat{K}_A = 3) = \lim_{n\to\infty} P(\hat{K}_C = 3) = P(3 \mid 2) = P(\chi^2_2 \le 4) \cdot P(\chi^2_4 > 8) \approx 0.0792.$$

The percentages given in Table 1 tend to increase as either the sample size n *or* θ_{min} increases. The percentages are usually larger than the percentage 7.92 obtained from the asymptotic theory when θ_{min} is appreciable. Table 2 and 3 present the results for Akaike's (A_k) and Mallows' (C_k) methods in terms of the percentage of correct decisions for normal distribution and for elliptical $t(5)$ distribution, respectively.

As seen from Table 1, 2, and 3, the percentages for the two methods are very close, especially for large sample size (n = 206 or n_2 = 200), supporting the result that the asymptotic distribution of K_A and K_C are the same. These criteria perform best for large values of θ_{min}. When $K = k_0 = m - 1 = 3$ we have

$$\lim_{n\to\infty} P(\hat{K}_A = 3) = \lim_{n\to\infty} P(\hat{K}_C = 3) = P(3 \mid 3) = P(\chi^2_2 \le 4) \approx 0.865$$

We also have $P(4 \mid 4) = 1$.

The Monte Carlo results for $K = 3$ and $K = 4$ agree quite well with the asymptotic theory when n and θ_{min} are large. Although the asymptotic distribution depends on k_0, m and n_1, the speed of convergence depends highly on the values of the population eigenvalues, especially the value of θ_{min}.

Overall the two criteria under normal and elliptical t(5) sampling have almost the same behaviours when n and θ_{min} are large. Our simulation study agrees quite well with theory. As expected the population eigenvalues have the greatest effect on the speed of convergence.

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Table 1 : The **Percentage** of **Overestimation** by **one** when K = m - 2 = 2, under **normal sampling** (m = 4,p = 6)

θ_1	θ_2	θ_3	θ_4	AKAIKE n_2 = 50	AKAIKE n_2 = 100	AKAIKE n_2 = 200	MALLOWS n_2 = 50	MALLOWS n_2 = 100	MALLOWS n_2 = 200
0.1	0.08	0	0	2.0	2.8	9.4	2.6	4.0	9.4
0.4	0.2	0	0	6.8	12.0	13.4	8.8	14.0	14.2
0.8	0.4	0	0	10.6	14.4	15.0	14.2	16.8	15.8
2.	0.8	0	0	12.8	16.0	15.6	16.6	18.2	16.0
6	2	0	0	14.0	16.4	15.4	17.0	18.4	16.0

Table 2 : The **Percentage** of **Correct Decision**, under **normal sampling** (m = 4,p = 6)

θ_1	θ_2	θ_3	θ_4	K	AKAIKE n_2 = 50	AKAIKE n_2 = 100	AKAIKE n_2 = 200	MALLOWS n_2 = 50	MALLOWS n_2 = 100	MALLOWS n_2 = 200
0.4	0.2	0.1	0	3	24.6	67.0	83.2	29.8	67.2	83.4
1.	0.8	0.4	0	3	85.8	86.6	83.2	85.8	86.4	83.2
2	1	0.8	0	3	85.8	85.2	83.0	84.2	85.0	82.8
6	4	2.	0	3	86.2	85.4	83.4	84.6	85.0	82.8
0.4	0.2	0.1	0.08	4	18.4	58.8	92.8	20.2	60.0	93.0
0.8	0.6	0.4	0.2	4	82.6	99.0	100	84.6	99.0	100
4.	2	1	0.8	4	100	100	100	100	100	100
6.	4	3	1	4	100	100	100	100	100	100

Table 3 : The **Percentage** of **Correct Decision**, for **elliptical t(5)**, (m = 4,p = 6)

θ_1	θ_2	θ_3	θ_4	K	AKAIKE n_2 = 50	AKAIKE n_2 = 100	AKAIKE n_2 = 200	MALLOWS n_2 = 50	MALLOWS n_2 = 100	MALLOWS n_2 = 200
0.4	0.2	0.1	0	3	6.0	6.8	14.2	9.2	8.8	15.4
1.	0.8	0.4	0	3	39.6	69.0	85.4	43.4	71.0	85.4
2	1	0.8	0	3	73.2	83.2	83.6	74.0	83.4	83.4
6	4	2.	0	3	81.0	83.8	83.4	80.6	83.0	83.0
0.4	0.2	0.1	0.08	4	5.6	13.6	15.2	6.8	14.4	15.8
0.8	0.6	0.4	0.2	4	13.2	17.0	15.8	14.0	17.4	16.2
4.	2	1	0.8	4	65.4	86.6	99.4	67.2	87.2	99.4
6.	4	3	1	4	98.0	100	100	98.2	100	100