A note on the null distributions of some test statistics for profile analysis under general conditions

Solomon W. Harrar* and Jin Xu†

Abstract

In this note, we present the asymptotic expansions of the null distributions of some test statistics for \( k \)-sample profile analysis under general conditions. It extends Maruyama (2007, Asymptotic expansions of the null distributions of some test statistics for profile analysis in general conditions. J. Statist. Plann. Inference, 137, 506-526)’s result of two-sample case to \( k \)-sample (\( k \geq 2 \)) situations. Further, two new test statistics are devised for testing flatness based on the normal theory likelihood ratio criterion under two different specifications for the parameter space. The asymptotic expansions for these statistics are obtained. Our derivations are much simpler and elegant in that they are based on a transformation on some known results for one-way MANOVA and Hotelling’s \( T^2 \) statistics, etc. The accuracy of the asymptotic expansions in approximating the exact null distributions of the test statistics is examined via simulation studies. An application to a real data set is illustrated.

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1 Introduction

Consider \( p \)-dimensional independent populations \( \mathbf{y}^{(1)}, \mathbf{y}^{(2)}, \ldots, \mathbf{y}^{(k)} \) with mean vectors \( \mu^{(1)}, \mu^{(2)}, \ldots, \mu^{(k)} \) and common covariance matrix \( \Sigma (> 0) \). The mean profile of \( \mathbf{y}^{(j)} \) can be treated graphically as a line connecting the points \( (1, \mu_{1}^{(j)}), \ldots, (p, \mu_{p}^{(j)}) \) where \( \mu_{i}^{(j)} \) is the \( i \)th component of \( \mu^{(j)} \). Profile analysis is the study of the relationship between these lines of mean vectors. For one-sample case, the problem of interest is whether the mean vector is flat; for two or more}

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sample case, the problem of primary interest is whether the profiles are (piecewise) parallel. And if the parallelism holds, then two follow-up questions are (1) whether the separation of the profiles, or the difference of means, is significant, and (2) whether the profiles are flat. (Rencher, 2002; Johnson and Wichern, 1988; Srivastava and Carter, 1983)

Let \( y^{(j)}_\alpha (\alpha = 1, \ldots, n_j) \) be independent identically distributed (i.i.d.) samples from the \( j \)th population \((j = 1, \ldots, k)\). Denote \( \bar{y}^{(j)} \) and \( S^{(j)} \) respectively as the sample mean and sample covariance of the \( j \)th sample, and denote \( \bar{y} = \frac{1}{n} \sum_{j=1}^{k} \sum_{\alpha=1}^{n_j} y^{(j)}_\alpha \), \( n = \sum_{j=1}^{k} n_j \), \( W = \sum_{j=1}^{k} (n_j - 1)S^{(j)} \), \( B = \sum_{j=1}^{k} n_j (\bar{y}^{(j)} - \bar{y})(\bar{y}^{(j)} - \bar{y})' \), \( S = W/(n-k) \). Let \( 1 \) be a \( p \times 1 \) vector of ones and \( C \) be a \((p-1) \times p\) matrix of rank \( p-1 \) such that \( C1 = 0 \). Then under the assumption of normality, the profile analysis for one- and two-sample cases can be summarized in Table 1.

Under normality, each of the test statistics for the three tests in profile analysis are known to be distributed as some constant multiple an \( F \) random variable. The tests are unaffected in term of size when the sample sizes are very large, even if the assumption of normality does not hold. However for moderate sample sizes, asymptotic expansions under non-normality that include terms of order up to \( O(n^{-1}) \) will provide fairly close approximations. In the context of profile analysis, Okamoto et al. (2006) used perturbation method and obtained the asymptotic expansions of the distributions of the test statistics under elliptical populations. Maruyama (2007) extended the results under more general conditions by a different method introduced by Kano (1995).

In this note, we will present the null distributions of some test statistics for profile analysis in the general \( k \)-sample case \((k \geq 2)\). However our technique is to simply apply a transformation on some known results of one-way MANOVA test and Hotelling’s \( T^2 \) statistic, etc. (Fujikoshi, 1997; Fujikoshi, 2002; and Kakizawa, 2008). This paper’s contribution goes beyond extending the results of Maruyama (2007) in that some new test statistics are proposed for the flatness test in contrast to the traditional one. The asymptotic expansion of one of the new statistics is the sum of quasi-independent Hotelling’s \( T^2 \) statistics whose asymptotic expansion is through a decent application of a recent result by Kakizawa (2008).

The rest of the paper is organized as follows. The main results of the paper, the asymptotic expansion for the null distribution of some tests in profile analysis, are presented in Section 2. In Section 3, the numerical accuracy of the approximations based on asymptotic expansions is investigated. The application of the results is illustrated with a real data example in Section 4.

2 Main results

2.1 Test statistics in \( k \)-sample case

We propose three statistics for testing parallelism, level and flatness for the \( k \)-sample profile analysis as described in Table 2 below.

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Table 1: Profile analysis (one- and two-sample cases)

<table>
<thead>
<tr>
<th>Null hypothesis</th>
<th>Test statistic</th>
<th>Null distribution under normality</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Equality</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_0^{EQ}: \mu_1^{(1)} = \mu_2^{(1)} = \cdots = \mu_p^{(1)}$</td>
<td>$T_{EQ} = n_1(C\bar{y}^{(1)})'(CS^{(1)}C')^{-1}(C\bar{y}^{(1)})$</td>
<td>$T^2(p - 1, n_1 - 1)$</td>
</tr>
<tr>
<td><strong>Parallelism</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_0^{PR}: C\mu^{(1)} = C\mu^{(2)}$</td>
<td>$T_{PR}(2) = \frac{n_1 n_2}{n_1 + n_2}(\bar{y}^{(1)} - \bar{y}^{(2)})'(CSC')^{-1}(\bar{y}^{(1)} - \bar{y}^{(2)})$</td>
<td>$T^2(p - 1, n_1 + n_2 - 2)$</td>
</tr>
<tr>
<td><strong>Level</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_0^{LE}: 1'\mu^{(1)} = 1'\mu^{(2)}$</td>
<td>$T_{LE}(2) = \frac{n_1 n_2}{n_1 + n_2}1'(\bar{y}^{(1)} - \bar{y}^{(2)})(1'S1)^{-1}(\bar{y}^{(1)} - \bar{y}^{(2)})1$</td>
<td>$F(1, n_1 + n_2 - 2)$</td>
</tr>
<tr>
<td><strong>Flatness</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_0^{FL}: C\mu^{(1)} = C\mu^{(2)} = 0$</td>
<td>$\tilde{T}_{FL}(2) = (n_1 + n_2)(C\bar{y})'(CSC')^{-1}(C\bar{y})$</td>
<td>$T^2(p - 1, n_1 + n_2 - 2)$</td>
</tr>
</tbody>
</table>

Here $T^2(p, n)$ means Hotelling’s $T^2$ distribution with relationship $\frac{n-p+1}{np}T^2(p, n) = F(p, n - p + 1)$, where $F(p, n - p + 1)$ is $F$ distribution with degrees of freedom $p$ and $n - p + 1$ (Anderson, 1984, p.163).
Table 2: Profile analysis (k-sample case)

<table>
<thead>
<tr>
<th>Null hypothesis</th>
<th>Test statistics</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_{0PR}^{PR}$ : $C\mu^{(1)} = C\mu^{(2)} = \cdots = C\mu^{(k)}$</td>
<td>$T_{PR}(k) = (n-k)\operatorname{tr}(CBC')(CW'C')^{-1}$</td>
</tr>
<tr>
<td>$H_{0LE}^{LE}$ : $1'\mu^{(1)} = 1'\mu^{(2)} = \cdots = 1'\mu^{(k)}$</td>
<td>$T_{LE}(k) = \frac{(B1)/(k-1)}{1\times(1/((n-k))}$</td>
</tr>
<tr>
<td>$H_{0FL}^{FL}$ : $C\mu^{(1)} = C\mu^{(2)} = \cdots = C\mu^{(k)} = 0$</td>
<td>$T_{FL}(k) = n(n-1)(C\bar{y}')(C(W + B)C')^{-1}(C\bar{y})$</td>
</tr>
</tbody>
</table>

Some comments are in order.

First, $T_{PR}(k)$ is the natural extension of $T_{PR}(2)$ in two-sample case. Its is called Lawley-Hotelling statistic in normal theory, whose distribution is denoted as $LH(p-1, k-1, n-k)$. (More specifically, $LH(p, k, n)$ with degrees of freedom $k$ and $n$ is defined as the distribution of $ntrHG^{-1}$ where $H$ and $G(>0)$ are $p \times p$ independent Wishart random matrices with distributions $W_p(\Sigma, k)$ and $W_p(\Sigma, n)$, respectively (Anderson, 1984, Sec. 8.6.2). While the $k$-sample version of the likelihood ratio statistic under normality is noted as $\Lambda_{PR} = |CW'C'|/|C(W + B)C'|$.

Second, $T_{LE}(k)$ is essentially an $F$ statistic (of one-way ANOVA). It is also extension of $T_{LE}(2)$ in two-sample case. It can be rewritten as $T_{LE}(k) = (k-1)(n-k)\operatorname{tr}(1'B1)(1'W1)^{-1}$ with distribution $F(k-1, n-k)$ under normality.

Third, we take a close look at the flatness test. It is noted that the flatness is subsequently tested provided parallelism holds, otherwise its treatment would be different. Therefore, for the moment we consider the parameter space to be the null hypothesis of parallelism, i.e., $\Omega = H_{0PR}^{PR}$. Under normality, the likelihood ratio criterion for flatness hypothesis yields the statistic

$$\Lambda_{FL} = \frac{|C(W + B)C'|}{|C(W + B + n\bar{y}\bar{y})C'|} = \frac{1}{1 + n(C\bar{y})'(C(W + B)C')^{-1}(C\bar{y})},$$

a monotone function of $T_{FL}(k)$. In this manner, $T_{FL}(k)$ can be viewed as a likelihood ratio statistic for testing the mean vector of the pooled transformed samples $C\bar{y}^{(j)} (j = 1, \ldots, k)$ equal zero. It is free of $k$ after conditioning on the parallelism. And it is easy to show the null distribution of $T_{FL}(k)$ is $T^2(p-1, n-1)$, which is different to that of $T_{PR}(2)$ (in the second degree of freedom) of two-sample case.

On the other hand, if one chooses the parameter space to be the unconditional space, denoted by $\Omega^* = \{\mu^{(j)} \in \mathbb{R}^p, j = 1, \ldots, k\}$, then the resulting likelihood ratio statistic under normality is

$$\Lambda_{FL}^* = \frac{|CW'C'|}{|C(W + B_0)C'|},$$

where $B_0 = \sum_{j=1}^k n_jy^{(j)}y^{(j)}$. Its null distribution is Wilk’s $\Lambda$ distribution $U(p-1, k, n-k)$ (Rencher, 2002, Section 6.1.3). It is noticed that $\Lambda_{FL}^* = \Lambda_{PR} \cdot \Lambda_{FL}$, revealing a structure of...
decomposition into the two tests. The counterpart of $\Lambda^*_{FL}$ under the Lawley-Hotelling criterion is
\[
T^*_{FL}(k) = (n - k)\text{tr}(CB_0C')(CWC')^{-1},
\]
whose null distribution is $LH(p - 1, k, n - k)$ which is also different from that of $\tilde{T}_{FL}(2)$ as $T^*_{FL}(2) = n_1(C\tilde{y}^{(1)})'(CSC')^{-1}(C\tilde{y}^{(1)}) + n_2(C\tilde{y}^{(2)})'(CSC')^{-1}(C\tilde{y}^{(2)}) \neq \tilde{T}_{FL}(2)$ in general. In neither cases of $\Omega$ and $\Omega^*$ can $T_{FL}(k)$ and $T^*_{FL}(k)$ reduce to the traditional two-sample version, $\tilde{T}_{FL}(2)$. Notice that the distribution of $T_{FL}(2)$ under the alternative hypothesis of non-flatness is the same as that of a constant multiple of non-central $F$ random variable with non-centrality parameter $(n_1 + n_2)\tilde{\mu}'C'(CSC)^{-1}C\tilde{\mu}$ where $\tilde{\mu} = (n_1\mu_1 + n_2\mu_2)/(n_1 + n_2)$. Hence $\tilde{T}_{FL}(2)$ tends to be large as long as $C\tilde{\mu} \neq 0$ and regardless of whether or not parallelism holds. Therefore, the rationale behind $\tilde{T}_{FL}(2)$ is not very clear. As a conclusion, from the sequential test point of view, we would prefer using $T_{FL}(k)$ as the statistic.

Fourth, the test statistics $T_{PR}(k)$ and $T_{FL}(k)$ are invariant to the choice of $C$ as long as it is a contrast matrix satisfying $C1 = 0$. This is easily seen by noting that two arbitrary contrast matrices $C_1$ and $C_2$ must be related by $C_1 = DC_2$ for some non-singular matrix $D_{(p - 1) \times (p - 1)}$.

Finally, it is noted that for parallelism test, other criteria such as likelihood ratio or Bartlett-Nanda-Pillai can be used too (Anderson, 1984). However, the resulting statistics are shown to be very close to Lawley-Hotelling statistic and their distributions can be obtained similarly (Fujikoshi, 2002). We will not pursue them here.

### 2.2 Null distributions in $k$-sample case

Since the primary concern of profile analysis is about the mean vectors, we assume the homogeneity of any high order moments or cumulants up to the degree required under general conditions.

Let $M$ be a $q \times p$ known matrix of rank $q(\leq p)$. Then the previous testing problems in profile analysis can equivalently be formulated as hypotheses based on the transformed populations $y^{(j)*} = My^{(j)}$ with mean $\mu^{(j)*} = M\mu^{(j)}$ and covariance $\Sigma^* = M\Sigma M'$. For instance, the parallelism hypothesis becomes $H^*_{0PR} : \mu^{(1)*} = \cdots = \mu^{(k)*}$, thus reduces to a standard one-way MANOVA problem.

Let $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_p)'$ be a random vector with zero mean vector and covariance matrix $I_p$. Denote
\[
\kappa_{abc} = E(\varepsilon_a\varepsilon_b\varepsilon_c) \quad \text{and} \quad \kappa_{abcd} = E(\varepsilon_a\varepsilon_b\varepsilon_c\varepsilon_d) - (\delta_{ab}\delta_{cd} + \delta_{ac}\delta_{bd} + \delta_{ad}\delta_{bc})
\]
as the third- and fourth- order cumulants where $\delta_{ab}$ is the Kronecker delta defined by $\delta_{ab} = 1$ if $a = b$ and $\delta_{ab} = 0$ if $a \neq b$. Define two matrices of third- and fourth- order cumulants of $\varepsilon$ by
\[
K_3(\varepsilon) = E[\text{vec}(\varepsilon\varepsilon')\varepsilon'] , \quad K_4(\varepsilon) = E[\text{vec}(\varepsilon\varepsilon')\text{vec}(\varepsilon\varepsilon')] - E_N[\text{vec}(\varepsilon\varepsilon')\text{vec}(\varepsilon\varepsilon')]', \tag{2.1}
\]

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where \( E_N \) stands for the expected value under normality. It can be verified that

\[
E_N[\text{vec}(\varepsilon \varepsilon')\text{vec}(\varepsilon \varepsilon')] = I_p^2 + K_{p,p} + \text{vec}(I_p)\text{vec}(I_p)',
\]

where \( K_{p,p} \) is the \( p^2 \times p^2 \) commutation matrix. (The reader is advised to refer to Magnus and Neudecker (1979) for the definition and properties of the commutation matrix.) Then the following measures of multivariate skewness and kurtosis can be expressed as

\[
\begin{align*}
\kappa_3^{(1)} &= \kappa_3^{(1)}(\varepsilon) = \sum_{a,b,c} \kappa_{abc}^2 = \text{tr} \{ K_3(\varepsilon)'K_3(\varepsilon) \}, \\
\kappa_3^{(2)} &= \kappa_3^{(2)}(\varepsilon) = \sum_{a,b,c} \kappa_{abc} \kappa_{idc} = \text{tr} \{ K_3(\varepsilon)'\text{vec}(I_p)\text{vec}(I_p)'K_3(\varepsilon) \}, \\
\kappa_4^{(1)} &= \kappa_4^{(1)}(\varepsilon) = \sum_{a,b} \kappa_{aabb}^2 = \text{vec}(I_p)'K_4(\varepsilon)\text{vec}(I_p) = E(\varepsilon'\varepsilon)^2 - p(p + 2).
\end{align*}
\]

The indices \( \kappa_3^{(1)} \) and \( \kappa_4^{(1)} \) measure multivariate skewness and kurtosis, respectively, and were introduced by Mardia (1970). Whereas \( \kappa_3^{(2)} \) is a measure of skewness and was introduced by Isogai (1983). The expressions in (2.2) are quite enlightening in showing the main difference between the two measures of multivariate skewness. It is clearly seen that both \( \kappa_3^{(1)} \) and \( \kappa_3^{(2)} \) are of the form \( \text{tr}\{K_3(\varepsilon)'AK_3(\varepsilon)\} \) where \( A = I_p \otimes I_p \) for \( \kappa_3^{(1)} \) and \( A = \text{vec}(I_p)\text{vec}(I_p)' \) for \( \kappa_3^{(2)} \).

The effect of pre-multiplication of \( \varepsilon \) by a full row rank matrix on the skewness and kurtosis is examined next.

**Lemma 2.1.** Let \( \varepsilon^* = M\varepsilon \), then we have

\[
\begin{align*}
\kappa_3^{(1)*} &= \kappa_3^{(1)}(\varepsilon^*) = \text{tr} \{ M'MK_3(\varepsilon)'[(M'M) \otimes (M'M)]K_3(\varepsilon) \}, \\
\kappa_3^{(2)*} &= \kappa_3^{(2)}(\varepsilon^*) = \text{tr} \{ M'MK_3(\varepsilon)'[\text{vec}(M'M)\text{vec}(M'M)']K_3(\varepsilon) \}, \\
\kappa_4^{(1)*} &= \kappa_4^{(1)}(\varepsilon^*) = E(\varepsilon'\varepsilon'M\varepsilon)^2 - 2\text{tr}(M'M)^2 - (\text{tr}(M'M))^2.
\end{align*}
\]

**Proof.** Notice that

\[
\begin{align*}
K_3(M\varepsilon) &= (M \otimes M)K_3(\varepsilon)M' \\
K_4(M\varepsilon) &= (M \otimes M)K_4(\varepsilon)(M' \otimes M')
\end{align*}
\]

which follow directly from the identity \( \text{vec}(ABC) = (C' \otimes A)\text{vec}(B) \). Then substituting these in (2.2) leads to the desired results noting the identity \( (A \otimes B)(C \otimes D) = (AC) \otimes (BD) \). \( \square \)

Now assume \( y^{(j)} - \mu^{(j)} = \Sigma^{1/2}\varepsilon \), then by setting \( M = \Sigma^{1/2} \), Lemma 2.1 gives the multivariate skewness and kurtosis indices for \( y^{(j)} \); by setting \( M = C\Sigma^{1/2} \). Lemma 2.1 gives the indices for \( Cy^{(j)} \). Moreover, it is noted that the test statistics based on the transformed populations \( y^{(j)*} \) are affine invariant. Hence by further setting \( M = (C\Sigma C)^{-1/2}C\Sigma^{1/2} \), we can get the indices for the standardized \( Cy^{(j)} \) in the following corollary.
Corollary 2.1. Let $M = (C'S'C')^{-1/2}CS^{1/2}$, then $\kappa_3^{(1)^*}$, $\kappa_3^{(2)^*}$ and $\kappa_4^{(1)^*}$ become

$$
\kappa_3^{(1)^*} = \text{tr} \{ \Sigma^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2} K_3(\varepsilon)' \times [ (\Sigma^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2}) \otimes (\Sigma^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2})] K_3(\varepsilon) \},
$$

$$
\kappa_3^{(2)^*} = \text{tr} \{ \Sigma^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2} K_3(\varepsilon)' \times [ \text{vec}(\Sigma^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2}) \text{vec}(\Sigma^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2})] K_3(\varepsilon) \},
$$

$$
\kappa_4^{(1)^*} = E(\varepsilon^{1/2} C'(C'S'C')^{-1} C \Sigma^{1/2} \varepsilon)^2 - (p - 1)(p + 1).
$$

In practice to obtain the estimates of the indices, we can first suitably choose a contrast matrix such that $CC' = I_{p-1}$, e.g.,

$$
C = \begin{pmatrix}
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 \\
\frac{1}{\sqrt{2}} & \frac{2}{\sqrt{6}} & \cdots & \cdots & \cdots \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \cdots & \cdots & \cdots \\
\frac{1}{\sqrt{p(p-1)}} & \frac{1}{\sqrt{p(p-1)}} & \cdots & \cdots & \frac{1}{\sqrt{p(p-1)}}
\end{pmatrix},
$$

then pre-multiply it to the pooled standardized samples (so that the resulting samples are still standardized with dimension of $p - 1$), and finally estimate $\kappa_3^{(1)^*}$, $\kappa_3^{(2)^*}$, $\kappa_4^{(1)^*}$ through (2.2).

Corollary 2.2. Let $M = (1'\Sigma 1)^{-1/2} 1'\Sigma^{1/2}$, then $\kappa_3^{(1)^*}$, $\kappa_3^{(2)^*}$ and $\kappa_4^{(1)^*}$ can be simplified as

$$
\kappa_3^{(1)^*} = \kappa_3^{(2)^*} = \frac{E(1'\Sigma^{1/2} \varepsilon)^2}{(1'\Sigma 1)^3}, \quad \kappa_4^{(1)^*} = \frac{E(1'\Sigma^{1/2} \varepsilon)^4}{(1'\Sigma 1)^4} - 3.
$$

Example 2.1. If $\varepsilon$ is elliptically contoured distribution with kurtosis parameter $\kappa$ (Fang and Zhang, 1990, Section 2.6), then $\kappa_3^{(1)^*} = \kappa_3^{(2)^*} = 0$; further $\kappa_4^{(1)^*} = \kappa(p - 1)(p + 1)$ in Corollary 2.1 and $\kappa_4^{(1)^*} = 3\kappa$ in Corollary 2.2.

Now the distributions of $T_{PR}(k)$, $T_{LE}(k)$ and $T_{PL}(k)$ can be readily obtained from the distributions of Lawley-Hotelling statistic and Hotelling’s $T^2$ under general conditions (Fujikoshi, 2002; Gupta et al., 2006; Fujikoshi, 1997). More specifically, the general conditions are given as follows, for each population, generically denoted as $y$,

C1: $E(\|y\|^8) < +\infty$;

C2: The characteristic function of $x = (y_1, \cdots, y_p, y_1^2, y_1y_2, \cdots, y_p^2)$ satisfies the Cramér’s condition, i.e., $\limsup_{t \to \infty} |E(\exp(i'tx))| < 1$,

where $\| \cdot \|$ is the Euclidean norm and $i = \sqrt{-1}$. The restriction of the second condition is based on one of the validity conditions (Bhattacharya and Ghosh, 1978) for asymptotic expansions. Note that the Cramér’s condition is satisfied if $y$ is a continuous type random vector.
Proposition 2.1. Under the conditions C1 and C2, the null distribution of $T_{PR}(k)$ can be expanded as

$$P(T_{PR}(k) \leq x) = G_{(p-1)(k-1)}(x) + n^{-1} \sum_{j=0}^{3} c_j G_{(p-1)(k-1)+2j}(x) + o(n^{-1}),$$

(2.3)

where

$$c_0 = \frac{1}{4} (p-1)(k-1)(k-p-1) - (a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*}) + a_1 \kappa_4^{(1)*},$$

$$c_1 = -\frac{1}{2} (p-1)(k-1)^2 + 3(a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*}) - 2a_1 \kappa_4^{(1)*},$$

$$c_2 = \frac{1}{4} (p-1)(k-1)(p-1+k) - 3(a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*}) + a_1 \kappa_4^{(1)*},$$

$$c_3 = a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*},$$

where $a_1 = \left(\sum_{\alpha=1}^{k} \rho_{\alpha}^{-2} - k^2 - 2k + 2\right)/8$, $a_2 = \left(\sum_{\alpha=1}^{k} \rho_{\alpha}^{-2} - 3k + 2\right)/12$, $a_3 = \left(\sum_{\alpha=1}^{k} \rho_{\alpha}^{-2} - k^2\right)/8$, $\rho_{\alpha} = \sqrt{n_{\alpha}/n}$ ($\alpha = 1, \ldots, k$), and $\kappa_3^{(1)*}$, $\kappa_3^{(2)*}$ and $\kappa_4^{(1)*}$ are given in Corollary 2.1.

Proposition 2.2. Under the conditions C1 and C2, the null distribution of $T_{LE}(k)$ can be expanded as

$$P((k-1)T_{LE}(k) \leq x) = G_{k-1}(x) + n^{-1} \sum_{j=0}^{3} c_j G_{k-1+2j}(x) + o(n^{-1}),$$

(2.5)

where

$$c_0 = \frac{1}{4} (k-1)(k-3) - (a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*}) + a_1 \kappa_4^{(1)*},$$

$$c_1 = -\frac{1}{2} (k-1)^2 + 3(a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*}) - 2a_1 \kappa_4^{(1)*},$$

$$c_2 = \frac{1}{4} (k-1)(k+1) - 3(a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*}) + a_1 \kappa_4^{(1)*},$$

$$c_3 = a_2 \kappa_3^{(1)*} + a_3 \kappa_3^{(2)*},$$

$a_1$, $a_2$, $a_3$ are defined as in Proposition 2.1, and $\kappa_3^{(1)*}$, $\kappa_3^{(2)*}$, and $\kappa_4^{(1)*}$ are given in Corollary 2.2.

Remark 2.1. Proposition 2.1 and Proposition 2.2 are obtained by applying Lemma 2.1 to the asymptotic expansion of Lawley-Hotelling statistic given by Fujikoshi (2002). When $k = 2$, Proposition 2.1 and Proposition 2.2 reduce to Proposition 4 and Proposition 5 of Maruyama (2007) respectively. Our derivation here is much simpler.

Proposition 2.3. Under the conditions C1 and C2, the null distribution of $T_{FL}(k)$ can be expanded as

$$P(T_{FL}(k) \leq x) = G_{p-1}(x) + n^{-1} \sum_{j=0}^{3} c_j G_{p-1+2j}(x) + o(n^{-1}),$$

(2.7)
where
\[
\begin{align*}
c_0 &= -\frac{1}{4}(p-1)^2 + \frac{1}{6}\kappa_3^{(1)*} - \frac{1}{4}\kappa_4^{(1)*}, \\
c_1 &= -\frac{1}{2}(p-1) - \frac{1}{2}\kappa_3^{(1)*} + \frac{1}{2}\kappa_4^{(1)*}, \\
c_2 &= \frac{1}{4}(p-1)(p+1) - \frac{1}{2}\kappa_3^{(2)*} - \frac{1}{4}\kappa_4^{(1)*}, \\
c_3 &= \frac{1}{3}\kappa_3^{(1)*} + \frac{1}{2}\kappa_3^{(2)*},
\end{align*}
\]
and \(\kappa_3^{(1)*}, \kappa_3^{(2)*}, \text{ and } \kappa_4^{(1)*}\) are given in Corollary 2.1.

**Remark 2.2.** Proposition 2.3 is obtained by applying Lemma 2.1 to the asymptotic expansion of Hotelling’s \(T^2\) statistic given by Kano (1995) and Fujikoshi (1997). It is different to the distribution of \(T_{PR}(k)\) in Proposition 2.1 as expected.

We also give the distribution of \(T_{FL}^*(k)\) under general conditions. Observe that
\[
T_{FL}^*(k) = \sum_{j=1}^{k} n_j(c\bar{y}^{(j)\prime}(CSC)^{-1}(c\bar{y}^{(j)})) = \sum_{j=1}^{k} T^{(j)},
\]
which is the sum of quasi-independent Hotelling’s \(T^2\) statistics, \(\{T^{(j)}, j = 1, \ldots, k\}\). Then its null distribution can be obtained by applying Lemma 2.1 to a simplified result of Kakizawa (2008, Theorem 3).

**Proposition 2.4.** Under the conditions \(C1\) and \(C2\), the null distribution of \(T_{FL}^*(k)\) can be expanded as
\[
P(T_{FL}^*(k) \leq x) = G_{(p-1)k}(x) + n^{-1} \sum_{j=0}^{3} c_j G_{(p-1)k+2j}(x) + o(n^{-1}),
\]
(2.9)
where
\[
\begin{align*}
c_0 &= \frac{1}{4}(p-1)k(k-p) - (a_2^*\kappa_3^{(1)*} + a_3^*\kappa_3^{(2)*}) + a_4^*\kappa_4^{(1)*}, \\
c_1 &= -\frac{1}{2}(p-1)k^2 + 3a_2^*\kappa_3^{(1)*} + 3a_3^*\kappa_3^{(2)*} - 2a_4^*\kappa_4^{(1)*}, \\
c_2 &= \frac{1}{4}(p-1)(p+k) - (3a_2^* + \frac{1}{2})\kappa_3^{(1)*} - (3a_3^* + \frac{1}{2})\kappa_3^{(2)*} + a_4^*\kappa_4^{(1)*}, \\
c_3 &= (a_2^* + \frac{1}{2})\kappa_3^{(1)*} + (a_3^* + \frac{1}{2})\kappa_3^{(2)*},
\end{align*}
\]
where \(a_1^* = (\sum_{\alpha=1}^{k} \rho_{\alpha}^{-2} - k^2 - 2k)/8, a_2^* = (\sum_{\alpha=1}^{k} \rho_{\alpha}^{-2} - 3k)/12, a_3^* = (\sum_{\alpha=1}^{k} \rho_{\alpha}^{-2} - k^2)/8,\) and \(\kappa_3^{(1)*}, \kappa_3^{(2)*}, \text{ and } \kappa_4^{(1)*}\) are given in Corollary 2.1.
Table 3: Theoretical values of $\kappa^{(1)*}_3$, $\kappa^{(2)*}_3$, and $\kappa^{(1)*}_4$ for M3, M4, M5

<table>
<thead>
<tr>
<th></th>
<th>$p = 3$</th>
<th>$p = 5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>M3</td>
<td>(0.0, 0.16)</td>
<td>(0.0, -3.84)</td>
</tr>
<tr>
<td>M4</td>
<td>(2.67, 0.8)</td>
<td>(9.6, 0.192)</td>
</tr>
<tr>
<td>M5</td>
<td>(0.67, 0.2)</td>
<td>(2.4, 0.48)</td>
</tr>
</tbody>
</table>

Remark 2.3. Although the null distributions of $T_{FL}(k)$ and $T_{FL}^*(k)$ under normality only differ by one degree of freedom, their asymptotic expansions under general conditions cannot be simply related by changing the first degree of freedom of $k$ to $k - 1$ or vice versa. Some subtle changes of coefficients of skewness and kurtosis also take place at level $n^{-1}$ (comparing $a_j$'s with $a_j^*$'s).

3 Numerical Accuracy

In this section, we examine the numerical accuracy of the test sizes approximated by different finiteness corrections based on the asymptotic expansions of the null distributions. The performance for the two-sample case has been reported in Maruyama (2007). Here we first study a three-sample case as an example for general $k$-sample case and then focus on the accuracy comparison between the new test statistics and the traditional one for the flatness test.

We adopt three nonnormal models considered in Maruyama (2007) as follows,

M3: $y = (y_1, \ldots, y_p)'$ with $y_j$ ($j = 1, \ldots, p$) independently from Uniform$(-5, 5)$,

M4: $y = (y_1, \ldots, y_p)'$ with $y_j$ ($j = 1, \ldots, p$) independently from Exp(1),

M5: $y = (y_1, \ldots, y_p)'$ with $y_j$ ($j = 1, \ldots, p$) independently from $\chi^2_8$.

The theoretical values of $\kappa^{(1)*}_3$, $\kappa^{(2)*}_3$, and $\kappa^{(1)*}_4$ for M3, M4, M5 are given in Table 3. It is noted that because the components of $y$ in these models are independent and identically distributed, we get $K_3 = \beta_3(e_1e_1' e_2e_2' \cdots e_pe_p)'$, where $\beta_3$ is the skewness of $y_i$ and $e_j$ is a $p \times 1$ constant vector with the $j$th element 1 and others 0. It is easy to verify $\kappa^{(2)*}_3 = 0$ by Corollary 2.1 in these cases. (There seems a misprint in Table 1 of Maruyama (2007).) Let $T_g$ be a generic test statistic whose asymptotic expansion of the distribution is of form

$$P(T_g \leq x) = G_f(x) + n^{-1} \sum_{j=0}^{3} c_j G_{f+2j}(x) + o(n^{-1}). \quad (3.1)$$

Then along with the size approximated by the large sample theory, i.e.,

$$\alpha_1 = P(T_g > u), \quad u = \chi^2_f(\alpha), \quad \text{the } \alpha \text{ upper percentile of } \chi^2_f,$$

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three correction methods based on the asymptotic expansion (3.1) are obtained as follows,

1) [percentile correction]

\[ \alpha_2 = P(T_g > \tau_u), \quad \tau_u = u + \frac{2u}{nf} \left\{ -c_0 + \frac{(c_2 + c_3)u}{f + 2} + \frac{c_3u^2}{(f + 2)(f + 4)} \right\}; \]  

(3.2)

2) [Bartlett correction]

\[ \alpha_3 = P(T_g > \tau_b), \quad \tau_b = u(1 - \frac{\lambda_b}{n})^{-1}, \quad \lambda_b = \frac{2}{f} \sum_{j=1}^{3} jc_j; \]  

(3.3)

3) [monotone transformation correction]

\[ \alpha_4 = P(T_g > \tau_m), \quad \tau_m = n\lambda_1(e^{\frac{u}{n\lambda_1+\lambda_2}}-1), \quad \lambda_1 = \frac{f(f + 2)}{4c_2 + 12c_3}, \quad \lambda_2 = \frac{-(f + 2)(c_1 + c_2)}{2c_2 + 6c_3}; \]  

(3.4)

The details can be found in Fujikoshi (2000) and Maruyama (2007) among others. It is noted that in the simulations and in practice \( \tau_u, \tau_b, \) and \( \tau_m \) are estimated by replacing the coefficients \( c_j \)s and \( \kappa_{3}^{(1)*}, \kappa_{3}^{(2)*}, \kappa_{4}^{(1)*} \) with their consistent estimators.

For every model, we set the number of groups, \( k \), to be 3, and compare the sizes of \( \alpha_1, \alpha_2, \alpha_3, \) and \( \alpha_4 \) for three types of hypothesis given the nominal size to be 0.05. We let the sample sizes vary in both balanced and unbalanced ways. To be specific, we choose \((n_1, n_2, n_3)\) to be \((5, 5, 5), (5, 5, 10), (10, 10, 10), (10, 20, 30), (20, 20, 20), (30, 30, 30)\). And we choose the dimension of random vector to be 3 and 5, respectively. The actual size in each case is estimated by the empirical size from 10,000 simulations. It should be noted that for the flatness test, as an adjustment for the sequentialness of the test, the actual sizes for the proposed statistic \( T_{FL}(k) \) is estimated by the empirical conditional probability

\[ \alpha = P(T_{FL}(k) > \tau_{FL}|T_{PR}(k) < \tau_{PR}), \]

where \( \tau_{FL} \) and \( \tau_{PR} \) take different values according to different correction methods. (The actual sizes without conditioning are also computed and are found to be indistinguishable from the conditional ones as the models satisfy the parallelism automatically. The details are available upon request.) The results are shown in Figure 1 and Figure 2, where symbol ‘+’ stands for \( \alpha_1 \) of large sample theory and the symbols ‘*’, ‘△’, ‘♦’ stand for \( \alpha_2 \) (percentile correction), \( \alpha_3 \) (Bartlett correction) and \( \alpha_4 \) (monotone transformation correction), respectively. Our findings are summarized as follows.

1) The test criteria for profile analysis under normality or large sample theory are not robust. They tend to have inflated type I error rates, i.e., they are liberal. (See lines of ‘+’ in Figures 1 and 2.)

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Figure 1: Actual sizes of profile analysis for three models when the dimension of random vector is 3. The three rows of the panel correspond to three models M3, M4 and M5, respectively. The four columns of the panel correspond to different types of testing indicated in the titles, where PR, LE, FL, FL* stand for parallelism test, level test, flatness test using $T_{FL}(k)$ and flatness test using $T^*_{FL}(k)$, respectively. Symbols ‘+’, ‘*’, ‘△’, ‘♦’ stand for $\alpha_1$ (large sample theory), $\alpha_2$ (percentile correction), $\alpha_3$ (Bartlett correction) and $\alpha_4$ (monotone transformation correction), respectively.

2) The overall improvement of accuracy of sizes through asymptotic expansions (‘*’, ‘△’, ‘♦’) is very significant compared to the size obtained from large sample theory (‘+’). The improvement of accuracy is appreciable in all three types of hypothesis testing, in all three models under consideration and in the balanced as well as unbalanced cases.

3) Among three correction methods, the Bartlett correction appears to be the best, especially in Model 3 (First rows of Figures 1 and 2).

4) Both $T_{FL}(k)$ and $T^*_{FL}(k)$ for flatness test work well. The former with sequential test scheme gains better accuracy toward the nominal size than the latter (Columns 3 and 4 of Figures 1 and 2).

We also carry out simulations on other multivariate distributions such as multivariate $t$ distribution and contaminated multivariate normal distribution. The results exhibit a similar pattern as found before, therefore are not displayed here.
Next, we compare the sizes of flatness test using the traditional statistic $\tilde{T}_{FL}(2)$ and two proposed statistics $T_{FL}(2)$ and $T_{FL}^*(2)$ in two-sample case in a similar fashion as before. In addition, we choose $(n_1, n_2)$ to be $(5, 5), (5, 10), (10, 10), (5, 20), (20, 20)$. The asymptotic expansion of the distribution of $\tilde{T}_{FL}(2)$ is claimed to be identical to that of $T_{PR}(2)$ in Maruyama (2007). The results are shown in Figures 3 and 4, where the same symbols are used as before to stand for sizes obtained by different correction methods. It is seen that the test statistic $\tilde{T}_{FL}(2)$ has a tendency of rejecting more null hypotheses than it should even after corrections. (See the first column of Figures 3 and 4.) While $T_{FL}(2)$ and its finiteness correction perform well in controlling the size to the desired level. (See the second column of Figures 3 and 4.) But $T_{FL}^*(2)$ behaves not as well as $T_{FL}(2)$ when comparing Column 3 and Column 4 in Figures 3 and 4. Again, the Bartlett correction appears to be the best among the three correction methods.

Furthermore, we compare the power of $\tilde{T}_{FL}(2), T_{FL}(2)$ and $T_{FL}^*(2)$ for model M5 under the situation when the nominal size is 0.05, the dimension of random vector is 5 and the Bartlett correction is used. The alternative models are chosen by adding $\delta = 0, 1, 2, \ldots, 5$ respectively.
Figure 3: Actual sizes of flatness test for three models when the dimension of random vector is 3. The three rows of the panel correspond to three models. The three columns of the panel correspond to different test statistics indicated in the titles, where FL0, FL, FL* stand for $\tilde{T}_{FL}(2)$, $T_{FL}(2)$ and $T^*_{FL}(2)$, respectively. Symbols ‘+’, ‘∗’, ‘△’, ‘♦’ stand for $\alpha_1$ (large sample theory), $\alpha_2$ (percentile correction), $\alpha_3$ (Bartlett correction) and $\alpha_4$ (monotone transformation correction), respectively.

to the first component of $y$ and the first and third components of $y$ so that only flatness is violated. The result is shown in Figure 5. We can see that when $\delta = 0$ the power is in fact the size (the third row of Figure 4 with pooled sample size 40) where $T_{FL}(2)$ beats the other two significantly. For alternative values near the null hypothesis, $T_{FL}(2)$ is better than $\tilde{T}_{FL}(2)$ and $T^*_{FL}(2)$ despite the slightly higher powers of the other two statistics. While as $\delta$ increases, so is the non-centrality parameter, $T^*_{FL}(2)$ appears to be superior to the other two. The graphs clearly suggest that if we make adjustment for size inflation, then $\tilde{T}_{FL}(2)$ and $T_{FL}(2)$ will have very similar power. The graphs also show that $\tilde{T}_{FL}(2)$ and $T_{FL}(2)$ are more sensitive to slight departures from the null than $T^*_{FL}(2)$. Furthermore, the graphs give evidence that the power curves exhibit similar patterns under different alternative structures. Finally, taking both size and power into consideration, two new statistics $T_{FL}(2)$ and $T^*_{FL}(2)$ outperform the traditional one $\tilde{T}_{FL}(2)$.

In conclusion, we assert that $T_{PR}(k)$, $T_{LE}(k)$, and $T_{FL}(k)$ can serve as a full extension of test statistics for $k$-sample profile analysis. The finiteness correction based on the asymptotic expansion is crucial to improve the accuracy of size under general conditions. We recommend
Figure 4: Actual sizes of flatness test for three models when the dimension of random vector is 5. The three rows of the panel correspond to three models. The three columns of the panel correspond to different test statistics indicated in the titles, where FL0, FL, FL* stand for $\bar{T}_{FL}(2)$, $T_{FL}(2)$ and $T^*_F(2)$, respectively. Symbols ‘+’, ‘∗’, ‘△’, ‘♦’ stand for $\alpha_1$ (large sample theory), $\alpha_2$ (percentile correction), $\alpha_3$ (Bartlett correction) and $\alpha_4$ (monotone transformation correction), respectively.

using Bartlett correction for its accuracy and simplicity. Furthermore, it is numerically possible that the $p$-values computed from the formulae (2.3), (2.5), (2.7) and (2.9) can be greater than 1 or negative because they are only asymptotic expansion results as opposed to convergence results (Yanagihara and Tonda, 2003). The expansions should mainly be used to obtain percentiles or Bartlett’s and monotone transformation corrections.

4 Application

The quality and quantity of rainfall on a 65-year old spruce stand in Upper-Solling near Götingen, Germany were manipulated for experimental purposes by constructing a permanent roof over two sections of the wood. The roofs are built underneath the canopy at 3.5 meter above the ground. In one of the two experimental areas the rain was collected and de-mineralized to treat with a nutritive substance and sodium salts and re-sprinkled under the de-acidification (D1) roof. The second roofed area (D2) is served as the control of roof effect. For this area, rain was collected and re-sprinkled without further manipulation. In this experiment, another control
Figure 5: Powers of flatness test obtained by $T_{FL}(2)$, $T_{FL}^*(2)$ and $T_{FL}^0(2)$ for model M5 when the nominal size is 0.05, the dimension of random vector is 5, and the Bartlett correction is used. The alternative models are chosen by adding $\delta = 0, 1, 2, \ldots, 5$ respectively to the first component of $y$ (left panel) and the first and third components of $y$ (right panel). Three statistics are denoted as FL0 (with red line of ‘+’), FL (with green line of ‘*’), and FL* (with blue line of ‘△’), respectively.

area (D0) was considered which does not have any roof and is subjected to the normal weather condition. Ten water samples were collected at a depth between 70 and 100 centimeters from each of the areas (D0, D1, D2) and for each of the winter months (November-February) in the years 1989/1990−1995/1996. For this example we use the average over the four winter months to represent the $SO_4$ concentration for the winter of a particular year. Therefore we have $k = 3$, $p = 7$ and $n_1 = n_2 = n_3 = 10$ for this case. See Brunner, Domhof and Langer (2002, Section 1.3.3 and Appendix A.3) for a detailed account of this data set.

The profiles of $SO_4$ concentrations (mg/l) of the individual sample observations over the seven years are plotted in Figure 6 (a). The boldface lines are the mean profiles for the three areas. A chi-square plot of the concentrations corrected for area mean is displayed in Figure 6 (b). It is clear from the profile plots that apart from one or two outliers, we do not see any marked deviation from parallelism or level hypotheses. On the other hand, the chi-squared plot provides a resounding evidence against normality. Mardia’s (1970) tests of multivariate normality based on skewness and kurtosis yielded p-values less than 0.0001 and 0.0001, respectively, which lead to the conclusion that the data does not appear to have come from multivariate normal
Figure 6: (a) $SO_4$ Concentrations (milligram/liter) in water samples taken from the three sites representing the three areas or treatments (D0, D1 and D2) for the seven winter seasons in the years 1989/1990 – 1995/1996. (b) Chi-square plot of the $SO_4$ concentrations data corrected for area mean.

We conducted the profile analysis tests based on four methods for approximating the exact null distributions of the test statistics. Two of the methods are based on the quantiles of the exact distribution of the test statistics assuming multivariate normality and the quantiles of the limiting chi-square distribution. The other two are based on quantiles from the asymptotic expansion with Bartlett’s and monotone transformation corrections given by (3.3) and (3.4), respectively. The p-values using all the four methods of approximations are presented in Table 4.

Clearly, p-values based on the multivariate normal assumption and the limiting distribution lead to the rejection of the parallelism hypothesis. When parallelism is rejected, the standard practice in profile analysis is to proceed with separate flatness test for each group. In which case we have to deal with the intricacies associated with multiple testing. At any rate, in light of the small sample sizes and the failure of the normality assumption, we obviously cannot have faith on the conclusions from these two approximations. On the other hand, based on the p-values from the asymptotic expansions, we conclude that there is no significant evidence against parallelism. We therefore can proceed with the test for the levelness and flatness of the mean profiles. The p-values for levelness unanimously indicate for the tenability of this
Table 4: Profile Analysis of $SO_4$ in the three experimental areas of the spruce forest roof project

<table>
<thead>
<tr>
<th>Approximation</th>
<th>Test Statistics</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$T_{PR}(3)$</td>
</tr>
<tr>
<td>Assuming Normality</td>
<td>0.0473</td>
</tr>
<tr>
<td>Limiting Distribution</td>
<td>0.0119</td>
</tr>
<tr>
<td>Bartlett Correction</td>
<td>0.0731</td>
</tr>
<tr>
<td>Monotone Transformation</td>
<td>0.0839</td>
</tr>
</tbody>
</table>

hypothesis. Furthermore, we see there is clear evidence that the mean profiles are not flat. Therefore, the $SO_4$ concentrations in the two roofed and the unroofed areas fluctuate in exactly the same way across time.

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References


