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Abstract

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1. GLRT

Suppose $\{X_{i1}, \dots, X_{in_i}\}$ are i.i.d. distributed as $N(\mu_i, \Sigma)$ for $1 \leq i \leq K$. Let $\mathbf{X}_i = (X_{i1}, \dots, X_{in_i})$ for $i = 1, \dots, k$. The k samples are independent. μ_i , $i = 1, \dots, k$ and $\Sigma > 0$ are unknown. An interesting problem in multivariate analysis is to test the hypotheses

$$H : \mu_1 = \mu_2 = \dots = \mu_k \quad v.s. \quad K : \mu_i \neq \mu_j \text{ for some } i \neq j. \quad (1)$$

Let $\mathbf{Z} = (X_1, \dots, X_k)$.

$$f(Z; \mu_1, \dots, \mu_k, \Sigma) = \prod_{i=1}^k \left[(2\pi)^{-n_i p/2} |\Sigma|^{-n_i/2} \exp\left(-\frac{1}{2} \text{tr} \Sigma^{-1} \sum_{j=1}^{n_i} (x_{ij} - \mu_i)(x_{ij} - \mu_i)^T\right) \right].$$

Assume $n = \sum_{i=1}^p n_i < p$. Let $a \in \mathbb{R}^p$ be a vector satisfying $a^T a = 1$. Then

$$f_a(a^T Z; \mu_1, \dots, \mu_k, \Sigma) = (2\pi)^{-n/2} |a^T \Sigma a|^{-n/2} \exp\left(-\frac{1}{2a^T \Sigma a} \sum_{i=1}^k \sum_{j=1}^{n_i} (a^T x_{ij} - a^T \mu_i)^2\right)$$

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$$\max_{\mu_1, \dots, \mu_k, \Sigma} f_a(a^T Z, \mu_1, \dots, \mu_k, \Sigma) = (2\pi)^{-n/2} \left(\sum_{i=1}^k \sum_{j=1}^{n_i} (a^T x_{ij} - a^T \bar{\mathbf{X}}_i)^2 \right)^{-n/2} e^{-n/2} \quad (2)$$

Let $S_i = \sum_{j=1}^{n_i} (x_{ij} - \bar{\mathbf{X}}_i)(x_{ij} - \bar{\mathbf{X}}_i)^T$ and $S = \sum_{i=1}^k S_i$.

Under H , we have

$$\max_{\mu, \Sigma} f_a(a^T Z, \mu, \dots, \mu, \Sigma) = (2\pi)^{-n/2} \left(\sum_{i=1}^k \sum_{j=1}^{n_i} (a^T x_{ij} - a^T \bar{\mathbf{X}})^2 \right)^{-n/2} e^{-n/2} \quad (3)$$

The generalized likelihood ratio test statistic is defined as

$$T(Z) = \max_{a^T a=1, a^T S a=0} a^T \sum_{i=1}^k n_i (\bar{\mathbf{X}}_i - \bar{\mathbf{X}})(\bar{\mathbf{X}}_i - \bar{\mathbf{X}})^T a \quad (4)$$

Let $J = \text{diag}(n_1^{-1/2} \mathbf{1}_{n_1}, \dots, n_k^{-1/2} \mathbf{1}_{n_k})$. Then $S = Z(I_n - JJ^T)Z^T$ and

$$\sum_{i=1}^k n_i (\bar{\mathbf{X}}_i - \bar{\mathbf{X}})(\bar{\mathbf{X}}_i - \bar{\mathbf{X}})^T = Z(JJ^T - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T)Z^T. \quad (5)$$

The matrix $I_n - JJ^T$, $JJ^T - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T$ and $\frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T$ are all projection matrix and pairwise orthogonal with rank $n - k$, $k - 1$ and 1.

Let \tilde{J} be a $n \times (n - k)$ matrix satisfied $\tilde{J}\tilde{J}^T = I - JJ^T$. Then $S = Z\tilde{J}\tilde{J}^T Z^T$ and Note that

$$Z(JJ^T - \frac{1}{n} \mathbf{1}_n \mathbf{1}_n^T)Z^T = ZJ(I_k - \frac{1}{n} J^T \mathbf{1}_n \mathbf{1}_n^T J)J^T Z^T.$$

5 Note that $I_k - \frac{1}{n} J^T \mathbf{1}_n \mathbf{1}_n^T J$ is a projection matrix with rank $k - 1$. Let C be a $k \times (k - 1)$ matrix satisfied $CC^T = I_k - \frac{1}{n} J^T \mathbf{1}_n \mathbf{1}_n^T J$.

In Proposition 1, letting $A = Z\tilde{J}$ and $B = ZJCC^T J^T Z^T$ yields

$$\begin{aligned} T(Z) &= \lambda_{\max}((I_p - Z\tilde{J}(\tilde{J}^T Z^T Z\tilde{J})^{-1} \tilde{J}^T Z^T)ZJCC^T J^T Z^T(I_p - Z\tilde{J}(\tilde{J}^T Z^T Z\tilde{J})^{-1} \tilde{J}^T Z^T)) \\ &= \lambda_{\max}(C^T J^T Z^T(I_p - Z\tilde{J}(\tilde{J}^T Z^T Z\tilde{J})^{-1} \tilde{J}^T Z^T)ZJC). \end{aligned}$$

Note that

$$\begin{aligned} &\left(\begin{pmatrix} J^T \\ \tilde{J}^T \end{pmatrix} Z^T Z \begin{pmatrix} J & \tilde{J} \end{pmatrix} \right)^{-1} \\ &= \begin{pmatrix} J^T Z^T Z J & J^T Z^T Z \tilde{J} \\ \tilde{J}^T Z^T Z J & \tilde{J}^T Z^T Z \tilde{J} \end{pmatrix}^{-1} = \begin{pmatrix} J^T (Z^T Z)^{-1} J & J^T (Z^T Z)^{-1} \tilde{J} \\ \tilde{J}^T (Z^T Z)^{-1} J & \tilde{J}^T (Z^T Z)^{-1} \tilde{J} \end{pmatrix}. \end{aligned} \quad (6)$$

It follows that

$$\begin{aligned}
& (J^T(Z^T Z)^{-1}J)^{-1} \\
&= J^T Z^T Z J - J^T Z^T Z \tilde{J}(\tilde{J}^T Z^T Z \tilde{J})^{-1} \tilde{J}^T Z^T Z J \\
&= J^T Z^T (I_p - Z \tilde{J}(\tilde{J}^T Z^T Z \tilde{J})^{-1} \tilde{J}^T Z^T) Z J
\end{aligned} \tag{7}$$

It follows that

$$T(Z) = \lambda_{\max}\left(C^T (J^T(Z^T Z)^{-1}J)^{-1}C\right) \tag{8}$$

Proposition 1. Suppose A is a $p \times r$ matrix with rank r and B is a $p \times p$ non-zero semi-definite matrix. Let $H_A = A(A^T A)^{-1}A^T$. Then

$$\max_{a^T a=1, a^T A A^T a=0} a^T B a = \lambda_{\max}((I_p - H_A)B(I_p - H_A)). \tag{9}$$

Proof. Note that $a^T A A^T a = 0$ is equivalent to $A^T a = 0$ and is in turn equivalent to $H_A a = 0$. In this circumstance, $a = (I_p - H_A)a$. Then

$$\begin{aligned}
\max_{a^T a=1, a^T A A^T a=0} a^T B a &= \max_{a^T a=1, H_A a=0} a^T B a \\
&= \max_{a^T a=1, H_A a=0} a^T (I_p - H_A)B(I_p - H_A)a.
\end{aligned} \tag{10}$$

It's obvious that $(10) \leq \lambda_{\max}((I - H_A)B(I - H_A))$. On the other hand, let α_1 be one eigenvector corresponding to the largest eigenvalue of $(I - H_A)B(I - H_A)$. Note that the row of H_A are all eigenvectors of $(I - H_A)B(I - H_A)$ corresponding to eigenvalue 0. It follows that $H_A \alpha_1 = 0$. Now that α_1 satisfies the constraint of (10), (10) is maximized when $a = \alpha_1$. □

2. Schott's method

$$E = Z Z^T - \sum_{i=1}^k n_i \bar{X}_i \bar{X}_i^T.$$

$$H = \sum_{i=1}^k n_i \bar{X}_i \bar{X}_i^T - n \bar{X} \bar{X}^T.$$

$$\text{tr } E = \text{tr } Z^T Z - \text{tr } J^T Z^T Z J.$$

$$\text{tr } H = \text{tr } J^T Z^T Z J - \frac{1}{n} 1_n^T Z^T Z 1_n$$

$$T_{SC} = \frac{1}{\sqrt{n-1}} \left(\frac{1}{k-1} \text{tr } H - \frac{1}{n-k} \text{tr } E \right)$$

3. Theory

15 Let $Z\tilde{J} = U_{Z\tilde{J}} D_{Z\tilde{J}} V_{Z\tilde{J}}^T$ be the singular value decomposition of $Z\tilde{J}$. Let $H_{Z\tilde{J}} = U_{Z\tilde{J}} U_{Z\tilde{J}}^T$. $T(Z) = \lambda_{\max}(C^T J^T Z^T (I_p - H_{Z\tilde{J}}) Z J C)$.
 ZJC is independent of $H_{Z\tilde{J}}$

$$\mathbb{E}(Z\tilde{J}) = O_{p \times (n-k)}$$

Let $\Sigma = U\Lambda U^T$. Then

$$Z\tilde{J} = U\Lambda^{1/2}G_1,$$

where G_1 is a $p \times (n-k)$ matrix with i.i.d. $N(0,1)$ entries.

$$\mathbb{E}(ZJ) = (\sqrt{n_1}\mu_1, \dots, \sqrt{n_k}\mu_k) \stackrel{\text{def}}{=} \mu_f$$

And

$$ZJC = \mu_f C + U\Lambda_{1/2}G_2$$

where G_2 is a $p \times (k-1)$ matrix with i.i.d. $N(0,1)$ entries.

Then

$$\begin{aligned} T(Z) \sim \lambda_{\max} & (G_2^T \Lambda^{1/2} U^T (I_p - H_{Z\tilde{J}}) U \Lambda_{1/2} G_2 + \mu_f^T (I_p - H_{Z\tilde{J}}) \mu_f + \\ & \mu_f^T (I_p - H_{Z\tilde{J}}) U \Lambda^{1/2} G_2 + G_2^T \Lambda^{1/2} U^T (I_p - H_{Z\tilde{J}}) \mu_f) \end{aligned}$$

We have

$$G_2^T \Lambda^{1/2} U^T (I_p - H_{Z\tilde{J}}) U \Lambda_{1/2} G_2 \sim \sum_{i=1}^p \lambda_i (\Lambda^{1/2} U^T (I_p - H_{Z\tilde{J}}) U \Lambda^{1/2}) \xi_i \xi_i^T$$

20 where $\xi_i \stackrel{i.i.d.}{\sim} N(0, I_{k-1})$.

The eigenvalues of $\Lambda^{1/2} U^T (I_p - H_{Z\tilde{J}}) U \Lambda^{1/2}$ equal to those of $(I_p - H_{Z\tilde{J}}) U \Lambda U^T (I_p - H_{Z\tilde{J}})$.

Let $U = (U_1, U_2)$ and $\Sigma = \text{diag}(\Lambda_1, \Lambda_2)$, where U_1 is $p \times r$ and Λ_1 is $r \times r$. Assume $cI_{p-r} \leq \Lambda_2 \leq CI_{p-r}$.

$$\begin{aligned} & (I_p - H_{Z\tilde{J}}) U \Lambda U^T (I_p - H_{Z\tilde{J}}) \\ &= (I_p - H_{Z\tilde{J}}) U_1 \Lambda_1 U_1^T (I_p - H_{Z\tilde{J}}) + (I_p - H_{Z\tilde{J}}) U_2 \Lambda_2 U_2^T (I_p - H_{Z\tilde{J}}) = R_1 + R_2 \\ & \lambda_{\max}((I_p - H_{Z\tilde{J}}) U_1 \Lambda_1 U_1^T (I_p - H_{Z\tilde{J}})) = \lambda_{\max}(\Lambda_1^{1/2} U_1^T (I_p - H_{Z\tilde{J}}) U_1 \Lambda_1^{1/2}) \\ & \leq \lambda_{\max}(\Lambda_1^{1/2} U_1^T (I_p - U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T) U_1 \Lambda_1^{1/2}) \leq \lambda_1 \lambda_{\max}(U_1^T (I_p - U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T) U_1) \\ & = \lambda_1 \lambda_{\max}(I_r - U_1^T U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T U_1) \end{aligned}$$

25 We need to investigate the behavior of $U_{Z\tilde{J}}$.

$$G_1^T \Lambda G_1 = \tilde{J}^T Z^T Z \tilde{J} = V_{Z\tilde{J}} D_{Z\tilde{J}}^2 V_{Z\tilde{J}}^T$$

Note that

$$G_1^T \Lambda G_1 = G_{1[1:r,]}^T \Lambda_1 G_{1[1:r,]} + G_{1[(r+1):p,]}^T \Lambda_2 G_{1[(r+1):p,]}$$

For $i = 1, \dots, r$,

$$\begin{aligned} & \lambda_i(G_{1[1:r,]}^T \Lambda_1 G_{1[1:r,]}) \geq \lambda_i(G_{1[1:r,]}^T \text{diag}(\lambda_i I_i, O_{(r-i) \times (r-i)}) G_{1[1:r,]}) \\ & = \lambda_i \lambda_i (G_{1[1:i,]}^T G_{1[1:i,]}^T) = \lambda_i n(1 + o_P(1)) \end{aligned}$$

The last equality holds since $n^{-1} G_{1[1:i,]}^T G_{1[1:i,]} \xrightarrow{P} I_i$ by law of large numbers.

On the other hand, for $i = 1, \dots, r$,

$$\begin{aligned} & \lambda_i(G_{1[1:r,]}^T \Lambda_1 G_{1[1:r,]}) \\ &= \lambda_i \left(G_{1[1:r,]}^T \left(\text{diag}(\lambda_1, \dots, \lambda_{i-1}, O_{(r-i+1) \times (r-i+1)}) + \text{diag}(O_{(i-1) \times (i-1)}, \lambda_i, \dots, \lambda_r) \right) G_{1[1:r,]} \right) \\ & \leq \lambda_1 (G_{1[1:r,]}^T \text{diag}(O_{(i-1) \times (i-1)}, \lambda_i, \dots, \lambda_r) G_{1[1:r,]}) \leq \lambda_1 (G_{1[1:r,]}^T \text{diag}(O_{(i-1) \times (i-1)}, \lambda_i I_{r-i+1}) G_{1[1:r,]}) \\ & = \lambda_i \lambda_1 (G_{1[i:r,]}^T G_{1[i:r,]}^T) = \lambda_i n(1 + o_P(1)) \end{aligned}$$

where the first inequality holds by Weyl's inequality. It follows that $\lambda_i(G_{1[1:r]}^T \Lambda_1 G_{1[1:r]}) = \lambda_i n(1 + o_P(1))$ for $i = 1, \dots, r$.

Note that $\lambda_{\max}(G_{1[(r+1):p]}^T \Lambda_2 G_{1[(r+1):p]}) \leq C \lambda_{\max}(G_{1[(r+1):p]}^T G_{1[(r+1):p]}) = O_P(p)$ by Bai-Yin's law, here we have assumed $n/p = O(1)$. Assume $p/(\lambda_r n) \rightarrow$
 30 0, we can deduce that $D_{Z\tilde{J}[i,i]}^2 = \lambda_i(G_1^T \Lambda G_1) = \lambda_i n(1 + o_P(1))$, $i = 1, \dots, r$.

Note that

$$U \Lambda^{1/2} G_1 G_1^T \Lambda^{1/2} U^T = U_{Z\tilde{J}} D_{Z\tilde{J}}^2 U_{Z\tilde{J}}^T$$

then

$$G_1 G_1^T = \Lambda^{-1/2} U^T U_{Z\tilde{J}} D_{Z\tilde{J}}^2 U_{Z\tilde{J}}^T U \Lambda^{-1/2}$$

and

$$\begin{aligned} G_{1[(r+1):p]} G_{1[(r+1):p]}^T &= \Lambda_2^{-1/2} U_{[(r+1):p]}^T U_{Z\tilde{J}} D_{Z\tilde{J}}^2 U_{Z\tilde{J}}^T U_{[(r+1):p]} \Lambda_2^{-1/2} \\ &\geq \Lambda_2^{-1/2} U_{[(r+1):p]}^T U_{Z\tilde{J}[1:r]} D_{Z\tilde{J}[1:r]}^2 U_{Z\tilde{J}[1:r]}^T U_{[(r+1):p]} \Lambda_2^{-1/2} \\ &\geq D_{Z\tilde{J}[r,r]}^2 \Lambda_2^{-1/2} U_{[(r+1):p]}^T U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T U_{[(r+1):p]} \Lambda_2^{-1/2} \end{aligned}$$

Thus,

$$\lambda_{\max}(U_{[(r+1):p]}^T U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T U_{[(r+1):p]}) \leq \frac{C}{D_{Z\tilde{J}[r,r]}^2} \lambda_1(G_{1[(r+1):p]} G_{1[(r+1):p]}^T) = O_P\left(\frac{p}{\lambda_r n}\right)$$

Note that

$$\begin{aligned} &\lambda_{\max}(U_{[(r+1):p]}^T U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T U_{[(r+1):p]}) = \lambda_{\max}(U_{Z\tilde{J}[1:r]}^T U_{[(r+1):p]} U_{[(r+1):p]}^T U_{Z\tilde{J}[1:r]}) \\ &= \lambda_{\max}(U_{Z\tilde{J}[1:r]}^T (I_p - U_1 U_1^T) U_{Z\tilde{J}[1:r]}) = \lambda_{\max}(I_r - U_{Z\tilde{J}[1:r]}^T U_1 U_1^T U_{Z\tilde{J}[1:r]}) \\ &= 1 - \lambda_{\min}(U_{Z\tilde{J}[1:r]}^T U_1 U_1^T U_{Z\tilde{J}[1:r]}) = 1 - \lambda_{\min}(U_1^T U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T U_1) \\ &= \lambda_{\max}(I_r - U_1^T U_{Z\tilde{J}[1:r]} U_{Z\tilde{J}[1:r]}^T U_1) \end{aligned}$$

Therefore $\lambda_{\max}(R_1) = O_P\left(\frac{\lambda_1 p}{\lambda_r n}\right)$

Having this, we can deal with $R_1 + R_2$

For $i = 1, \dots, r$,

$$\lambda_i(R_1 + R_2) \leq \lambda_1(R_1 + R_2) \leq \lambda_1(R_1) + \lambda_1(R_2) \leq O_P\left(\frac{\lambda_1 p}{\lambda_r n}\right) + C$$

For $i = r+1, \dots, p-r$,

$$\lambda_i(R_1 + R_2) \leq \lambda_{i-r}(R_2) = \lambda_{i-r}(\Lambda_2^{1/2} U_2^T (I_p - H_{Z\tilde{J}}) U_2 \Lambda_2^{1/2}) \leq \lambda_{i-r}(\Lambda_2) = \lambda_i$$

On the other hand, for $i = 1, \dots, p - r - n + k$,

$$\begin{aligned}\lambda_i(R_1 + R_2) &\geq \lambda_i(R_2) = \lambda_i(\Lambda_2^{1/2} U_2^T (I_p - H_{Z\bar{J}}) U_2 \Lambda_2^{1/2}) \\ &= \lambda_i(\Lambda_2 - \Lambda_2^{1/2} U_2^T H_{Z\bar{J}} U_2 \Lambda_2^{1/2}) \geq \lambda_{i+n-k}\end{aligned}$$

The last equality holds since $U_2^T H_{Z\bar{J}} U_2$ is at most of rank $n - k$.

$$\sum_{i=1}^{p-r-n+k} \lambda_{i+n-k}^2 \leq \text{tr}[(R_1 + R_2)^2] \leq r(O_P(\frac{\lambda_1 p}{\lambda_r n}) + C)^2 + \sum_{i=r+1}^{p-r} \lambda_i^2$$

Or

$$|\text{tr}[(R_1 + R_2)^2] - \sum_{i=r+1}^p \lambda_i^2| \leq \sum_{i=r+1}^{n-k} \lambda_i^2 + \sum_{i=p-r+1}^p \lambda_i^2 + r(O_P(\frac{\lambda_1 p}{\lambda_r n}) + C)^2$$

Similarly,

$$|\text{tr}[(R_1 + R_2)] - \sum_{i=r+1}^p \lambda_i| \leq \sum_{i=r+1}^{n-k} \lambda_i + \sum_{i=p-r+1}^p \lambda_i + r(O_P(\frac{\lambda_1 p}{\lambda_r n}) + C)$$

Therefore, assume $\lim p/n \rightarrow \infty$ and $\frac{\lambda_1^2 p}{\lambda_r^2 n^2} \rightarrow 0$, we have

$$\text{tr}[(R_1 + R_2)^2] = (1 + o_P(1)) \sum_{i=r+1}^p \lambda_i^2$$

and

$$\text{tr}[(R_1 + R_2)] = \sum_{i=r+1}^p \lambda_i + O(n) + O_P(\frac{\lambda_1 p}{\lambda_r n}).$$

Note that

$$\frac{\lambda_1[(R_1 + R_2)^2]}{\text{tr}[(R_1 + R_2)^2]} = \frac{(O_P(\frac{\lambda_1 p}{\lambda_r n}) + C)^2}{(1 + o_P(1)) \sum_{i=r+1}^p \lambda_i^2} \xrightarrow{P} 0.$$

Apply Lyapunov central limit theorem conditioning on $H_{Z\bar{J}}$, we have

$$(\text{tr}[(R_1 + R_2)^2])^{-1/2} (G_2^T \Lambda^{1/2} U^T (I_p - H_{Z\bar{J}}) U \Lambda_{1/2} G_2 - \text{tr}(R_1 + R_2) I_{k-1}) \xrightarrow{\mathcal{L}} W_{k-1}$$

where W_{k-1} is a $(k-1) \times (k-1)$ symmetric random matrix whose entries above the main diagonal are i.i.d. $N(0, 1)$ and the entries on the diagonal are i.i.d.

$N(0, 2)$. By Slutsky's theorem, we have

$$(\sum_{i=r+1}^p \lambda_i^2)^{-1/2} (G_2^T \Lambda^{1/2} U^T (I_p - H_{Z\bar{J}}) U \Lambda_{1/2} G_2 - \sum_{i=r+1}^p \lambda_i^2) \xrightarrow{\mathcal{L}} W_{k-1}$$

And

$$\begin{aligned}
& \mathbb{E}[\|\mu_f^T(I_p - H_{Z\tilde{J}})U\Lambda^{1/2}G_2\|_F^2 | Z, \tilde{J}] \\
&= (k-1) \text{tr}(\mu_f^T(I_p - H_{Z\tilde{J}})U\Lambda U^T(I_p - H_{Z\tilde{J}})\mu_f) \\
&\leq (k-1)\lambda_1((I_p - H_{Z\tilde{J}})U\Lambda U^T(I_p - H_{Z\tilde{J}}))\|\mu_f\|_F^2 \\
&= (k-1)O_P\left(\frac{\lambda_1 p}{\lambda_r n}\right)\|\mu_f\|_F^2 \\
&= (k-1)O_P\left(\frac{\lambda_1 \sqrt{p}}{\lambda_r n}\right)\sqrt{p}\|\mu_f\|_F^2 = o_P(p)
\end{aligned}$$

³⁵ The last equality holds when we assume $\frac{1}{\sqrt{p}}\|\mu_f\|_F^2 = O(1)$. Hence $\|\mu_f^T(I_p - H_{Z\tilde{J}})U\Lambda^{1/2}G_2\|_F^2 = o_P(p)$.

References