Principal Components Analysis in the Complex Case[1])

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1. Introduction

KSHIRSAGAR [1961] has developed the goodness of fit test of a single non-isotropic principal component when the observations are from a multivariate normal distribution. GUPTA and KSHIRSAGAR [1965] generalized these results to the k non-isotropic principal components. KSHIRSAGAR [1961] has also derived the distribution of latent roots of the covariance matrix of normal variables, when the hypothetical linear function of the variables is eliminated. In the same paper he has also given the relation between original roots and the residual roots. In this paper an attempt has been made to develop a similar theory when the observations are from a "complex multivariate normal distribution". These latter distributions and the sampling distributions derived from it are studied by GOODMAN [1963] and KHATRI [1965].

2. Complex Multivariate Normal Distribution

Let

$$\xi' = [\xi_1 | \xi_2 | \cdots | \xi_p]$$
$$\xi_j = x_j + i y_j \quad (j = 1,2,\ldots,p) \tag{2.1}$$

and $\eta' = (x_1\, y_1\, x_2\, y_2 \ldots x_p\, y_p)$.

We assume $E(\eta) = 0$ and $V(\eta')$ where V stands for the variance-covariance matrix equal to

$$\begin{aligned} \Sigma_\eta = E(\eta'\eta) &= \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \quad \text{if} \quad j = k \\ &= \begin{bmatrix} \frac{1}{2}\alpha_{jk} & -\frac{1}{2}\beta_{jk} \\ \frac{1}{2}\beta_{jk} & \frac{1}{2}\alpha_{jk} \end{bmatrix} \sigma_j \sigma_k \quad \text{if} \quad j \neq k\,. \end{aligned} \tag{2.2}$$

It can be easily seen that the covariance matrix of the complex vector, ξ, is

$$\Sigma_\xi = E(\xi \bar{\xi}')$$

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where $\bar{\xi}$ is the complex conjugate of ξ and has its elements in the j-th row and k-th column to be

$$\begin{array}{ll} \sigma_k^2 & \text{if} \quad j = k \\ (\alpha_{jk} + i\beta_{jk})\sigma_j\sigma_k & \text{if} \quad j \neq k\,. \end{array} \tag{2.3}$$

GOODMAN [1963] has shown the density of ξ to be

$$p(\xi) = \frac{1}{\pi^p|\Sigma_\xi|}\exp\{-(\bar{\xi}'\bar{\Sigma}_\xi^1\xi\}\,. \tag{2.4}$$

Let (ξ_{js}) be a sample of size n from the distribution of ξ. The maximum likelihood estimate of Σ_ξ is

$$S = \frac{1}{N}A \tag{2.5}$$

where

$$A = \sum_{j=1}^{N}\xi_{js}\bar{\xi}_{js} \tag{2.6}$$

is the matrix of sum of squares and sum of products of the sample observations.

A follows the complex WISHART distribution and its density function is given by GOODMAN [1963] and GUPTA [1964]

$$\frac{|A|^{n-p}\exp(-\operatorname{tr}\bar{\Sigma}_\xi^1 A)}{|\Sigma_\xi|^n\pi^{p(p-1)/2}\Gamma(n)\ldots\Gamma(n-p+1)}\,. \tag{2.7}$$

3. Principal Components

As $\xi' = (\xi_1,\xi_2,\ldots,\xi_p)$ is a p-component vector having complex multivariate normal distribution, there exists an unitary matrix, Γ, such that

$$\Sigma_\xi = \bar{\Gamma}'\operatorname{diag}(\sigma_1,\sigma_2,\ldots,\sigma_p)\Gamma\,. \tag{3.1}$$

If the roots of the HERMITian matrix, Σ_ξ, are arranged in descending order of magnitude as

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p$$

then $\bar{\Gamma}_i'\xi$ is called the i-th principal component.

As Γ is an unitary matrix from (3.1), it follows

$$\bar{\Gamma}'\Sigma_\xi\Gamma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_p \end{bmatrix}.$$

The maximum likelihood estimate of Γ_i's and σ_i's are provided by C_i's and θ_i's which are respectively the latent roots and vector of the sample matrix S. We assume C_i's are normalized and hence

$$C = [C_1|C_2|\ldots|C_p]' \tag{3.3}$$

is a unitary matrix. As before

$$S = C\Theta\bar{C}' = C\,\mathrm{diag}\,(\theta_1,\theta_2,\ldots,\theta_p)\bar{C}'$$

or (3.4)

$$\bar{C}'SC = \Theta$$

and hence

$$Z_i = \bar{C}_i'\xi \tag{3.5}$$

are the sample principal components.

4. Goodness of Fit Test for Two Non-isotropic Principal Components

If all the roots of the HERMITian matrix, Σ_ξ, except the first two are equal, then the latent vectors corresponding to these anomolous roots are the two non-isotropic principal components and

$$\Sigma_\xi = (\sigma_1 - \sigma)\Gamma_1\bar{\Gamma}_1' + (\sigma_2 - \sigma)\Gamma_2\bar{\Gamma}_2' + \sigma I \tag{4.1}$$

where $\sigma_3 = \sigma_4 = \cdots = \sigma_p = \sigma$ (say).

We set up the following hypotheses: H: – (H_1). All the roots of Σ_ξ except the first two are equal, and (H_2) the latent vector and corresponding to the two anomolous roots are Γ_1^* and Γ_2^*, i.e.,

$$\Gamma_1 = \Gamma_1^* \quad \text{and} \quad \Gamma_2 = \Gamma_2^*.$$

Make the transformation

$$U = \bar{\Gamma}'\xi$$

where

$$\xi = (\xi_{jk}) \quad \begin{array}{l} j = 1,\ldots,p \\ k = 1,\ldots,p \end{array}$$

then

$$\chi_H^2 = \sum_{j=3}^{p}\sum_{t=1}^{n} U_{jt}\bar{U}_{jt}' = \mathrm{tr}\, U\bar{U}' - \sum_{t=1}^{n} U_{1t}\bar{U}_{1t}' - \sum_{t=1}^{n} U_{2t}\bar{U}_{2t}' = \mathrm{tr}\, B - \lambda_1^2 - \lambda_2^2 \tag{4.2}$$

where

$$U\bar{U}' = B$$

and λ_1^2/n and λ_2^2/n have independent χ^2 with $2n$ degrees of freedom each.

Consider the partial regression coefficient of $\bar{\Gamma}_j'\xi$, $(j = 3,\ldots,p)$ on $\bar{\Gamma}_2'\xi$ when $\bar{\Gamma}_1'\xi$ is fixed, viz

$$\frac{\bar{\Gamma}_j' A\Gamma_2 - \rho\dfrac{\lambda_2}{\lambda_1}\bar{\Gamma}_j' A\Gamma_1}{\lambda_2(1-\rho^2)^{\frac{1}{2}}} \tag{4.3}$$

where

$$\rho = \frac{\bar{\Gamma}_1' A\Gamma_2}{\{(\bar{\Gamma}_1' A\Gamma_1)(\bar{\Gamma}_2' A\Gamma_2)\}^{\frac{1}{2}}}.$$

Then

$$\chi_1^2 = \sum_{j=3}^{p} \left\{ \frac{\bar{\Gamma}_j' A \Gamma_2 - \rho \frac{\lambda_2}{\lambda_1} \bar{\Gamma}_j' A \Gamma_1}{\lambda_2 (1-\rho^2)^{\frac{1}{2}}} \right\}^2$$

$$= \frac{\bar{\Gamma}_2' A \Gamma_2 + \rho^2 \frac{\lambda_2^2}{\lambda_1^2} \bar{\Gamma}_1' A \Gamma_1 - 2\rho \frac{\lambda_2}{\lambda_1} \bar{\Gamma}_2' A \Gamma_1}{\lambda_2^2 (1-\rho^2)} - \lambda_2^2 (1-\rho^2) \tag{4.4}$$

is a $\chi^2 \sigma$ with $2(p-2)$ degrees of freedom and which is the direction factor.

It is clear that the angle between two hypothetical principal components will be

$$\rho \frac{\lambda_2}{\lambda_1} \text{ and}$$

$$\chi_3^2 = \rho^2 \frac{\lambda_2^2}{\lambda_1^2} \tag{4.5}$$

follows a $\chi^2 \sigma$ with one degree of freedom. Hence

$$\chi_2^2 = \frac{\bar{\Gamma}_1' A \Gamma_1}{\lambda_1^2} - \lambda_1^2 - \rho^2 \frac{\lambda_2^2}{\lambda_1^2} \tag{4.6}$$

is a $\chi^2 \sigma$ with $2(p-2)$ degrees of freedom and is also the direction factor.

5. Residual Roots

In the case of a single non-isotropic principal component, if $\bar{h}'\xi$ is the hypothetical component we desire to test the hypothesis that $\bar{h}'\xi$ is the same as $\bar{\Gamma}'\xi$.

The hypothetical function

$$\begin{aligned} \eta &= \bar{\Gamma}'\xi \\ &= \bar{\Gamma}'\bar{C}'z \quad \text{(from 3.5)} \\ &= \bar{w}'z \end{aligned} \tag{5.1}$$

where

$$w = C\Gamma \tag{5.2}$$

and we assume the normalization

$$\bar{w}'w = 1 .$$

The sample conditional covariance matrix when η is eliminated is

$$\frac{1}{n}\left[\theta_j \delta_{jk} - \frac{\bar{w}_j \theta_j \bar{w}_k \theta_k}{\lambda^2}\right] \quad (j,k = 1, \ldots, p) \tag{5.3}$$

where δ_{jk} is the KRONCKER delta.

The roots of the above matrix are called the residual roots of ξ in the complex case. Thus the residual roots are $1/n$ times the roots of the determinantal equation in φ.

$$\left| \theta_j \sigma_{jk} - \frac{1}{\lambda^2} \bar{w}_j w_k \theta_j \theta_k - \varphi \sigma_{jk} \right| = 0 .$$

After little simplification, we get

$$\bar{w}_j^2 = \frac{\lambda^2}{\theta_j^2} \frac{\prod_k (\varphi_k - \theta_j)}{\prod_{l \neq k} (\varphi_k - \theta_j)}. \tag{5.4}$$

6. Distribution of Residual Roots

When Σ_ξ has one root, $\sigma_1 > 1$, and the remaining roots are all equal to unity, the s.s and s.p. matrix of the true principal components is

$$B = \Gamma A \bar{\Gamma}' \tag{6.1}$$

and the distribution of B is the complex WISHART distribution

$$\text{Const.} |B|^{n-p} \exp\left\{ - \left(\frac{b_{11}}{\sigma_1} + b_{22} + \cdots + b_{pp} \right) \right\} \mathrm{d}B. \tag{6.2}$$

B can also be given by

$$B = w \Theta \bar{w}' \quad \text{(by 5.2)}. \tag{6.3}$$

TAMURA [1965] has given the JACOBian of the transformation from B to w and θ in terms of rotation angles in the real case, whereas the orthogonal matrix has been represented by the rotational angles. KHATRI [1965] has also given the JACOBian of this transformation in the complex case. It is easy to deal with the KHATRI's transformation.

$$J(B; \theta, w) = \frac{\prod_{k=1}^{p-1} \prod_{j=k+1}^{p} (\theta_j - \theta_k)^2}{\prod_{g=1}^{p-1} |w_g|} \tag{6.4}$$

where w_g is the matrix of the first g rows and g columns of w.

Therefore, the joint distribution of λ and w comes out to be

$$\text{const. } p(\theta)\ \bar{\sigma}_1^n \exp\left\{ - \lambda^2 \left(\frac{1}{\sigma_1} - 1 \right) \right\} \prod_1^{p-1} |w_g^{-1}| \,\mathrm{d}\theta \,\mathrm{d}w. \tag{6.5}$$

Integrating all the elements of w except in its first row we get

$$\text{const.} p(\theta) \sigma_1^{-n} \exp\left\{ - \lambda^2 \left(\frac{1}{\sigma_1} - 1 \right) \right\} \frac{2}{w_{11}} \mathrm{d}\theta \cdot \prod_2^p \mathrm{d}w_{1i}. \tag{6.6}$$

We now make the transformation from $\bar{w}_j$ ($j = 2, \ldots, p$) to φ_k^2 ($k = 1, \ldots, p-1$) by (5.4) and get the joint distribution of φ_k^2 and Θ,

$$\frac{\text{const.} p(\Theta) \exp\left[- \lambda^2 \left(\frac{1}{\sigma_1} - 1 \right) \right] \prod_j (w_j \theta_j) \prod (\theta_j - \theta_k | \prod (\varphi_h - \varphi_k)}{\sigma_1^n w_{11} \prod_k \varphi_k \prod_j \prod_k |\varphi_k - \theta_j|}$$

$$\cdot \frac{\prod_k |\varphi_k - \theta_1| \,\mathrm{d}\Theta \,\mathrm{d}\varphi}{\prod_{j \neq 1} (\theta_1 - \theta_j)}. \tag{6.7}$$

Substituting for all w_i from (5.4) in terms of φ_k and making the use of

$$\prod_{k=1}^{p-1} \varphi_k = \frac{1}{\lambda_2} \prod_{j=1}^{p} \theta_j$$

(6.7) reduces to

$$\frac{\text{const.}\, p(\Theta) \exp\left[-\lambda^2\left(\frac{1}{\sigma_1} - 1\right)\right] (\lambda^2)^p \prod_{h \neq k} |\varphi_h - \varphi_k| \, d\Theta \, d\varphi}{\sigma_1^n \prod_j \theta_j \prod_{k,j} |\varphi_k - \theta_j|}$$

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