

THE GOODNESS OF FIT OF TWO (OR MORE) HYPOTHETICAL PRINCIPAL COMPONENTS

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1. Introduction

If all the latent roots except the largest one of Σ , the covariance matrix of a multinormal population are equal, the corresponding latent vector gives rise to a single non-isotropic principal component. A goodness of fit test for a hypothetical principal component was derived by Kshirsagar [11]. He considered the following two aspects: (1) Departure from the hypothesis due to there being more than one non-isotropic principal component and (2) departure due to deviation in direction of the true principal component from the hypothetical one. By removing the contribution due to (1) to the over all statistic, he gave an exact test dealing with the direction aspect of the hypothetical principal component. The procedure was analogous to Bartlett's ([4], [5], [6]) direction and collinearity tests in discriminant analysis. However, in practice, it will be only rarely true that only one non-isotropic principal component adequately represents Σ . In other words Σ will have two or more unequal roots, the remaining being all equal. There will, therefore, be two or more non-isotropic principal components. In this paper, it is proposed to extend Kshirsagar's test to suit this situation by considering the goodness of fit of two or more hypothetical principal components. The case of two principal components is considered in detail first. Further generalization is outlined in section 5.

2. Two non-isotropic principal components

Let $\mathbf{x}' = (x_1, x_2, \dots, x_p)$ be the row vector of p multinormal variables measured from their true means and covariance matrix Σ . Let $\sigma_{(i)}^2$ and $\mathbf{l}_{(i)}$ ($i=1, \dots, p$) be the latent roots and corresponding orthonormal latent vectors of Σ respectively. We assume that $\sigma_3^2 = \dots = \sigma_p^2 (= \sigma^2)$ and $\sigma_1^2 > \sigma_2^2 > \sigma^2$. This means that $\mathbf{l}_1\mathbf{x}$ and $\mathbf{l}_2\mathbf{x}$ are the (true) two non-isotropic principal components. Let $\mathbf{l}_{(i)}$ ($i=1, \dots, p$) form the columns of a matrix L' . Obviously L is orthogonal. As in Kshirsagar [11] we define

$$(2.1) \quad \mathbf{y}' = \mathbf{x}'\mathbf{L}' = (y_1, y_2, \dots, y_p)$$

and also it can be readily seen that

$$(2.2) \quad \begin{aligned} \Sigma &= \sigma_1^2 \mathbf{l}_1 \mathbf{l}_1' + \sigma_2^2 \mathbf{l}_2 \mathbf{l}_2' + \sigma^2 (\mathbf{I} - \mathbf{l}_1 \mathbf{l}_1' - \mathbf{l}_2 \mathbf{l}_2') \\ &= (\sigma_1^2 - \sigma^2) \mathbf{l}_1 \mathbf{l}_1' + (\sigma_2^2 - \sigma^2) \mathbf{l}_2 \mathbf{l}_2' + \sigma^2 \mathbf{I} \end{aligned}$$

i.e., Σ is completely determined by \mathbf{l}_1 , \mathbf{l}_2 , σ_1^2 , σ_2^2 and σ^2 where \mathbf{I} is the identity matrix.

Let

$$(2.3) \quad \mathbf{X} = (x_{ir}) \quad (i=1, \dots, p) \quad (r=1, \dots, n)$$

be a sample of size n from the distribution of \mathbf{x} . Then Σ is estimated by $\frac{1}{n} \mathbf{A}$ where

$$(2.4) \quad \mathbf{A} = (a_{ij}) = \mathbf{X}'\mathbf{X}$$

is the matrix of the sums of squares and products of the observations in the sample.

Suppose now, we have two hypothetical linear functions $\mathbf{l}_1^{*\prime} \mathbf{x}$ and $\mathbf{l}_2^{*\prime} \mathbf{x}$ satisfying

$$(2.5) \quad \mathbf{l}_1^{*\prime} \mathbf{l}_1 = 1 \quad \mathbf{l}_2^{*\prime} \mathbf{l}_2 = 1 \quad \text{and} \quad \mathbf{l}_1^{*\prime} \mathbf{l}_2^* = 0.$$

We now set up the following null hypothesis. $H: (H_1)$ all the roots of Σ except the first two are equal and (H_2) the latent vectors corresponding to the two anomalous roots are \mathbf{l}_1^* and \mathbf{l}_2^* , i.e.,

$$\mathbf{l}_1 = \mathbf{l}_1^* \quad \text{and} \quad \mathbf{l}_2 = \mathbf{l}_2^*.$$

It should be noted that H consists of both H_1 and H_2 . However, we are more interested in H_2 rather than H_1 . H_2 deals with the direction aspect of the first two principal components, while H_1 simply deals with the adequacy of only two nonisotropic components. A hypothesis about the goodness of two assigned principal components is meaningful only when H_1 is true. If H_1 is not true, two components are not fully adequate to represent Σ , but they may do so only approximately. One, therefore, will wish to test H_1 by a preliminary test and will proceed to H_2 only when there is reason to believe in the validity of H_1 or else we are prepared to ignore the effect of the non-validity of H_1 . Consequently it is necessary to remove the contribution of H_1 to the over all test criterion of H and obtain a more precise test for H_2 , as done by Bartlett ([4], [5], [6]). If H is true $\mathbf{l}_{(i)} = \mathbf{l}_{(i)}^*$ ($i=1, 2$). Consequently we can suppress the stars in the foregoing discussion. $\mathbf{l}_{(1)}$ and $\mathbf{l}_{(2)}$ satisfy orthogonality conditions (2.5) and hence we can find $p-2$ suitable other

vectors $l_{(i)} (i=3, 4, \dots, p)$ such that

$$(2.6) \quad L' = (l_{(1)} \vdots l_{(2)} \vdots \dots \vdots l_{(p)})$$

is an orthogonal matrix. Then it can be easily seen from (2.1) that

$$(2.7) \quad y_1 \text{ is } N(0, \sigma_1), y_2 \text{ is } N(0, \sigma_2) \text{ while } y_i (i=3, \dots, p) \text{ are } N(0, \sigma),$$

all being independent. Consequently,

$$(2.8) \quad \chi_H^2 = \frac{1}{\sigma^2} \sum_{i=3}^p \sum_{r=1}^n y_{ir}^2$$

where

$$(2.9) \quad Y = (y_{ir}) = XL'$$

has a χ^2 distribution with $n(p-2)$ d.f. This is the over all criterion for H which is $H_1 \cap H_2$. The test can be applied if σ^2 is known. The criterion can also be expressed as

$$(2.10) \quad (\text{putting } B = Y'Y = LX'XL' = LAL')$$

$$(2.11) \quad \begin{aligned} \sigma^2 \chi_H^2 &= \text{tr } Y'Y - \sum_{i=1}^2 \sum_{r=1}^n y_{ir}^2 \\ &= \text{tr } B - b_{11} - b_{22} \\ &= \text{tr } A - \lambda_1^2 - \lambda_2^2 \end{aligned}$$

where

$$(2.12) \quad b_{ii} = \lambda_i^2 = \sum_{r=1}^n y_{ir}^2 = l_{(i)}' A l_{(i)}, \quad (i=1, 2).$$

From (2.7) it is obvious that $\frac{\lambda_1^2}{\sigma_1^2}$ has a χ^2 distribution with n d.f. $\frac{\lambda_2^2}{\sigma_2^2}$ has a χ^2 distribution with n d.f. and both are independently distributed.

We now want to isolate the contribution of H_1 to this over-all χ_H^2 as we are more interested in the direction aspect of the hypothetical components.

3. Partitioning of χ_H^2

From (2.7) it follows that $B = Y'Y$ has the Wishart distribution

$$\text{Const } |B|^{-\frac{n-p-1}{2}} e^{-\frac{1}{2} \left(\frac{b_{11}}{\sigma_1^2} + \frac{b_{22}}{\sigma_2^2} + \frac{b_{33} + \dots + b_{pp}}{\sigma^2} \right)} dB$$

where $d\mathbf{B}$ stands for the volume element. As in Kshirsagar [11], we transform to the rectangular coordinates

$$(3.2) \quad \mathbf{T} = \begin{pmatrix} t_{11} & 0 & \cdots & 0 \\ t_{21} & t_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ t_{p1} & t_{p2} & \cdots & t_{pp} \end{pmatrix}$$

by

$$(3.3) \quad \mathbf{B} = \mathbf{T}\mathbf{T}'$$

and find that

$$(3.4) \quad \begin{aligned} (1) \quad & \frac{t_{11}^2}{\sigma_1^2} \text{ is a } \chi^2 \text{ with } n \text{ d.f.} \\ (2) \quad & \frac{t_{22}^2}{\sigma_2^2} \text{ is a } \chi^2 \text{ with } n-1 \text{ d.f., } (i=3, \dots, p) \\ (3) \quad & \frac{t_{ii}^2}{\sigma^2} \text{ is a } \chi^2 \text{ with } n-(i-1) \text{ d.f.} \\ (4) \quad & t_{21} \text{ is } N(0, \sigma_2) \\ (5) \quad & t_{ij} (i > j) \text{ are } N(0, \sigma), \quad i, j=3, \dots, p. \end{aligned}$$

All these are independently distributed.

χ_H^2 of section (2) can now be written as

$$(3.5) \quad \begin{aligned} \chi_H^2 &= \text{tr } \mathbf{B} - \lambda_1^2 - \lambda_2^2 \\ &= \text{tr } \mathbf{T}\mathbf{T}' - t_{11}^2 - (t_{21}^2 + t_{22}^2) \\ &= \sum_{i=3}^p \sum_{j=1}^i t_{ij}^2. \end{aligned}$$

In the case of a single nonisotropic principal component Kshirsagar [11] proved by a geometrical argument that the direction factor is obtained by selecting only those t 's from the sum (3.5) which have the second subscript unity. It can, therefore, be easily conjectured that in the present case the directions factor for the two hypothetical principal components will be obtained by selecting those t 's from the sum (3.5) which have the second subscript (1) one and (2) two. Thus

$$(3.6) \quad \begin{aligned} \chi_1^2 &= t_{31}^2 + \cdots + t_{p1}^2 \\ \chi_2^2 &= t_{32}^2 + \cdots + t_{p2}^2 \end{aligned}$$

will be the two direction factors while

$$(3.7) \quad \chi_3^2 = t_{21}^2$$

will correspond to the angle between the two components. (This is explained later.) From (3.4) we see that

$$\frac{\chi_1^2}{\sigma^2} \text{ is a } \chi^2 \text{ with } p-2 \text{ d.f.}$$

$$\frac{\chi_2^2}{\sigma^2} \text{ is a } \chi^2 \text{ with } p-2 \text{ d.f.}$$

and $\frac{\chi_3^2}{\sigma^2}$ is a χ^2 with 1 d.f.

These tests give direction aspect of the goodness of $l_{(1)}^*$ and l_2^* respectively.

In the next section we express these χ^2 's in terms of known quantities and in section (5) we shall parallel Kshirsagar's [11] arguments to give an alternative derivation of these direction tests.

4. An alternative geometrical derivation

We have already seen that $l_i\mathbf{x}$ ($i=1, \dots, p$) are all normally independently distributed. In the case of one hypothetical principal component $l_1\mathbf{x}$ Kshirsagar [11] considered the sample projection of $l_i\mathbf{x}$ ($i=2, \dots, p$) on $l_1\mathbf{x}$ and constructed the direction test. The sample projection is equivalent to the sample regression coefficient.

In the present case of two hypothetical components, we consider the partial regression coefficients of $l_i\mathbf{x}$ ($i=3, \dots, p$) on $l_2\mathbf{x}$ when $l_1\mathbf{x}$ is fixed. This is as good as considering the sample projection of $l_i\mathbf{x}$ on $l_2\mathbf{x}$ in a space orthogonal to $l_1\mathbf{x}$.

A little calculation shows that the partial regression coefficient under consideration is

$$(4.1) \quad \frac{l_i A l_2 - \rho \lambda_2 l_i A l_1 / \lambda_1}{\lambda_2^2 (1 - \rho^2)}$$

where

$$\rho = \frac{l_1 A l_2}{\sqrt{(l_1 A l_1)(l_2 A l_2)}}$$

is the sample correlation coefficient between $l_1\mathbf{x}$ and $l_2\mathbf{x}$. As $l_i\mathbf{x}$ are all independently distributed, the above regression coefficient are all also independently normally distributed and consequently

$$(4.2) \quad \sum_{i=3}^p \left\{ \frac{l_i A l_2 - \rho \frac{\lambda_2 l_i A l_1}{\lambda_1}}{\lambda_2 (1 - \rho^2)^{1/2}} \right\}^2$$

is distributed as $\chi^2 \sigma^2$ with $p-2$ d.f. Since we consider projections on $l_2 x$, the above statistic gives weight to the direction of the hypothetical function $l_2 x$ and consequently can be taken as the direction factor. We now show that this is nothing but χ_2^2 of section (3). From (3.3) and (2.10)

$$(4.3) \quad T T' = L A L'$$

as each is equal to the matrix B . Equating elements on both sides we have

$$(4.4) \quad t_{11}^2 = l_1 A l_1 = \lambda_1^2$$

$$(4.5) \quad t_{1i} t_{i1} = l_i A l_1 \quad (i=2, \dots, p)$$

$$(4.6) \quad t_{21}^2 + t_{22}^2 = l_2 A l_2 = \lambda_2^2$$

$$(4.7) \quad t_{2i} t_{i2} + t_{22} t_{i2} = l_i A l_2 \quad (i=3, \dots, p).$$

From these it can be easily seen that

$$(4.8) \quad t_{11}^2 = \lambda_1^2$$

$$(4.9) \quad t_{22}^2 = \lambda_2^2 - \frac{(l_1 A l_2)^2}{\lambda_1^2} = \lambda_2^2 (1 - \rho^2)$$

and

$$(4.10) \quad t_{i2} = \frac{l_i A l_2 - \rho \frac{\lambda_2}{\lambda_1} l_i A l_1}{\lambda_2 \sqrt{(1 - \rho^2)}}.$$

Hence

$$(4.11) \quad \sum_{i=3}^p t_{i2}^2 = \sum_{i=3}^p \frac{\left(l_i A l_2 - \rho \frac{\lambda_2}{\lambda_1} l_i A l_1 \right)^2}{\lambda_2^2 (1 - \rho^2)}$$

which is the same expression as (4.2) and is the direction factor χ_2^2 of section (3). For practical applications, however, the above χ_2^2 can also be put in a more convenient form by expanding the square in (4.11) and using the orthogonality of L , viz., $\sum_{i=3}^p l_i l_i' = I - l_1 l_1' - l_2 l_2'$. After a little

simplification we obtain

$$(4.12) \quad \chi_2^2 = \frac{l_2 A^2 l_2 + \rho^2 \frac{\lambda_2^2}{\lambda_1^2} l_1 A^2 l_1 - 2\rho \frac{\lambda_2}{\lambda_1} l_2 A^2 l_1}{\lambda_2^2(1-\rho^2)} - \lambda_2^2(1-\rho^2).$$

The expression of χ_1^2 and its geometrical derivation is almost the same as Kshirsagar's expression except for the minor change that χ_1^2 is now not $t_{21}^2 + \dots + t_{p1}^2$ but $t_{31}^2 + \dots + t_{p1}^2$ as it is necessary to remove t_{21} in the present case as we are dealing with two hypothetical principal components l_1x and l_2x . In fact

$$t_{21} = \frac{l_1 A l_2}{t_{11}} = \rho \frac{\lambda_2}{\lambda_1}$$

represents the regression coefficient of l_2x on l_1x , i.e., t_{21} corresponds to the sample projection of l_2x on l_1x . $\frac{t_{21}^2}{\sigma_2^2} = \chi_3^2$ is a χ^2 with 1 d.f. and will test the orthogonality of l_1 and l_2 . However, both l_1 and l_2 have been assigned to us in the hypothesis as orthogonal and consequently this is of little interest for testing the hypothesis under consideration.

Thus in the present case

$$(4.13) \quad \begin{aligned} \chi_1^2 &= \text{Kshirsagar's expression of } \chi_2^2 \text{ in the} \\ &\quad \text{case of one component} - t_{21}^2 \\ &= \frac{l_1 A^2 l_1}{\lambda_1^2} - \lambda_1^2 - \rho^2 \frac{\lambda_2^2}{\lambda_1^2}. \end{aligned}$$

If σ^2 is assumed to be known, we can use the above two χ^2 tests for our hypothesis about the directions of the two assigned functions l_1x and l_2x . However, if it is unknown, we note from (3.5) that $\chi_H^2 = \sum_{i=3}^p \sum_{j=1}^i t_{ij}^2$ is $\chi^2 \sigma^2$ with $n(p-2)$ d.f. and χ_1^2 , χ_2^2 and χ_3^2 are parts of it, consequently $\chi_H^2 - \chi_1^2 - \chi_2^2 - \chi_3^2 = \text{tr}A - \lambda_1^2 - \lambda_2^2 - \lambda_1^2 - \lambda_2^2$ is independently distributed of χ_1^2 , χ_2^2 and χ_3^2 as $\chi^2 \sigma^2$ with d.f. = $n(p-2) - (p-2) - (p-2) = (n-2)(p-2)$. This can be used to obtain an independent estimate of σ^2 and hence using this estimate we may employ F -tests instead of two χ^2 tests based on χ_1^2 and χ_2^2 .

5. Generalization to more than two assigned principal components

The generalization of the above test procedure to the case of $k (< p)$ hypothetical principal components $l_i x$ ($i=1, \dots, k$), $l_i l_j = \delta_{ij}$ ($i, j=1, \dots, k$); δ_{ij} is the Kronecker delta, is straightforward. As before, we can obtain $(p-k)$ mutually orthogonal vectors l_j ($j=k+1, \dots, p$) such that they

are also orthogonal to the assigned vectors l_i ($i=1, \dots, k$). These vectors will now constitute the orthogonal matrix L of section (2). As before by transferring from $B=LAL'$ to TT' where T is lower triangular, we can show that t_{ii}^2 ($i=k+1, \dots, p$) are $\chi^2\sigma^2$ variables with $n-(i-1)$ d.f. and t_{ij} ($i>j$) are normal variables. The direction statistics for the k assigned function are therefore provided by

$$\begin{aligned}
 \chi_1^2 &= t_{k+1, 1}^2 + \dots + t_{p, 1}^2 \\
 \chi_2^2 &= t_{k+1, 2}^2 + \dots + t_{p, 2}^2 \\
 &\dots \dots \dots \dots \dots \\
 &\dots \dots \dots \dots \dots
 \end{aligned}
 \tag{5.1}$$

The d.f. in each case are obviously $p-k$. If σ^2 is not known, it can be estimated as before by

$$\text{tr}A - \lambda_1^2 - \lambda_2^2 - \dots - \lambda_k^2 - \chi_1^2 - \dots - \chi_k^2$$

based on $(n-k)(p-k)$ d.f. λ_i^2 represents the sample sum of squares for $l_i x$, viz., $l_i A l_i$. It is theoretically possible to express the above χ^2 's in terms of A and the given l_i 's only. But the resulting expression will be complicated. A geometrical deviation of these χ^2 's can also be given by sample projections of $l_j x$ ($j=k+1, \dots, p$) on $l_i x$ ($i=1, \dots, k$) when the remaining $l_r x$ ($r \neq i=1, \dots, k$) are fixed. But it is not necessary to spell out this as it is implicit in the Bartlett decomposition TT' of the Wishart matrix B .

6. Numerical illustration

To illustrate the use of the test outlined in section 4, we apply it to a random sample of size $n=50$ from a multivariate normal distribution (using Wold's [17] random normal deviates) of four variables x_1, x_2, x_3, x_4 of zero means and variance-covariance matrix

$$\Sigma = (\sigma_1^2 - \sigma^2) l_1 l_1' + (\sigma_2^2 - \sigma^2) l_2 l_2' + \sigma^2 I$$

where $\sigma_1^2 > \sigma_2^2 > \sigma^2$. σ^2 is taken to be unity. l_1 and l_2 were taken proportional to

$$m_1 = (1, -2, 3, 1) \quad \text{and} \quad m_2 = (2, 5, 1, 5)$$

respectively. The matrix A of sums of squares and products of the sample values was found to be

$$\begin{pmatrix} 62.9852 & 23.5025 & 3.2115 & .8449 \\ 23.5025 & 84.9415 & -22.4047 & -.8951 \\ 3.2115 & -22.4047 & 42.9952 & 4.8939 \\ .8449 & -.8951 & 4.8939 & 45.9578 \end{pmatrix}.$$

The latent roots of $\frac{A}{n}$, the estimate of Σ are

$$\theta'_1=2.0492, \theta'_2=1.1118, \theta'_3=.9172, \theta'_4=.8068.$$

The assumption that Σ has only two latent roots >1 and all others are equal to unity can be tested by using Bartlett's Statistic [3] (see also Lawley [13])

$$\left\{ (n-2) - \frac{1}{6} \left(2p-3 - \frac{2}{p-1} \right) - \frac{4}{p-1} \right\} \left\{ -\log_e \theta'_3 \theta'_4 + \theta'_3 + \theta'_4 - (p-2) \right\}.$$

The values of this statistic in this example comes out to be 0.8367. Comparing this with 5% value of a χ^2 with $\frac{1}{2}(p-2)(p-1)=6$ d.f. we find that it is not significant.

We shall now test the hypothesis that the second nonisotropic principal component U_2x is proportional to m'_2x where $m_2=(2, 5, 1, 5)$. The over all criterion value is

$$\begin{aligned} \chi^2 &= \text{tr } A - \lambda_1^2 - \lambda_2^2 \\ &= 100.5647 \end{aligned}$$

for $n(p-2)=100$ d.f. and is not significant. Its direction components are given by

$$\begin{aligned} \chi_1^2 &= \frac{U_1 A^2 U_1}{\lambda_1^2} - \lambda_1^2 - \frac{(U_2 A U_1)^2}{\lambda_1^2} = 1.4265 \\ \chi_2^2 &= \left\{ \frac{U_3 A U_2 - \rho \frac{\lambda_2}{\lambda_1} U_3 A U_1}{\lambda_2 \sqrt{1-\rho^2}} \right\}^2 + \left\{ \frac{U_4 A U_2 - \rho \frac{\lambda_2}{\lambda_1} U_4 A U_1}{\lambda_2 \sqrt{1-\rho^2}} \right\}^2 = 0.28098 \end{aligned}$$

for $(p-2)=2$ d.f. each and both are not significant.

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