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Abstract

The analysis of the covariance structure is a key topic in many fields of Statistics. Due to the complicated structure of the exact distributions of the test statistics involved, the required tests are often not performed or rather are performed using approximations for the distributions of the test statistics which, in most cases, are unable to guarantee the necessary accuracy of the results. These problems become even more evident and serious when one intends to perform tests of elaborate structures. In this work we intend to give an overview of the latest results on this topic and in particular we aim to clarify and illustrate the two following points: i) how it is possible to create a procedure to test elaborate block-structures in covariance matrices by splitting the null hypothesis into a set of conditionally independent hypotheses; ii) how does the proposed procedure make it easy the development of very precise near-exact approximations which allow the easy implementation and execution of the different tests. Several examples of elaborate structures are presented. The numerical studies carried out illustrate the quality of the near-exact approximations developed.

Keywords: hypotheses testing; Generalized Near-Integer Gamma distributions; likelihood ratio tests; mixtures; near-exact distributions.

1. Introduction

In different statistical techniques it is very important, from a modeling point of view, to consider specific and elaborate structures for the covariance matrices. Some examples are: i) the sphericity covariance structure for the error structure in linear models, ii) the block-matrix sphericity structure in multivariate regression, iii) the block-circular covariance structure in Hierarchical Models (Liang et al., 2014), iv) the equicorrelation covariance structure to model corneal curvature maps (Viana, 1995), and v) different covariance structures that may be represented by Kronecker products (Roy & Khattree, 2005; Srivastava et al., 2008; Kim & Hero, 2001; Naik & Rao, 2001). However due to the complicated expressions of the exact distribution of the likelihood ratio test (LRT) statistics involved, the tests of these elaborate structures are often not performed or performed using approximations for the distribution of the LRT statistics which are unable to guarantee the required accuracy of the results, mainly for small samples and/or large number of variables. This can lead to erroneous conclusions. For the simpler cases there are several known techniques to approximate the distribution of the LRT statistics; the most well known are the Chi-squared (Wilks, 1938) and Box type (Box, 1949) approximations, which are very simple to use but do not perform well specially when small samples and/or large number of variables are considered. To overcome this problem it is possible to use a recent and innovative technique, which enables the development of accurate approximations. These are the so-called near-exact approximations (Coelho, 2004). These approximations may be used to test elaborate structures on covariance matrices and/or conditions on the mean vectors. In recent literature it is possible to verify that these near-exact approximations exhibit a very good performance even in extreme cases such as when very small samples and/or large number of real or complex random variables are considered.

2. How to handle tests on elaborate structures

The main question is: Is it possible to test, with precision and at one time, elaborate structures on covariance matrices and/or conditions on mean vectors? The answer is clearly yes! In Coelho & Marques (2009), in Section 3.3, the authors illustrated how one could proceed in the following two tests: i) the multi-sample block-matrix sphericity test, and ii) the multi-sample block-scalar sphericity test, but we will try to go a bit further. Suppose we have a p-variate Normal population, $N_p(\underline{\mu}, \Sigma)$, and that we want to test if the covariance matrix has a block-diagonal structure with $\Sigma = \mathrm{diag}(\Sigma_{11}, \ldots, \Sigma_{kk}, \ldots, \Sigma_{mm})$ which is the well known test of independence of groups of variables. But, what if we also want to test if the matrices Σ_{ii} have a circular structure (Marques & Coelho, 2013; Olkin & Press, 1969)? Still, what if we want to test if in q populations all the covariance matrices have this kind of structure and if the q mean vectors are all equal? One can go a little bit further, what if one wants to test the existence of different structures on some or on all of the block diagonal covariance matrices Σ_{ii}, such as the circular and/or equivariance and equicorrelation structures! To address these elaborated structures and to test them, the key idea is to decompose, in an adequate manner, the null hypothesis of the overall test. More precisely, suppose we want to test an elaborate structure for the covariance matrix, and that it is possible to decompose the corresponding null hypothesis into a sequence of m partial null hypotheses in the following way $H_0 \equiv H_{0m|1,\ldots,m-1} \circ \ldots \circ H_{02|1} \circ H_{01}$ (see Coelho & Marques (2009) for the notation). Given the above decomposition, the LRT statistic of the overall test may be given by $\Lambda = \Lambda_{m|1,\ldots,m-1} \times \ldots \times \Lambda_{2|1} \times \Lambda_1$, where $\Lambda_{i|1,\ldots,i-1}$ is the LRT statistic to test $H_{0i|1,\ldots,i-1}$ $(i = 1, \ldots, m)$; note that for $i = 1$ we have the LRT statistic associated with the first test in the sequence which is simply represented by Λ_1. If it is possible to ensure the independence of the LRT statistics under H_0 we may obtain both the expression of the h-th moment of the overall LRT statistic and the characteristic function (CF) of its logarithm from the expressions of the moments of LRT statistics for the sub-hypotheses. More precisely we have $E[\Lambda^h] = \prod_{i=1}^m E[(\Lambda_{i|1,\ldots,i-1})^h]$ and, for $W = -\log \Lambda$, the CF of W given by

$$\Phi_W(t) = E[\mathrm{e}^{\mathrm{i}tW}] = E[\Lambda^{-\mathrm{i}t}] = \prod_{i=1}^m E[(\Lambda_{i|1,\ldots,i-1})^{-\mathrm{i}t}] = \prod_{i=1}^m E[\mathrm{e}^{\mathrm{i}tW_{i|1,\ldots,i-1}}] = \prod_{i=1}^m \Phi_{W_{i|1,\ldots,i-1}}(t)$$

where $\Phi_{W_{i|1,\ldots,i-1}}(t)$ is the CF of $W_{i|1,\ldots,i-1} = -\log \Lambda_{i|1,\ldots,i-1}$ $(i = 1, \ldots, m)$. This is the starting factorization on which the development of the near-exact approximations for the LRT statistic of the overall test is based. In what follows we will use an example to show how it is possible to implement the above procedure.

As suggested in Kim & Hero (2001) there are applications on which it is important to be able to test if in a covariance matrix we have different patterns. For example, Kim & Hero (2001) considered the following diagonal structures: $\mathrm{diag}(\Sigma_A, \Sigma_B)$, with (i) $R_A > 0, R_B > 0$, (ii) $R_A > 0, R_B = \sigma^2\mathbf{I}$, or (iii) $R_A > 0, R_B = \mathbf{I}$ in a target detection problem. We may consider even more complex cases. For example, given a sample of size N from a $p-$variate normal population, $N_p(\underline{\mu}\,, \Sigma)$, we may be interested in testing if the covariance matrix has the following structure

$$H_0 :\ \Sigma = \begin{bmatrix} \Sigma_{11} & 0 & 0 \\ 0 & \sigma^2\mathbf{I}_{p_2} & 0 \\ 0 & 0 & \Sigma_{\mathrm{C}} \end{bmatrix}$$

where $\Sigma_{11} > 0$ has no special structure, $\sigma^2\mathbf{I}_{p_2}$ has a spherical structure (Marques & Coelho, 2008) and Σ_{C} has a circular structure (Marques & Coelho, 2013; Olkin & Press, 1969), and where the matrices Σ_{11}, $\mathbf{I}_{p_2}$ and Σ_{C} are of order p_i $(i = 1, 2, 3)$ respectively, with $p = p_1 + p_2 + p_3$. Using the general procedure described in Section 2.1 we may decompose H_0 as $H_0 \equiv H_{03|1} \circ H_{02|1} \circ H_{01}$, where

$$H_{01} \;:\; \Sigma_{ij} = 0 \;\text{ for }\; i \neq j \quad (i,j = 1,\dots,3)\,, \tag{1}$$

is the null hypothesis to test the independence of the three groups of random variables,

$$H_{02|1} \;:\; \Sigma_{22} = \sigma^2 \mathbf{I}_{p_2} \quad (\text{assuming that } H_{01} \text{ is true }) \tag{2}$$

is the null hypothesis to test the sphericity of the second group of variables, and finally

$$H_{03|1} \;:\; \Sigma_{33} = \Sigma_{\mathrm{C}} \quad (\text{assuming that } H_{01} \text{ is true }) \tag{3}$$

is the null hypothesis to test the circularity of the covariance matrix for the third group with p_3 variables. Note that in this case there is indeed no specific requirement concerning the order to test $H_{02|1}$ and $H_{03|1}$. Following, again, the results in Section 2.1, the LRT is given by the product of the LRT statistics used to test H_{01}, $H_{02|1}$ and $H_{03|1}$ respectively in (1), (2) and (3) and ahead denoted by Λ_1, $\Lambda_{2|1}$ and $\Lambda_{3|1}$ (for the expressions of these LRT statistics please see Anderson (2003), Coelho (2004), Marques & Coelho (2008), Marques & Coelho (2013) and Olkin & Press (1969)). Thus, the LRT statistic is given by

$$\Lambda = \Lambda_1\Lambda_{2|1}\Lambda_{3|1} = \underbrace{\frac{|A|}{\prod_{i=1}^{3} A_{ii}}}_{\Lambda_1}\;\underbrace{\frac{|A_{22}|}{\left(\frac{1}{p_2}tr(A_{22})\right)^{p_2}}}_{\Lambda_{2|1}}\;\underbrace{2^{2(p_3-m-1)}\frac{|V|}{\prod_{j=1}^{p_3} v_j}}_{\Lambda_{3|1}} \tag{4}$$

where A is the maximum likelihood estimator of Σ, A_{ii} $(i = 1,2,3)$ is the i-th diagonal block, of order p_i, of A and $m = \left\lfloor \frac{p_3}{2} \right\rfloor$. The expressions of V and v_j are given in (32), (33) and (34) in Marques and Coelho (2013). The independence of the LRT statistics under H_0 allows the obtainment of the expression of the h-th moment of Λ through the product of the expressions h-th moment of the LRT statistics Λ_1, $\Lambda_{2|1}$, $\Lambda_{3|1}$ in (4) (for the expression of h-th moment of these LRT statistics please see Anderson (2003), Coelho (2004), Marques & Coelho (2008), Marques & Coelho (2013) and Olkin & Press (1969)), thus

$$\begin{aligned} E[\Lambda^h] &= E\left[\Lambda_1^h\right] E\left[\Lambda_{2|1}^h\right] E\left[\Lambda_{3|1}^h\right] \\ &= \underbrace{\prod_{k=1}^{2}\prod_{j=1}^{p_k} \frac{\Gamma\left(\frac{n+1-j}{2}\right)\Gamma\left(\frac{n+1-q_k-j}{2}+h\right)}{\Gamma\left(\frac{n+1-q_k-j}{2}\right)\Gamma\left(\frac{n+1-j}{2}+h\right)}}_{E\left[\Lambda_1^h\right]} \times \underbrace{\prod_{j=2}^{p_2} \frac{\Gamma\left(\frac{n}{2}+\frac{j-1}{p_2}\right)}{\Gamma\left(\frac{n}{2}+\frac{j-1}{p_2}+h\right)} \frac{\Gamma\left(\frac{n+1-j}{2}+h\right)}{\Gamma\left(\frac{n+1-j}{2}\right)}}_{E\left[\Lambda_{2|1}^h\right]} \\ &\quad \times \underbrace{\frac{\Gamma\left(\frac{n}{2}\right)^m \Gamma\left(\frac{n+1}{2}\right)^{p_3-m-1}}{\prod_{j=1}^{p_3-1}\Gamma\left(\frac{n-j}{2}\right)} \frac{\prod_{j=1}^{p_3-1}\Gamma\left(\frac{n-j}{2}-\mathrm{i}t\right)}{\Gamma\left(\frac{n}{2}-\mathrm{i}t\right)^m \Gamma\left(\frac{n+1}{2}-\mathrm{i}t\right)^{p_3-m-1}}}_{E\left[\Lambda_{3|1}^h\right]}\,, \end{aligned} \tag{5}$$

where $q_1 = p_2 + p_3$, $q_2 = p_3$ and $m = \left\lfloor \frac{p_3}{2} \right\rfloor$. Although this expression may be simplified, this simplification does not bring any advantage for our purposes, as we will see in the next sections.

3. Near-exact approximations and numerical studies

Using the example considered in the previous section, we will now explain how it is possible to develop precise near-exact distributions for the LRT statistic in (4). Based on the expression of the

h-th moment of Λ in (5) it is possible to obtain the CF of $W = -\log\Lambda$ which will be given by the product of the CFs of $W_1 = -\log\Lambda_1$, $W_{2|1} = -\log\Lambda_{2|1}$ and $W_{3|1} = -\log\Lambda_{3|1}$, that is

$$\Phi_W(t) = E[\Lambda^{-\mathrm{i}t}] = E[\Lambda_1^{-\mathrm{i}t}]E[\Lambda_{2|1}^{-\mathrm{i}t}]E[\Lambda_{3|1}^{-\mathrm{i}t}] = \Phi_{W_1}(t)\Phi_{W_{2|1}}(t)\Phi_{W_{3|1}}(t)\,.$$

Furthermore, considering as a starting point the factorizations of the CFs of W_1, $W_{2|1}$ and $W_{3|1}$ in Marques et al. (2011), Marques & Coelho (2008) and Marques & Coelho (2013) we may rewrite the CF of W as

$$\begin{aligned}
\Phi_W(t) \;=\; & \underbrace{\prod_{j=2}^{p}\left(\frac{n+1-j}{2}\right)^{r_{1j}}\left(\frac{n+1-j}{2}-\mathrm{i}t\right)^{-r_{1j}}}_{\Phi_{W_{1,a}}(t)} \times \underbrace{\left(\frac{\Gamma\left(\frac{n}{2}\right)\Gamma\left(\frac{n-1}{2}-\mathrm{i}t\right)}{\Gamma\left(\frac{n}{2}-\mathrm{i}t\right)\Gamma\left(\frac{n-1}{2}\right)}\right)^{k^\star}}_{\Phi_{W_{1,b}}(t)} \\
& \times \underbrace{\prod_{j=2}^{p_2}\left(\frac{n+1-j}{2}\right)^{r_{2j}}\left(\frac{n+1-j}{2}-\mathrm{i}t\right)^{-r_{2j}}}_{\Phi_{W_{21,a}}(t)} \times \underbrace{\prod_{j=2}^{p_2}\frac{\Gamma\left(\frac{n}{2}+\frac{j-1}{p_2}\right)\Gamma\left(\frac{n+1-j}{2}+\left\lfloor\frac{j-1}{p_2}+\frac{j-1}{2}\right\rfloor-\mathrm{i}t\right)}{\Gamma\left(\frac{n}{2}+\frac{j-1}{p_2}-\mathrm{i}t\right)\Gamma\left(\frac{n+1-j}{2}+\left\lfloor\frac{j-1}{p_2}+\frac{j-1}{2}\right\rfloor\right)}}_{\Phi_{W_{21,b}}(t)} \\
& \times \underbrace{\prod_{j=2}^{p_3}\left(\frac{n+1-j}{2}\right)^{r_{3j}}\left(\frac{n+1-j}{2}-\mathrm{i}t\right)^{-r_{3j}}}_{\Phi_{W_{31,a}}(t)} \times \underbrace{\left(\frac{\Gamma\left(\frac{n}{2}\right)\Gamma\left(\frac{n-1}{2}-\mathrm{i}t\right)}{\Gamma\left(\frac{n}{2}-\mathrm{i}t\right)\Gamma\left(\frac{n-1}{2}\right)}\right)^{(p_3-1)\bmod 2}}_{\Phi_{W_{31,b}}(t)}
\end{aligned}$$

where

$$\Phi_{W_1}(t) = \Phi_{W_{1,a}}(t)\times\Phi_{W_{1,b}}(t)\ ,\ \ \Phi_{W_{2|1}}(t) = \Phi_{W_{21,a}}(t)\times\Phi_{W_{21,b}}(t)\ \text{ and }\ \Phi_{W_{3|1}}(t) = \Phi_{W_{31,a}}(t)\times\Phi_{W_{31,b}}(t)$$

and where r_{1j} $(j = 2,\ldots,p)$ is given in expression (A.2) of Marques et al. (2011), r_{2j} $(j = 2,\ldots,p_2)$ is equal to $s_{j,p}$ in expression (14) of Marques & Coelho (2008), r_{3j} $(j = 2,\ldots,p_3)$ is given, for odd p_3 in expression (7) and for even p_3 in expression (11), in Marques & Coelho (2013), and $k^\star = \left\lfloor\frac{\ell}{2}\right\rfloor$ with ℓ denoting the number of groups with an odd number of variates. Clearly, now it is possible to rewrite the CF of W in the following form

$$\Phi_W(t) = \underbrace{\prod_{j=2}^{p}\left(\frac{n+1-j}{2}\right)^{r_j^\star}\left(\frac{n+1-j}{2}-\mathrm{i}t\right)^{-r_j^\star}}_{\Phi_{W_1}(t)} \times \underbrace{\Phi_{W_{1,b}}(t)\Phi_{W_{21,b}}(t)\Phi_{W_{31,b}}(t)}_{\Phi_{W_2}(t)} \tag{6}$$

with $r_j^\star = r_{1j} + r_{2j} + r_{3j}$ $(j = 2,\ldots,p)$; we consider $r_{2j} = 0$ for $j > p_2$ and $r_{3j} = 0$ for $j > p_3$. In (6), Φ_{W_1} is the CF of a Generalized Integer Gamma (GIG) distribution Coelho (1998), and Φ_{W_2} is the CF of the sum of independent Logbeta distributions. Based on this representation of Φ_W it is possible to obtain near-exact distributions for W and for Λ, by approximating the CF of W_2 in (6) by an asymptotic approximating CF which will be denoted by $\Phi^\star_{W_2}$. As a result we obtain the following near-exact CF

$$\Phi_{NE}(t) = \Phi_{W_1}(t)\times\Phi_{W_2^\star}(t)\,. \tag{7}$$

In (7) $\Phi_{W_2^\star}$ is the CF of a finite mixture of Gamma distributions

$$\Phi_{W_2^\star}(t) = \sum_{j=0}^{m^\star}\pi_j(\lambda)^{r+j}(\lambda-\mathrm{i}t)^{-(r+j)}\,, \tag{8}$$

all with the same rate parameter λ and with shape parameters $r+i$, $i = 0,\ldots,m^\star$, where $m^\star$ is the number of exact moments matched and r is given in (10) ahead. The parameter λ is equal to the rate parameter of a mixture of two Gamma distributions which matches the first four moments of the exact distribution of W_2, being thus determined, together with r_1, r_2 and p, as solution of

$$\frac{\partial^h}{\partial t^h}\,\Phi_{W_2}(t)\bigg|_{t=0} = \frac{\partial^h}{\partial t^h}\,\left\{p(\lambda)^{r_1}(\lambda-\mathrm{i}t)^{-r_1}+(1-p)(\lambda)^{r_2}(\lambda-\mathrm{i}t)^{-r_2}\right\}\bigg|_{t=0}, h=1,\ldots,4 \qquad (9)$$

and the shape parameter r is equal to the sum of the second parameter of all the Logbeta distributions in Φ_{W_2}, and is given by

$$r=\frac{k^\star+(p_3-1)\bmod 2}{2}+\left\{\sum_{j=2}^{p_2}\frac{j-1}{p_2}+\frac{j-1}{2}-\left\lfloor\frac{j-1}{p_2}+\frac{j-1}{2}\right\rfloor\right\} \qquad (10)$$

the weights, π_j, in the mixture, are obtained as a solution of the system

$$\frac{\partial^h}{\partial t^h}\,\Phi_{W_2}(t)\bigg|_{t=0} = \frac{\partial^h}{\partial t^h}\,\Phi^\star_{W_2}(t)\bigg|_{t=0}, h=1,\ldots,m^\star \text{ with } \pi_{m^\star}=1-\sum_{j=0}^{m^\star-1}\pi_j\,. \qquad (11)$$

ensuring this way that the first $m^\star$ moments of $W_2^\star$ are equal to the first corresponding $m^\star$ exact moments.This approach is based on the results of Tricomi & Erdélyi(1951) for the ratio of to Gamma functions which can be use to show that a single Logbeta distribution may be well approximated by a mixture of Gamma distributions, and which have been applied we considerable success (Marques & Coelho(2008), Marques & Coelho(2013) and Marques et al.(2011)). Given the above construction we obtain the following representation for the near-exact CF in (7)

$$\begin{aligned}\Phi_{NE}(t) &= \Phi_{W_1}(t)\times\Phi^\star_{W_2}(t)=\prod_{j=2}^{p}\left(\frac{n+1-j}{2}\right)^{r_j^\star}\left(\frac{n+1-j}{2}-\mathrm{i}t\right)^{-r_j^\star}\sum_{j=0}^{m^\star}\pi_j(\lambda)^{r+j}(\lambda-\mathrm{i}t)^{-(r+j)}\\ &= \sum_{j=0}^{m^\star}\pi_j\prod_{j=2}^{p}\left(\frac{n+1-j}{2}\right)^{r_j^\star}\left(\frac{n+1-j}{2}-\mathrm{i}t\right)^{-r_j^\star}(\lambda)^{r+j}(\lambda-\mathrm{i}t)^{-(r+j)} \qquad (12)\end{aligned}$$

This is the CF of: i) a mixture of GNIG distributions if r is non-integer, ii) a mixture of GIG distributions if r is integer. The corresponding cumulative and density functions can be easily implemented computationally. In order to assess the precision of the approximation provided by Φ_{NE} we will use the measure

$$\Delta=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left|\frac{\Phi_W(t)-\Phi_{NE}(t)}{t}\right|\,\mathrm{d}t\,, \qquad (13)$$

which gives an upper bound on the proximity between the near-exact and the exact distribution functions being Φ_{NE} and Φ_W the corresponding CFs.
In Table 1 we may analyze the values of Δ for different scenarios and different values of $m^\star$. This table brings out the extremely low values of the measure which confirm the high quality of the near-exact approximations. Also it is possible to observe the good asymptotic properties of these approximations for increasing values of n and p.

4. Conclusions

In this paper it is described an effective procedure to implement LRTs on elaborate covariance structures. This procedure is based on a decomposition of the overall null hypothesis into a sequence simpler hypotheses which facilitates the obtainment of the expression of the LRT statistic, the expression of its h-th moment and the expression for the CF of its logarithm. The induced

Table 1: Values of Δ for the near-exact approximations

$\{p_1, p_2, p_3\}$	p	n	$NE(m^\star = 4)$	$NE(m^\star = 8)$	$NE(m^\star = 12)$	$NE(m^\star = 16)$
$\{3, 3, 4\}$		12	9.9×10^{-12}	2.3×10^{-16}	5.5×10^{-21}	2.1×10^{-23}
		50	7.2×10^{-14}	6.4×10^{-21}	2.9×10^{-27}	7.8×10^{-32}
		100	2.6×10^{-15}	1.8×10^{-23}	1.6×10^{-30}	5.4×10^{-37}
$\{3, 3, 4\}$	10	12	9.9×10^{-12}	2.3×10^{-16}	5.5×10^{-21}	2.1×10^{-23}
$\{5, 5, 6\}$	16	18	7.7×10^{-14}	5.1×10^{-21}	9.7×10^{-26}	1.9×10^{-31}
$\{8, 7, 6\}$	21	23	5.8×10^{-16}	3.4×10^{-23}	3.6×10^{-30}	4.5×10^{-35}

factorization on the CF enables the development of near-exact distributions for the LRT statistic. These near-exact distributions are extremely precise, have good asymptotic properties and may be easily implemented.

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