Approximation and Quantiles of the Distribution of the Modified Likelihood Ratio Criteria for Covariance Matrix Hypothesis Testing and Monitoring

Mario Antonio Gneri, Emanuel Pimentel Barbosa[1] & Ariane Meneguetti

Depto Estatística, IMECC-UNICAMP, Cidade Universitária Zeferino Vaz,
Distrito de Barão Geraldo, CEP 13083-859, Campinas, SP, Brazil

Abstract

Sugiura(1969) gives an asymptotic expansion of the modified likelihood ratio criteria for testing the hypothesis that a covariance matrix is equal to a given matrix. An improvement of this expansion is presented here. Numerical comparisons via simulation with the original Sugiura's approximation to the distribution of the criteria confirm the superiority of our expansion. This enable us to use the proposed method in usual hypotheses testing and in applications where extreme tail quantiles are necessary, as for instance, for monitoring dispersion in multivariate processes quality control charts.

1 Introduction

First consider the problem of monitoring dispersion in the univariate case. Let s^2 denote the umbiased estimate of variance for a random sample of size N. If the process variance is σ_0^2 then the assumption of normality implies that $\frac{(N-1)s^2}{\sigma_0^2}$ has a chi-square distribution with $N-1$ degrees of freedom and the usual s^2 chart is obtained by pivoting on this expression.

The multivariate analogue of this chart is obtained by means of the likelihood ratio criteria for testing that a covariance matrix is equal to a given matrix. This statistic has been obtained by various approaches, see for example Anderson [1] (page 434).

If $X_1, X_2, \ldots, X_N$ is a simple random sample of a p-variate normal distribution with positive definite covariance matrix Σ, the likelihood ratio criterion for testing the equality of Σ with a simmetric positive definite matrix Σ_0 is given by

$$\lambda = (\frac{e}{N})^{\frac{Np}{2}} |S\Sigma_0^{-1}|^{\frac{N}{2}} \; exp \; tr(-\frac{1}{2}\Sigma_0^{-1}S) \qquad (1)$$

where $\bar{X} = \frac{1}{N}\sum_{j=1}^{N} X_j$ and
$S = \sum_{j=1}^{N}(X_j - \bar{X})(X_j - \bar{X})^t$.

[1]Corresponding author. E-mail adress: emanuel@ime.unicamp.br

Also may be used the modified likelihood ratio criteria λ^*, obtained by substituing in formula (1) the size N of the sample by $n = N-1$.

First the distribution of λ^* was approximated by the assymptotic null distribution of the LR criteria (the qui-square distribution with $\frac{p(p+1)}{2}$ degrees of freedom). Afterwards was introduced the Satterthwaite's correction [8] [9], that approximates the distribution of a quadratic form by a multiple of a chi-square distribution (the constant and the degrees of freedom calculated by matching the first two moments of the quadratic form and the approximating distribution). But, as espected, these methods doesn't work well especially for low values of N.

Korin [4] [5] and Sugiura [11] derived very similar asymptotic expansions for the null distribution of the test criteria λ^*. In both papers ([4] and [11]) the null distribution of $(-2)\log\lambda^*$ is expressed in the form of asymptotic series of central qui-square distributions. Sugiura's paper is more transparent than Korin's one. In particular, the algoritm of calculus of the cumulative distribution function of the criteria is explicit. As a consequence of this fact improvements of the former are easier to implement.

The expansions available work well in ordinary hypotheses testing (α risk between $0,05$ and $0,01$, say) but not necessarily for monitoring α risk in certain applications such as quality control ($\alpha = 0,0027$), where the interest is in lower values of α. In the latter case the variance of the sample quantiles uses to be greater than in the former one due to lower values of the density (Kendall and Stuart [3]). Then the improvement of an existing expansion is a natural way to look for more precision.

In this paper an improvement of Sugiura's asymptotic expansion is obtained by adding two terms to the original one. Numerical comparisons between the original Sugiuras's method and the improved one are performed. These results enable the use of the improved Sugiura's approximation in the usual hypotheses testing context and (in adition) for monitoring dispersion in multivariate processes quality control . The improved Sugiura's approximation is used here in the calculation of the upper 0,0027 quantiles of $(-2)\ log\lambda^*$ for dimension p between 2 and 4 and some small values of the sample size N.

Since for larger values of N the available methods work well, Pham-Gia and Turkkan (2009) [7] tried to obtain the exact null density function of the test criteria, but this density does not have an easy representation or a practical way of implementation. As other authors, Pham-Gia and Turkkan present, for some small values of N and p, the upper 1 and 5 percentiles but not the 0,27 one, used in quality control charts.

Other authors (Nagarsenker and Pillai [6], for instance) claim to have found the exact distribution of $(\lambda^*)^{\frac{2}{n}}$, but we see in this paper the same type of problems that in the work of Pham-Gia and Turkkan. Also they show only the upper 1 and 5 percentiles.

The organization of this paper is as follows. In Section 2 we introduce some notacion and matemathical tools (Bernoulli polynomials). In Section 3 we present Sugiura's expansion and our improvement procedure. Section 4 presents some numerical comparisons between the two methods as well as a table of quantiles. The conclussions are in Section 5. The references are imediatly after the consclusions. Section 6 (Appendix 1) contains the formulas of the constants B_j for $j = 1, 2, ..., 6$, defined in function of the Bernoulli polynomials and refered in Section 3. Section 7 contain the tables of the comparisons and the quantiles.

2 Notation and mathematical tools

The Bernoulli polynomial $B_r(h)$ of order 1 and degree r is defined by the equation (Kendall and Stuart [3]):

$$\frac{ze^{hz}}{(e^z-1)} = \sum_{j=1}^{\infty}(\frac{z^r}{r!})B_r(h). \quad (2)$$

From the above formula and after some simple algebra is possible to obtain explicit expressions of the polynomials. The Bernoulli polinomials of degrees 1 to 6 to be used in this paper are listed below:

$\mathrm{B}_1(h) = h - \frac{1}{2}$,
$\mathrm{B}_2(h) = h^2 - h + \frac{1}{6}$,
$\mathrm{B}_3(h) = h^3 - \frac{3}{2}\ h^2 + \frac{1}{2}\ h$,
$\mathrm{B}_4(h) = h_4 - 2\ h^3 + h^2 - \frac{1}{30}$,
$\mathrm{B}_5(h) = h^5 - \frac{5}{2}\ h^4 + \frac{5}{3}\ h^3 - \frac{1}{6}\ h$,
$\mathrm{B}_6(h) = h^6 - 3\ h^5 + \frac{5}{2}\ h^4 - \frac{1}{2}\ h^2 + \frac{1}{42}(3)$

The constants B_j are defined in terms of the $B_j(h), j = 1, 2, ..., r+1$ by

$$B_{r+1} = \sum_{j=1}^{p} B_{r+1}(\tfrac{1-j}{2}).$$

We give here the formulas of B_2, B_3, B_4, B_5 and B_6, which will be useful in the next section:

$$\begin{aligned}
B_2 &= \frac{p(2p^2+3p-1)}{24}, \\
B_3 &= \frac{-p(p-1)(p+1)(p+2)}{32}, \\
B_4 &= \frac{p(6p^4+15p^3-10p^2-30p+3)}{480}, \\
B_5 &= \frac{(p-1)p(p+1)(-2p^3-6p^2+3p+14)}{384}, \\
B_6 &= \frac{(p-1)p(6p^5+27p^4+6p^3-99p^2-78p-69)}{2688} + \frac{p}{42}.
\end{aligned}$$

3 Approximations to the distribution of the criteria

3.1 Sugiura's expansion

Let $X_1, X_2, \ldots, X_N$ be a simple random sample of a p-variate normal distribution with positive definite covariance matrix Σ. Consider the modified LR criterion

$$\lambda^* = (\frac{e}{n})^{\frac{np}{2}} |S\Sigma_0^{-1}|^{\frac{n}{2}}\ exp\ tr(-\frac{1}{2}\Sigma_0^{-1}S) \quad (4)$$

where $n = N-1$, $\bar{X} = \frac{1}{N}\sum_{j=1}^{N} X_j$ and $S = \sum_{j=1}^{N}(X_j - \bar{X})(X_j - \bar{X})^t$.

The modified likelihood ratio criteria for testing the null hypotheses $\Sigma = \Sigma_0$ against $\Sigma \neq \Sigma_0$ was shown to be umbiased by Sugiura and Nagao [10]. In Anderson [1] may be seen that, under the null hypotheses, the limiting distribution of $(-2)\ log\lambda^*$ is the qui-square distribution with $\frac{p(p+1)}{2}$ degrees of freedom and also that the characteristic function of $(-2)\ log\lambda^*$ is

$$C(t) = (\frac{n}{2e})^{itpn}\ \frac{\Gamma_p(\frac{n(1-2it)}{2})}{\Gamma_p(\frac{n}{2})}\ (1-2it)^{\frac{np(1-2it)}{2}} \quad (5)$$

where $\Gamma_p(t)$ is the multivariate gamma function given by

$$\Gamma_p(t) = \pi^{\frac{p(p-1)}{4}} \prod_{j=1}^{p} \Gamma \frac{(t-(j-1))}{2}. \quad (6)$$

Sugiura [11], substituing in (5) the expression of $\Gamma_p(t)$ given in (6), derived an expansion of the form:

$$P((-2)log\lambda^* \leq z) = A'_0 P(\chi^2_f \leq z) + A'_1 P(\chi^2_{f+2} \leq z) + A'_2 P(\chi^2_{f+4} \leq z + A'_3 P(\chi^2_{f+6} \leq z) + O(n^{-4}) \quad (7)$$

where $f = \frac{p(p+1)}{2}$, χ^2_g denotes the qui-square distribution with g degrees of freedom and the constants A'_j depend exclusively on p and n.

3.2 The improved expansion

Sugiura (1969) obtained an aproximation at most of the order n^{-4} of the characteristic function $C(t)$ of $(-2)\ log\lambda^*$ as a particular case of the following formula:

$$C(t) = (1-2it)^{-\frac{p(p+1)}{4}} \exp(-\sum_{r=1}^{k}(-2)^r \frac{B_{r+1}}{[r(r+1)n^r]}$$

(1-2it)$^{-r} - 1) + O(n^{-k-1})$(8)

Now, after some tedious but simple calculations, we write the exponent in formula (8) as a linear combination of $(1-2it)^{-r}$ for $r = 1, 2, ..., 5$ and $O(n^{-6})$ and obtain the following aproximation at most of the order n^{-6} of $C(t)$:

$$C(t) = (1-2it)^{-\frac{p(p+1)}{4}} \exp(A_0 + \sum_{r=1}^{5} A_j (1-2it)^{-j}) + O(n^{-6}) \quad (9)$$

where the constants A_j, for $j = 1, 2, ..., 5$ (depending on $B_1, B_2, ..., B_6$ and n) are given in Appendix 1.

After that, by inversion of the characteristic function $C(t)$, we obtain the following expansion of the distribution fuction of $(-2)log\lambda^*$:

$$P((-2)log\lambda^* \leq z) = \sum_{j=0}^{5} A_j P(\chi^2_{f+2j} \leq z) + O(n^{-6})$$

where $f = \frac{p(p+1)}{2}$ and χ^2_g denotes the qui-square distribution with g degrees of freedom.

4 Numerical results

4.1 Comparisons by simulation

We compare in this section the original method of Sugiura and the improved one. Table 1 (Appendix 2) is based on means of 10 replicates of 1.000.000 Matlab simulations of the modified likelihood ratio criteria supported on random Wishart matrices, for any combination of sample size (N) and dimension(p) (N assuming the values 3,4,5, 6, 7, 8, 9, 10,15, 20 and 30 and p being equal to $2, 3$ and 4). We remark that the numerical comparisons are restricted to the case $\alpha = 0,0027$.

If the dimension $p = 2$ an error less or equal to $0,00005$ is reached begining at $N = 8$ for the original method (if $N = 7$ the error is 0,000055) and $N = 5$ for the improved one. If $p = 3$ the respective values of N are 20 and 10. If $p = 4$ the sample sizes that attain error less or equal to $0,00005$ are $N = 30$ and $N = 15$, respectively. The picture is similar for any value of the error, with the improved method reaching the aimed precision before than the original one. In all cases the behavior becomes worse with increasing p. Then, as espected, the performance of the improved method is better than that of the original one. This conclusion enables us to use the improved method for the calculations of some quantiles of λ^*.

4.2 Upper Quantiles of λ^* for $\alpha = 0,0027$

In this section we give the 0,0027 upper quantiles of λ^* for some low values of the simple size N and dimension p betweeen 2 and 4. The calculations were made by means of an inversion process (numerical solution of the quantile equation) based on our method, except in the cases marked with an asterisk. In these particular cases the calculations were made via simulation, because when the quocient N/p is near 1 (say, $N/p \leq 1,5$) the approximation methods doesn't work very well. In the inversion process of the distribution fuction of λ^* we used the software R. For all the remaning entries of Table 2 (Appendix 2) the values were calculated by applying our proposed method.

5 Conclusions

It was very comfortable to take the paper of Sugiura [11] as a starting point, because of its simplicity and transparency. As espected, our expansion works better than the original of Sugiura, as is easyly verified looking at Table 1. We remark that the original Sugiura's expansion is an approximation at most of order n^{-4} and our method is an approximation at most of order n^{-6}. This paper was not conceived for direct applications of our expansion, but the good performance of our proposed method enabled us to construct Table 2, with the 0,0027 upper quantiles of λ^* (the limits of usual quality control charts), which is ready to be used in monitoring multivariate processes dispersion.

References

[1] Anderson, T. W.,1971. An Introduction to Multivariate Statistical Analysis, John Wiley and Sons.

[2] Ha, H.T. and Provost, S.B., H., 2007. A Viable Alternative To Resorting to Statistical Tables, *Communications in Statistics - Simulation and Computation* 36: 1135-1151.

[3] Kendall, M. and Stuart, A., 1977, The Advanced Theory of Statistics, Volume 1, p. 82-83, Fourth edition, MacMillan Publishing Co., Inc., New York.

[4] Korin, B.P., 1968. On the distribution of a statistic used for testing a covariance matrix, *Biometrika*, 55, 1, 171-178.

[5] Korin, B.P, 1967, umpublished Ph.D. Thesis.

[6] Nagarsenker, B.N. and Pillai, K.C.S., 1973. Distribution of the likelihood ratio criterion for testing an hypothesis specifying a covariance matrix, *Biometrika*, 60, 359-364.

[7] Pham-Gia, T. and Turkkan, N., 2009, Testing a covariance matrix: exact null distribution of its likelihood criterion, *Journal of Statistical Computation and Simulation*, Vol 79, No 11, 1331-1340.

[8] Satterthwaite, F.E., 1941, Synthesis of Variance, Psychometrika 66, 507-515.

[9] Satterthwaite, F.E., 1946, An Approximate Distribution of Estimates of Variance, Biometrics Bulletin 2, 110-114.

[10] Sugiura, N. and Nagao, H., 1968. Umbiasedness of some test criteria for the equality of one or two covariance matrices, *The Annals of Mathemathical Statistics*, Vol. 39, 1686-1692.

[11] Sugiura, N., 1969. Asymptotic expansions of the distributions of the likelihood ratio criteria for covariance matrix. *The Annals of Mathemathical Statistics*, Vol. 40, No 6, 2051-2063.

6 Appendix 1: The constants A_j

We give here the formulas of the constants A_j, $j = 1, 2, ..., 5$ introduced in Subsection 3.2 defined in terms os the constants B_j of Section 2. The A_j's are used in the expression of the distribution function of $(-2)log(\lambda^*)$ as a series of central qui-square distributions (formula (10)).

$$\begin{aligned}A_0 = 1 - \frac{B_2}{n} + \frac{4B_3 + 3B_2^2}{6n^2} - \frac{4B_4 + 4B_2B_3 + B_2^3}{6n^3} + \frac{288B_5 + 80B_3^2 + 240B_2B_4 + 120B_2^2B_3 + 15B_2^4}{360n^4} \\ - \frac{384B_6 + 288B_2B_5 + 160B_3B_4 + 120B_2^2B_4 + 80B_2B_3^2 + 40B_2^3B_3 + 3B_2^5}{360n^5},\end{aligned}$$

$$A_1 = \frac{B_2}{n} - \frac{B_2^2}{n^2} + \frac{4B_2B_3 + 3B_2^3}{6n^3} - \frac{4B_2B_4 + 4B_2^2B_3 + B_2^4}{6n^4} + \frac{288B_2B_5 + 240B_2^2B_4 + 80B_2B_3^2 + 120B_2^3B_3 + 15B_2^5}{360n^5},$$

$$A_2 = \frac{3B_2^2 - 4B_3}{6n^2} + \frac{4B_2B_3 - 3B_2^3}{6n^3} + \frac{-16B_3^2 + 9B_2^4}{36n^4} + \frac{16B_3B_4 - 12B_2^2B_4 + 16B_2B_3^2 - 8B_2^3B_3 - 3B_2^5}{36n^5},$$

$$A_3 = \frac{4B_4 - 4B_2B_3 + B_2^3}{6n^3} + \frac{-4B_2B_4 + 4B_2^2B_3 - B_2^4}{6n^4} + \frac{16B_3B_4 + 12B_2^2B_4 - 16B_2B_3^2 - 8B_2^3B_3 + 3B_2^5}{36n^5},$$

$$A_4 = \frac{-288B_5 + 80B_3^2 + 240B_2B_4 - 120B_2^2B_3 + 15B_2^4}{360n^4} + \frac{288B_2B_5 - 240B_2^2B_4 - 80B_2B_3^2 + 120B_2^3B_3 - 15B_2^5}{360n^5},$$

$$A_5 = \frac{384B_6 - 288B_2B_5 - 160B_3B_4 + 120B_2^2B_4 + 80B_2B_3^2 - 40B_2^3B_3 + 3B_2^5}{360n5}.$$

7 Appendix 2: the tables

Table 1: Alpha Risk

	$p=2$		$p=3$		$p=4$	
N	Sugiura	Improved	Sugiura	Improved	Sugiura	Improved
3	0,008274	0,004884	-	-	-	-
4	0,003728	0,002973	0,025768	0,014027	-	-
5	0,003054	0,002749	0,007396	0,004420	0,054918	0,031385
6	0,002846	0,002690	0,004469	0,003184	0,014387	0,007811
7	0,002755	0,002690	0,003589	0,002811	0,007213	0,004318
8	0,002728	0,002682	0,003179	0,002782	0,005051	0,003432
9	0,002726	0,002707	0,003020	0,002759	0,004101	0,003071
10	0,002749	0,002685	0,002890	0,002723	0,003582	0,002849
15	0,002681	0,002685	0,002751	0,002687	0,002856	0,002717
20	0,002715	0,002716	0,002716	0,002712	0,002781	0,002703
30	0,002702	0,002701	0,002701	0,002700	0,002693	0,002712

Table 2: Upper Quantiles ($\alpha = 0,0027$)

N	$p=2$	$p=3$	$p=4$
3	25,195874 *	-	-
4	19,525525	42,346016 *	-
5	17,701035	30,937658	61,689276 *
6	16,805205	27,229300	44,432783 *
7	16,255047	25,486631	38,677972
8	15,909704	24,365813	35,885929
9	15,642290	23,681838	34,184662
10	15,466429	23,134330	33,016720
15	14,923143	21,874310	30,271052
20	14,723554	21,336168	29,276714
30	14,522508	20,864480	28,342020