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Goodness of fit procedures for the multivariate linear model based on spherical harmonics

Pruebas de bondad de ajuste para el modelo lineal multivariado basadas en armónicas esféricas

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Abstract

The theory of the goodness of fit procedures for multivariate normality based on spherical harmonics, introduced in [6], is extended to cover the context of the multivariate linear model (MLM). The limiting distribution of the statistics considered does depend on the distribution of the covariates in the MLM, and our results provide a complete description of the manner in which the covariate distribution affects the goodness of fit statistics. We provide two methods for approximation of the limiting distributions when, as is usually the case, the covariate distribution is unknown, and evaluate their performance in simulations.
Key words and phrases: Conditional models, empirical processes, Goodness of fit testing.

Resumen

La teoría de los métodos de bondad de ajuste para la familia normal multivariada, basados en armónicas esféricas, presentada en [6], se extiende, en el presente trabajo, al contexto del modelo lineal multivariado (MLM). Nuestros resultados proporcionan una descripción completa

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de la distribución límite de los estadísticos considerados, incluyendo la manera en que la distribución de la covariable afecta dicha distribución límite. Describimos dos métodos para la obtención de cuantiles aproximados para los estadísticos considerados (cuando se desconoce la distribución de la covariable) y evaluamos el desempeño de estos métodos mediante simulaciones.
Palabras y frases clave: Modelos condicionales, procesos empíricos, pruebas de bondad de ajuste.

1 Introduction

In recent years, a number of meaningful and effective methods have been developed for testing the null hypothesis of multivariate normality. Among these, we would like to mention the statistics obtained from kernel density estimators of Bowman and Foster [3], the statistics that use the empirical characteristic function of Henze and Wagner [4] and the statistics based on spherical harmonics and radial functions studied by Manzotti and Quiroz [6]. These statistics join the classic procedures of Mardia [7] among the best tools for deciding on the question of multivariate normality.

It seems natural to try to adapt the best of the test statistics for multivariate normality to the problem of testing for the adequacy of the Multivariate Linear Model (MLM, also referred to as the General Linear Model [1]) in the context of models with covariates, by applying the tests for multivariate normality to the residuals of the fitted conditional model. In doing so, some caution must be exerted, since the covariate distribution could affect the distribution of the test statistics being used.

When assessing goodness of fit of the MLM, it is common practice to informally examine the residuals for lack of uniformity, that is often associated with lack of independence between the radial and directional components of the residuals. In this respect the statistics proposed in [6] and, in particular, their $Z^2_{2,n}$, is well suited to detect this kind of departures from multivariate normality. Thus, the main goal of the present article is to carry out the adaptation of this statistic to the context of goodness of fit for the MLM. For this purpose we will describe a generalization of Theorem 2 in [8] and provide procedures for estimation of quantiles under minimal assumptions when the covariate distribution is unknown.

In order to present the statistic that we will consider, we will first introduce some notation. Let $(X_1, Y_1), \ldots, (X_n, Y_n)$ be an i.i.d. sample from the probability law P on $I\!R^p \times I\!R^q$. The X_i's (resp. the Y_i's) are assumed to be random vectors in $I\!R^p$ (resp. $I\!R^q$). In the MLM, the conditional assumption (the null hypothesis that we want to test) is that, given X_i,

$$Y_i = B\,X_i + Z_i \tag{1}$$

where B is a $q \times p$ parameter matrix and $Z_i \in I\!R^q$ has distribution $\mathrm{N}(0, \Sigma)$, for an unknown positive definite covariance matrix Σ. Let us denote by μ the marginal distribution (on $I\!R^p$) of X_1 and by $P = P_0$ the joint distribution of the pair (X_1, Y_1) under the null distribution. Let $\mathbf{X}$ (resp. $\mathbf{Y}$) denote the X (resp. Y) sample written in matrix form: $\mathbf{X}$ is an $n \times p$ matrix in which each X_i appears as a row. Then, as is well known (see, for example, [1]), the MLE for $\theta_0 = (B, \Sigma)$, namely, $\hat{\theta} = (\hat{B}, S)$, is given by

$$\hat{B}^t = (\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Y} \text{ and } S = \frac{1}{n}\mathbf{Y}^t Q \mathbf{Y} \tag{2}$$

where $Q = I - \mathbf{X}(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t$. Denote by $P_{\hat{\theta}}$ the joint distribution of a vector (X, Y) for which X has distribution μ and the conditional distribution of Y given X is $\mathrm{N}(\hat{B}\,X, S)$. The standardized residuals are the vectors $S^{-1/2}(Y_i - \hat{B}X_i)$.

The statistic we want to consider is obtained by application, to the standardized residuals, of radial functions and spherical harmonics described next. Let $\Omega_q = \{y \in I\!R^q : \|y\| = 1\}$ be the q-dimensional unit sphere. A spherical harmonic of degree j is the restriction to Ω_q of a homogeneous polynomial $p(y)$ on $I\!R^q$, of degree j, such that $\Delta(p) \equiv 0$ on $I\!R^q$, where Δ denotes the Laplace operator $\sum_{i=1}^q \partial^2/\partial x_i^2$. In dimension 2, the spherical harmonics coincide with the trigonometric functions on the unit circle. In higher dimensions, as in dimension 2, their linear combinations are dense, with respect to the sup norm, in the space of continuous functions on Ω_q [9]. In [6] closed form formulae have been worked out for the spherical harmonics of degree up to 4, in an orthonormal basis with respect to the uniform probability measure on the unit sphere. We will denote $\mathcal{E}_j$ the set of spherical harmonics of degree j in this orthonormal basis. The number of linearly independent spherical harmonics of degree j, in dimension q, is given by $\mathrm{LI}(q, j) = \binom{q+j-1}{j} - \binom{q+j-3}{j-2}$, with $\mathrm{LI}(q, 0) = 1$ and $\mathrm{LI}(q, 1) = q$, for all q.

In what follows, x and y denote points in $I\!R^p$ and $I\!R^q$, respectively. For $y \neq 0$ in and a positive integer j, define the functions

$$r_j(y) = \|y\|^j \text{ and } u(y) = y/\|y\|. \tag{3}$$

r_1 and u give the polar coordinates of y. For n large enough (to guarantee that S is, with high probability, non singular), let us define the sample standardization transformation by

$$T_n(x,y) = S^{-1/2}(y - \hat{B}x). \tag{4}$$

It is convenient to define, as well, the asymptotic transformation

$$T_\infty(x,y) = \Sigma^{-1/2}(y - Bx). \tag{5}$$

We will apply to the sample pairs (X_i, Y_i), functions which are products of spherical harmonics and powers of the radial component: $(r_j \circ T_n)(p \circ u \circ T_n)$, where p is a harmonic spheric in $\mathcal{E}_l$, $0 \leq l \leq 2$, and r_j and u are as defined in (3). Based on power considerations, we will use, specifically, the functions

$$(r_3 \circ T_n)(p \circ u \circ T_n),\ \ r_1 \circ T_n \text{ and } r_3 \circ T_n, \tag{6}$$

where $p \in \mathcal{E}_1 \cup \mathcal{E}_2$, and these spherical harmonics are listed in the same order as in Table 1 of [6]. This gives a total of $k = \binom{q+1}{2} + q + 1$ functions. The functions just introduced will be denoted $h_{j,n}, 1 \leq j \leq k$. Under the null hypothesis, we have consistency of $\hat{\theta}$ and the functions $h_{j,n}$ converge, in $L^2(P)$, to the limiting $h_{j,\infty}$, obtained by replacing T_∞ for T_n in (6). Denote by $\underline{h}_n$ the vector of functions $(h_{1,n}, \ldots, h_{k,n})^t$ and by $\underline{h}_\infty$ the corresponding vector of the $h_{j,\infty}$. For each function $h \in L^2(P)$, let

$$Ph = \int\int h(x,y)\, dP(x,y),\ \ P_{\hat{\theta}}h = \int\int h(x,y)\, dP_{\hat{\theta}}(x,y)$$

$$P_n h = \frac{1}{n}\sum_{i \leq n} h(X_i, Y_i),\ \ \nu_n(h) = \sqrt{n}(P_n h - Ph)$$

$$\text{and } \ \hat{\nu}_n(h) = \sqrt{n}(P_n h - P_{\hat{\theta}}h). \tag{7}$$

For the vector $\underline{h}_n$ defined above, let $\hat{\nu}_n(\underline{h}_n) = (\hat{\nu}_n(h_{1,n}), \ldots, \hat{\nu}_n(h_{k,n}))$ and define, similarly, $\nu_n(\underline{h}_\infty) = (\nu_n(h_{1,\infty}), \ldots, \nu_n(h_{k,\infty}))$. The functions in $\underline{h}_\infty$ are fixed, as opposed to those in $\underline{h}_n$ that depend on the sample through the estimates $\hat{B}$ and S. Thus, the covariance matrix, under the null hypothesis, of the vector $\underline{h}_\infty$, can, in principle, be calculated in advance. Call M_0 this covariance matrix that, in our case, due to our particular choice of functions, turns out to be computable in closed form and coincides with matrix V of formula (2.18) in [6]. Then, the statistic that we will consider is the quadratic form

$$Z_n^2 = \hat{\nu}_n^t(\underline{h}_n)\, M_0^{-1}\, \hat{\nu}_n(\underline{h}_n). \tag{8}$$

In the following section we present some properties of the statistic Z_n^2, including its asymptotic distribution and, in Section 3, we discuss bootstrap procedures for getting approximate quantiles of Z_n^2.

2 Invariance and limit distribution of Z_n^2

We will now state, without proofs, some results regarding the calculation and distribution of Z_n^2. These results generalize those obtained in [6] and show how the covariate distribution affects the distribution of the statistic considered. Proofs, based mostly on methods from empirical processes (as described, for instance, in [11]), will appear elsewhere [10].

By our choice of functions, a simplification occurs in the computation of $\hat{\nu}_n(\underline{h}_n)$. When calculating $P_{\hat{\theta}} h_{j,n}$, we need to average, with respect to μ, the integral

$$\int (r_3 \circ T_n)(p \circ u \circ T_n)(x, y) \mathrm{d}N(\hat{B}x, S)(y). \tag{9}$$

Noticing that the estimators $\hat{B}$ and S appear both in the definition of T_n and in the $N(\hat{B}x, S)$ distribution, we get, through a change of variables, that the integral in (9) takes the value $\int r_3(y)p(y/\|y\|)\mathrm{d}N(0, I_q)(y)$. This last expression is straightforward to compute and not random!. Our process $\hat{\nu}_n$ can be decomposed as

$$\hat{\nu}_n\, h_{j,n} = \nu_n\, h_{j,n} + \sqrt{n}(P h_{j,n} - P_{\hat{\theta}} h_{j,n}). \tag{10}$$

Always assuming the null hypothesis, write $Y_i = BX_i + \Sigma^{1/2} U_i$, where the U_i have the standard Gaussian distribution in $I\!R^q$. Let $\hat{B}_U$ and S_U be the estimators of the parameters B and Σ for the sample $(X_1, U_1), \ldots, (X_n, U_n)$. (For this hypothetical sample, B is the zero matrix and $\Sigma = I_q$). It is not difficult to verify that these estimators relate to those for the original sample through $\hat{B} = B + \Sigma^{1/2}\hat{B}_U$ and $S = \Sigma^{1/2} S_U \Sigma^{1/2}$. It follows that the standardized residuals $S^{-1/2}(Y_i - \hat{B}X_i)$ relate to the corresponding residuals for the (X_i, U_i) sample via

$$S^{-1/2}(Y_i - \hat{B}X_i) = \rho S_U^{-1/2}(U_i - \hat{B}_U X_i) \tag{11}$$

where $\rho = (\Sigma^{1/2} S_U \Sigma^{1/2})^{-1/2} \Sigma^{1/2} S_U^{1/2}$. Since ρ is an orthogonal matrix and the functions applied to the residuals are products of radial functions and spherical harmonics, it follows as in [8], Proposition 8, that the distribution of our Z_n^2 does not depend on the underlying parameters B and Σ. Thus, we have a further simplification in the analysis of Z_n^2 in the sense that we can assume, in what follows, that the true parameters are $B = \mathbf{0}$ and $\Sigma = I_q$.

We will now introduce some definitions needed to describe the limiting distribution of Z_n^2. Let $\xi^2(x, u)$ denote the q-dimensional $N(Bx, \Sigma)$ density evaluated at u. Put $\xi_0(x,u) = \xi(x,u)\,|_{B=0,\Sigma=I_q}$. Let us give an order to the parameters in our model (entries of $B = (b_{ij})$ and $\Sigma = (\sigma_{ij})$) as follows:

$$\begin{gathered} b_{11}, \dots b_{1p}, b_{21}, \dots b_{2p}, \dots b_{q1}, \dots b_{qp}, \\ \sigma_{12}, \dots \sigma_{1q}, \sigma_{23}, \dots \sigma_{2q}, \dots \sigma_{q-1,q}, \sigma_{11}, \dots \sigma_{qq}. \end{gathered} \tag{12}$$

Notice that we have a total of $s = pq + \binom{q+1}{2}$ parameters. Denote by $\dot{\xi}(x,u)$ the vector of partial derivatives of $\xi(x,u)$ with respect to the parameters listed above (in the order just given), evaluated at $B = 0, \Sigma = I_q$. For each $j \leq k$, let $c(h_{j,\infty})$ be the (s-dimensional) vector given by

$$c(h_{j,\infty}) = 2 \int \int h_{j,\infty}(x,u) \xi_0(x,u) \dot{\xi}(x,u) du\, d\mu(x). \tag{13}$$

Also, let $J = (J_{i,j})_{1 \leq i,j \leq s}$ be the Fisher information matrix for the MLM at θ_0, given by

$$J_{i,j} = 4P(\dot{\xi}_i \dot{\xi}_j / \xi_0^2), \tag{14}$$

where $\dot{\xi}_i$ denotes the i-th component of the vector $\dot{\xi}$. Let C be the $k \times s$ matrix in which the j-th row is $c(h_{j,\infty})$. In our case, complete expressions for both J and the matrix C can be worked out in terms of moments of the covariate, as follows: Let $\tau = (\mu(X_{1,1}), \dots, \mu(X_{1,p}))$ (a row vector of moments) and $M_X = (\mu(X_{1,i} X_{1,j}))_{1 \leq i,j \leq p}$ (matrix of crossed moments). Then

$$J = \begin{pmatrix} M_X & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ & \ddots & & & \\ \mathbf{0} & \cdots & M_X & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & I_{\binom{q}{2}} & \mathbf{0} \\ \mathbf{0} & & \cdots & \mathbf{0} & \frac{1}{2} I_q \end{pmatrix} \tag{15}$$

and

$$C = \begin{pmatrix} d_0\, \tau & \mathbf{0} & & \cdots & \mathbf{0} \\ & \ddots & & & \\ \mathbf{0} & \cdots & d_0\, \tau & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & d_1\, I_{\binom{q}{2}} & \mathbf{0} \\ \mathbf{0} & & \cdots & \mathbf{0} & A_{3,3} \end{pmatrix}, \tag{16}$$

where the block M_X appears q times in the diagonal of J, as does the vector $d_0\, \tau$ in the 'diagonal' of C; $d_0 = \sqrt{q}(q+2)$, $d_1 = \sqrt{2}(q+1)(q+3)\beta/\sqrt{q(q+2)}$ and the block $A_{3,3}$ is as in [6], equation (2.20).

Generalizing Theorem 2 in [8], we have that the limiting distribution of $\hat{\nu}_n(\underline{h}_n)$ is k-dimensional Gaussian with mean zero and covariance matrix $M_0 - CJ^{-1}C^t$, and, therefore the distribution of Z_n^2 converges to that of

$$\sum_{j=1}^{k} \delta_j W_j^2 \tag{17}$$

where the W_j are i.i.d. $N(0,1)$ variables and the δ_j are the eigenvalues of

$$I - M_0^{-1/2} C J^{-1} C^t M_0^{-1/2}. \tag{18}$$

From this result and the formulas for J and C in (15) and (16), we see how the covariate moments enter the distribution of our statistic, although it has been computed on 'residuals'. Since we do not assume a distributional form for the covariate, the moments that appear in τ and M_X must be estimated from the sample. That the null distribution of Z_n^2 can indeed be effectively estimated without knowing the covariate distribution is illustrated in the simulations that we describe next.

3 Bootstrapping quantiles of Z_n^2

We will now describe a Monte Carlo experiment, performed to evaluate the convergence of Z_n^2 to its limiting distribution and the influence of the covariate distribution on it. We will also present a parametric bootstrap procedure that approximates very closely the null finite sample distribution of Z_n^2. Our setting is as follows: we take $p = 3$ and $q = 4$. Without loss of generality, we assume $B = \mathbf{0}$ and $\Sigma = I_q$. For our first example, we generate the 3-dimensional covariate from the one parameter multivariate Burr-Pareto-Logistic distribution whose density is given in [5], formula (9.10), with parameter $\lambda = 0.5$. In our second example the covariate has independent coordinates with the student's t_4 distribution. The first distribution considered has bounded support and correlated coordinates, while the second distribution has relatively heavier tails and independent coordinates.

To approximate the finite sample null distribution of Z_n^2, for different sample sizes ranging from $n = 20$ to $n = 200$, and each of the two covariate distributions considered, we generated (using the R Statistical Language) 10,000 samples of X_is. Then, the Y_is were generated according to the MLM (1). For each sample, $\tilde{\nu}_n(\underline{h}_n)$ and Z_n^2 were computed (with code in the R language available from the authors) and finite sample quantiles were extracted. These quantiles are displayed in Tables 1 and 2, in rows labeled Z_n^2.

Assuming no knowledge of the covariate distribution, the limit distribution can be approximated as follows: We take one sample (the 'actual sample') and from the X_is we estimate the moments that go in the definitions of τ and M_X. Then we plug these estimates in (15) and (16), and we can compute an approximation to the matrix in (18). Call the eigenvalues of this matrix $\hat{\delta}_j$, $j \leq k$. Then, we can use Monte Carlo quantiles of $\sum_{j=1}^{k} \hat{\delta}_j W_j^2$ (based on 10,000 samples of W_js) as approximate quantiles for the limit distribution. This procedure was implemented for the sample sizes and covariate distributions considered (using only the first covariate sample) and the quantiles obtained are displayed in Tables 1 and 2 in the rows labelled Z_∞^2.

Finally, a different approximation to the finite sample quantiles of Z_n^2 can be obtained through a parametric bootstrap, conditioning on the observed X_i sample. For $l = 1$ to 10,000 generate the null Y_i sample according to (1), using $B = \mathbf{0}$ and $\Sigma = I_q$ (recall that this does not affect the distribution of our statistic). Then, compute the corresponding Z_n^2 for these 10,000 samples and extract quantiles. This method will produce quantiles that converge, as $n \to \infty$, to the limiting quantiles of Z_n^2 (a justification can be obtained with arguments similar to those in [2]). This bootstrap approximation was implemented (again, based on just one covariate sample for each sample size) and the quantiles obtained are displayed in Tables 1 and 2 in rows labeled $Z_{n,b}^2$.

From the results of these simulations we can conclude the following: In the case of the Burr-Pareto-Logistic distribution with bounded support, the limiting quantiles (rows Z_∞^2) display little variability with sample size, suggesting that, in this case, a good approximation to the limiting distribution can be attained even with small samples. There is more variability among these rows in Table 2, as could be expected. Still, in both cases, the finite sample quantiles of Z_n^2 are approaching the approximate limiting quantiles from below, as n grows. Thus, use of the approximate asymptotic quantiles will produce a conservative procedure, as is usually the case with this type of statistics. In both cases, the agreement between approximate finite sample quantiles, Z_n^2, and limiting quantiles, Z_∞^2, becomes fairly acceptable for $n \geq 200$. On the other hand, for both distributions of the covariate, the parametric bootstrap procedure seems to provide a good approximation to the finite sample distribution of Z_n^2 for all the sample sizes considered. This could be expected, since the parametric bootstrap is simulating the finite sample statistic and not the asymptotic distribution. On the other hand, the approximate asymptotic quantiles are significantly less expensive from the computational viewpoint. Each number in the Z_∞^2 rows takes a couple of seconds of computation on a desktop PC, while the corresponding numbers in row $Z_{n,b}^2$, for $n = 200$, require about 15 mins of computation on the same machine. The code in the R statistical language that implements the test statistics and the bootstrap procedures described here is available from the authors.

One important conclusion we can extract from these simulations is that the distribution of Z_n^2 is significantly affected by the covariate distribution, as we can judge by the differences between corresponding entries in Tables 1 and 2. This result is a bit surprising, considering that the spherical harmonics and radial functions are applied to the standardized residuals. In this regard, the theory presented in this article is useful in telling us how the covariate effect appears, and how to obtain valid approximate quantiles for Z_n^2 by appropriately using the information contained in the covariate sample.

Table 1: MC quantile approximations for Z_n^2, $p = 3, q = 4$, $m = 10^4$, X ∼MultivB-P-L(0.5)

Sample size	Approx.	90%	92.5%	95%	97.5%	99%
20	Z_n^2	4.431	4.731	5.114	5.845	6.972
20	$Z_{n,b}^2$	4.545	4.817	5.197	5.900	6.883
20	Z_∞^2	5.524	6.005	6.607	7.684	9.294
50	Z_n^2	4.981	5.344	5.917	6.928	8.549
50	$Z_{n,b}^2$	4.721	5.136	5.700	6.672	8.348
50	Z_∞^2	5.599	6.062	6.726	7.844	9.403
100	Z_n^2	5.217	5.655	6.287	7.526	9.563
100	$Z_{n,b}^2$	5.120	5.529	6.112	7.115	8.768
100	Z_∞^2	5.680	6.175	6.797	8.024	9.619
200	Z_n^2	5.367	5.787	6.459	7.656	9.347
200	$Z_{n,b}^2$	5.303	5.752	6.390	7.653	9.209
200	Z_∞^2	5.590	6.071	6.759	7.960	9.616

Table 2: MC quantile approximations for Z_n^2, $p = 3, q = 4, m = 10^4$, X: independent coordinates t_4

Sample size	Approx.	90%	92.5%	95%	97.5%	99%
20	Z_n^2	6.789	7.125	7.548	8.205	9.177
20	$Z_{n,b}^2$	6.581	6.894	7.313	7.882	8.831
20	Z_∞^2	8.489	9.149	10.03	11.55	13.45
50	Z_n^2	8.434	8.969	9.704	11.00	12.87
50	$Z_{n,b}^2$	8.131	8.730	9.588	11.08	13.41
50	Z_∞^2	9.634	10.42	11.50	13.14	15.25
100	Z_n^2	8.851	9.503	10.41	11.96	13.98
100	$Z_{n,b}^2$	9.040	9.686	10.59	12.21	14.06
100	Z_∞^2	9.231	9.948	10.90	12.57	14.46
200	Z_n^2	9.341	10.17	11.14	12.81	14.96
200	$Z_{n,b}^2$	9.465	10.10	11.02	12.60	14.73
200	Z_∞^2	9.705	10.48	11.58	13.33	15.38

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