THE BEST LINEAR UNBIASED ESTIMATORS OF REGRESSION COEFFICIENTS IN A MULTIVARIATE GROWTH-CURVE MODEL. A COORDINATE-FREE APPROACH

by

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Abstract

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The problems of the existence of the best linear unbiased estimators (BLUE) and of their equality to the ordinary least squares estimators (OLSE) of the expected value of the observations are treated in a coordinate-free approach using a multivariate growth-curve model. It will be proved that the alternative forms of the necessary and sufficient conditions used in solving of these problems are independent on the between-individuals design matrix of the model.

Key words: Ordinary least squares estimator, best linear unbiased estimator, orthogonal projections.

Resumen

Se discute el problema de existencia del mejor estimador lineal insesgado (BLUE) para el valor esperado de una distribución en un contexto libre de coordenadas, usando un modelo de curvas de crecimiento multivariado. Se presenta además la igualdad del estimador anterior con el estimador de mínimos cuadrados ordinarios (OLSE). Se prueba que las diferentes

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formas de expresar las condiciones necesarias y suficientes para demostrar las propiedades anteriores son independientes de la matriz de diseño del modelo entre individuos.

Palabras clave: Estimador de mínimos cuadrados ordinarios, mejor estimador lineal insesgado, proyecciones ortogonales.

1. Introduction

For the general linear model $y = X\beta + e$, where X is an $n \times p$ known design matrix of rank $r \leq p, \beta$ is a $p \times 1$ vector of unknown parameters and e is an $n \times 1$ vector of disturbances, it is assumed that y (vector of observations) has the expectation $E(y) = \mu = X\beta$ and the covariance matrix $\text{cov}(y) = \sigma^2 V$, with $\sigma^2 > 0$ a known or unknown number and V an $n \times n$ symmetric positive definite known matrix. When $V = I_n$ (the $n \times n$ identity matrix) the classical Gauss-Markov theorem states that the BLUE (or Gauss-Markov estimator) is the OLSE of μ which is obtained for any solution $\widehat{\beta}_{\text{OLSE}}$ of the normal equations $X'X\beta = X'y$.

When V is a positive definite matrix and $r = p$, **Aitken** [1] extended the former result proving that the BLUE is the generalized least squares estimator of μ obtained for the solution $\widehat{\beta}_{GLSE}$ of the generalized normal equations $X'V^{-1}X\beta = X'V^{-1}y$.

Some other extensions of the Gauss-Markov theorem have been made by **Zyskind** and **Martin** [30] for a nonnegative covariance matrix and **Harville** [15] for general mixed linear model.

In the multivariate case of linear regression models the covariance structure is more complicated than $\sigma^2 V$ and it has to be also treated the existence of BLUE of μ. These problems: the existence of the BLUE and the equality between OLSE and BLUE of $E(y)$ in linear regression models represented important subjects in statistics.

Seminal contributions in their solving expressed in geometrical form were obtained by **Kruskal** [17], **Eaton** [13], **Milliken** [19], **Haberman** [14], **Arnold** [2], **Kleffe** [16]. Some alternative proofs were given: **Seely** [27], [28] restricted the choice of the BLUE of $E(y)$ to a finite-dimensional linear space; **Drygas** [11], [12] dealt with conditions under which the BLUE of μ is independent on V for multivariate linear models in locally convex topological vector space; **Beganu** [5], [7], [10] considered the existence conditions of the BLUE for the fixed effects in multivariate mixed linear models; **Qian** and **Tian** [22] established some properties for the BLUE of a subset of regression coefficients in general linear model.

Developments of the several conditions for the OLSE to be the BLUE have been made by **Baksalary** and **van Eijnsbergen** [4] and **Puntanen** and **Styan** [20]. **Puntanen** *et al.* [21] introduced a new representation for the rank of the difference between the covariance matrices corresponding to the OLSE and the BLUE of μ in the general linear model.

The purpose of this article is to extend to a multivariate growth curve model some of the results obtained for the general univariate linear model regarding the existence of the BLUE and the equality between the OLSE and the BLUE of μ. Some necessary and sufficient conditions for the OLSE to be the BLUE are obtained using a coordinate-free approach and it will be proved that the both problems do not depend on the between-individuals design matrix of the considered model.

The article is structured as follows. In Section 2 the necessary and sufficient condition obtained by **Eaton** [13] is expressed in order to prove the existence of the BLUE of μ in a family of multivariate growth curve models with random effects proposed by **Reinsel** [25], [26]. In Section 3 some of the necessary and sufficient conditions given by **Zyskind** [29] and **Haberman** [14] for the OLSE to be the BLUE in the general linear model will be verified in the considered multivariate linear model. It will be proved by means of the orthogonal projections onto the corresponding linear manifolds that these conditions can be expressed only in terms of the within-individual design matrix. Two examples are presented and it is proved that the BLUE of μ exists and it is equal to the OLSE independently on the between-individuals design matrix of these models.

2. The existence of the BLUE

The problem of the existence of the BLUE is treated in a specific multivariate linear model. This question was approached by **Eaton** [13] who extended the **Kruskal**'s theorem [17] to the case of the general multivariate linear model.

In the sequel it will be used a coordinate-free approach for which some algebraical notions are necessary to be denoted (see [24]).

Let $\mathcal{L}_{p_1,p_2}$ be the linear space of $p_2 \times p_1$ real matrices endowed with the inner product $< C, D >= \mathrm{tr}(CD')$ for all $C, D \in \mathcal{L}_{p_1,p_2}$. The Kronecker matrix product is defined as usual: if $C \in \mathcal{L}_{p_1,p_2}$ and $D \in \mathcal{L}_{q_1,q_2}$ then $C \otimes D = (c_{ij}D)$ is an element in $\mathcal{L}_{p_1q_1,p_2q_2}$.

The same notation $\mathcal{L}_{p_1,p_2}$ will be used for the real vector space of linear transformations on M_1 to M_2, where M_1 and M_2 stand for p_1 and p_2-dimensional real inner product spaces, respectively. If T and S are linear operators in $\mathcal{L}_{p_2,p_2}$ and $\mathcal{L}_{p_1,p_1}$, respectively, then the Kroneker operators product $T©S$ is the linear transformation on $\mathcal{L}_{p_1,p_2}$ to $\mathcal{L}_{p_1,p_2}$ such that $(T©S)Q = TQS^*$ where S^* is the adjoint of S relative to the inner product in M_1. The composition of two linear operators is

$$(T_1©S_1) \circ (T_2©S_2) = (T_1T_2)©(S_1S_2)$$

and the adjoint relative to the usual trace inner product is

$$(T©S)^* = T^*©S^* .$$

The particular linear regression model used in the following belongs to a family of multivariate linear growth curve models with random effects and it was considered by **Reinsel** [25], [26] and **Lange** and **Laird** [18] as a special case of the linear mixed models.

This model consists in m characteristics measured at p occasions on each of n individual sampling units. If the within-individual and the between-individuals design matrices $X \in \mathcal{L}_{q,p}$ and $A \in \mathcal{L}_{r,n}$, respectively, are known matrices of full column ranks $(q \leq p, r < n)$, $B \in \mathcal{L}_{qm,r}$ is a matrix of unknown parameters and $\Lambda \in \mathcal{L}_{qm,n}$ is a matrix of random effects, then the observable random matrix is

$$Y = AB(X' \otimes I_m) + \Lambda(X' \otimes I_m) + E \qquad (1)$$

where $E \in \mathcal{L}_{pm,n}$ is the random matrix of errors. It is assumed that the lines of E and Λ are independent random vectors of each other and between them, identically distributed with zero expected means and the same covariance matrices Σ_e and Σ_λ, respectively. Then the expected mean of the observations is

$$\mu = E(Y) = AB(X' \otimes I_m) \qquad (2)$$

and the covariance matrix is

$$\Sigma = \mathrm{cov}(\mathrm{vec}Y) = I_n \otimes [(XX') \otimes \Sigma_\lambda + I_p \otimes \Sigma_e] \qquad (3)$$

where

$$V = (XX') \otimes \Sigma_\lambda + I_p \otimes \Sigma_e \qquad (4)$$

For $A \in \mathcal{L}_{r,n}$ and $X \in \mathcal{L}_{q,p}$ of full column rank let

$$\Omega = \{\mu = AB(X' \otimes I_m) \mid B \in \mathcal{L}_{qm,r}\} \qquad (5)$$

be a linear manifold in $\mathcal{L}_{pm,n}$ and $\mathcal{X} \subset R^{pm}$, $\mathcal{A} \in R^n$ be the ranges corresponding to the operators $X \otimes I_m \in \mathcal{L}_{qm,pm}$. and $A \in \mathcal{L}_{r,n}$, respectively.

The sets of symmetric and positive definite linear mapings V from $\mathcal{L}_{m,p}$ to $\mathcal{L}_{m,p}$ and Σ from $\mathcal{L}_{pm,n}$ to $\mathcal{L}_{pm,n}$ will be denoted by Θ and $\mathcal{S}$, respectively, such that $I_{pm} \in \Theta$ and $I_{npm} \in \mathcal{S}$. V and Σ are the covariance operators in (4) and (3) respectively.

Then the description of the regression model (1) with the assumptions (2), (3) and (4) in a coordinate-free form is that $E(Y) = \mu \in \Omega$ and $\mathrm{cov}\,(\vec{Y}) = \Sigma = I_n©V \in \mathcal{S}$, when $V \in \Theta$. Therefore the family of the modfel (1) will be the set of all $n \times pm$ random matrix Y whose expectation belongs to Ω given by (5) and whose covariance operator (or matrix) lies in a certain set $\mathcal{S}$ definite above.

It is known (see [13]) that the linear operator in $\mathcal{L}_{pm,n}$ to $\mathcal{L}_{pm,n}$

$$P_\Omega = P_A©P_{X\otimes I_m} \qquad (6)$$

is the orthogonal projection onto Ω, where

$$P_A = A(A'A)^{-1}A' \qquad (7)$$

and

$$P_{X\otimes I_m} = [X(X'X)^{-1}X']©I_m \qquad (8)$$

are the orthogonal projections onto $\mathcal{A}$ and $\mathcal{X}$, respectively. It can be noticed that $P_{X\otimes I_m} = P_X \otimes I_m$, where P_X is the orthogonal projection on the range of X.

Theorem 1. *The linear manifold $\mathcal{X}$ is invariant under V if and only if Ω is invariant under $\Sigma = I_n©V \in \mathcal{S}$ for all $V \in \Theta$.*

Proof. It is assumed that Ω is invariant under the linear transformation Σ which means $(I_n©V)\Omega = \Omega$.

Let $B \in \mathcal{L}_{qm,r}$ such that $\mu = AB(X' \otimes I_m) \in \Omega$. Then, using the definition of the Kronecker operators product and the symmetry of V, it can be written that

$$(I_n©V)\mu = \mu V = AB(X' \otimes I_m)V \in \Omega$$

The last relation means that

$$P_\Omega[AB(X' \otimes I_m)V] = AB(X' \otimes I_m)V$$

or

$$P_A AB(X' \otimes I_m)VP_{X\otimes I_m} = AB(X' \otimes I_m)V$$

because P_Ω given by (6) is the orthogonal projection on Ω. But P_A being the orthogonal projection on the linear space $\mathcal{A}$, it can be obtained that

$$AB(X' \otimes I_m)VP_{X\otimes I_m} = AB(X' \otimes I_m)$$

for all $B \in \mathcal{L}_{qm,r}$. This relation is equivalent to

$$(X' \otimes I_m)VP_{X\otimes I_m} = (X' \otimes I_m)V$$

which is the same as

$$P_{X\otimes I_m}V(X \otimes I_m)\alpha = V(X \otimes I_m)\alpha$$

for all $\alpha \in R^{qm}$. Since $P_{X\otimes I_m}$ is the orthogonal projection on $\mathcal{X}$ the last equality means that $V(X\otimes I_m)\alpha \in \mathcal{X}$, which can be expressed as: for all $\alpha \in R^{qm}$ there is $\beta \in R^{qm}$ such that

$$V(X \otimes I_m)\alpha = (X \otimes I_m)\beta \tag{9}$$

and this is the property for $\mathcal{X}$ to be invariant under V. The proof is complete because the equivalent relations were stated for all $V \in \Theta$.

Corollary 1. *The BLUE of $E(Y)$ exists in the family of models (1) if and only if $\mathcal{X}$ is invariant under V, for all $V \in \Theta$.*

Proof. **Eaton** [13] proved that the BLUE of $E(Y)$ exists in the general multivariate linear model if and only if $\Sigma\Omega = \Omega$ for all $\Sigma = I_n © V \in \mathcal{S}$, which is equivalent to $V\mathcal{X} = \mathcal{X}$, for all $V \in \Theta$ by Theorem 1.

Corollary 2. *The linear manifold $\mathcal{X}$ is invariant under V if and only if there exists the linear operator $Q \in \mathcal{L}_{qm,qm}$ such that*

$$V(X \otimes I_m) = (X \otimes I_m)Q \tag{10}$$

for all $V \in \Theta$.

Proof. The relation (9) is equivalent to the following condition: for all $\alpha \in R^{qm}$, there exists $\beta = Q(\alpha) \in R^{qm}$ such that

$$V(X \otimes I_m)\alpha = (X \otimes I_m)Q(\alpha)$$

for all $V \in \Theta$.

Corollary 3. *For the model (1) the linear transformation $Q \in \mathcal{L}_{qm,qm}$ verifying the condition (10) is*

$$Q = (X'X) \otimes \Sigma_\lambda + I_q \otimes \Sigma_e \tag{11}$$

Proof. By means of Theorem 1 and Corollary 2, the existence of the matrix Q with the property (10) is equivalent to the invariance of the linear manifold Ω under all $\Sigma = I_n © V \in \mathcal{S}$. Hence, for $V \in \Theta$ given by (4), we have

$$\begin{aligned}\Sigma\mu &= (I_n © V)[AB(X' \otimes I_m)]\\ &= AB(X' \otimes I_m)V\\ &= AB(X' \otimes I_m)[(XX') \otimes \Sigma_\lambda + I_p \otimes \Sigma_e]\\ &= AB[(XX') \otimes \Sigma_\lambda + I_q \otimes \Sigma_e](X' \otimes I_m)\\ &= ABQ(X' \otimes I_m) \in \Omega\,,\end{aligned}$$

for all $B \in \mathcal{L}_{qm,r}$. Therefore Q expressed in (11) being a $qm \times qm$ symmetric matrix, it verifies the relation (10).

3. The equality between OLSE and BLUE

The OLSE and the BLUE of $E(Y)$ corresponding to the model (1) are given in **Reinsel** [25], [26], **Lange** and **Laird** [18] and **Beganu** [10] as

$$\widehat{\mu}_{\text{OLSE}} = A(A'A)^{-1}A'Y[X(X'X)^{-1}X' \otimes I_m] \tag{12}$$

$$\widehat{\mu}_{\text{BLUE}} = A(A'A)^{-1}A'YV^{-1}(X \otimes I_m)\cdot [(X'\otimes I_m)V^{-1}(X\otimes I_m)]^{-1}(X'\otimes I_m). \tag{13}$$

In the following some of the alternative forms of the necessary and sufficient conditions for the OLSE to equal the BLUE of μ given by **Rao** [23], **Zyskind** [29] and **Haberman** [14] will be verified. These conditions were chosen for their accessibility and their geometrical representation.

Theorem 2. *In the model (1)*

$$\widehat{\mu}_{\text{OLSE}} = \widehat{\mu}_{\text{BLUE}} \tag{14}$$

if and only if the linear manifold $\mathcal{X}$ is invariant under V for all $A \in \mathcal{A}$ and $V \in \Theta$.

Proof. It is known ([17]) that the equality (14) holds if and only if Ω is invariant under $\Sigma \in \mathcal{S}$, which is equivalent through Theorem 1 to $V\mathcal{X} = \mathcal{X}$ for all $V \in \Theta$. It can be noticed that the proof of the relation (9) is independent on $A \in \mathcal{A}$.

Theorem 3. *The equality (14) corresponding to model (1) holds if and only if*

$$P_{X\otimes I_m}V = VP_{X\otimes I_m} \tag{15}$$

for all $A \in \mathcal{A}$ and $V \in \Theta$.

Proof. One of the necessary and sufficient conditions proved by **Zyskind** [29] to establish (14) is written for the model (1) as

$$P_\Omega \circ \Sigma = \Sigma \circ P_\Omega \qquad (16)$$

for all $\Sigma = I_n Ⓒ V \in \mathcal{S}$. Let $B \in \mathcal{L}_{qm,r}$ such that $\mu = AB(X' \otimes I_m) \in \Omega$. Then using Corollary 2, we have that

$$\begin{aligned}(P_\Omega \circ \Sigma)\mu &= [(P_A Ⓒ P_{X\otimes I_m}) \circ (I_n Ⓒ V)]\mu \\ &= [P_A Ⓒ (P_{X\otimes I_m} V)]\mu \\ &= P_A \mu V P_{X\otimes I_m} \\ &= ABQ(X' \otimes I_m) P_X \otimes I_m \\ &= ABQ(X' \otimes I_m)\end{aligned}$$

and

$$\begin{aligned}(\Sigma \circ P_\Omega)\mu &= [(I_n Ⓒ V) \circ (P_A Ⓒ P_{X\otimes I_m})]\mu \\ &= [P_A Ⓒ V P_{X\otimes I_m}]\mu \\ &= P_A \mu P_{X\otimes I_m} V \\ &= P_A AB(X' \otimes I_m) P_{X\otimes I_m} V \\ &= AB(X' \otimes I_m)V = ABQ(X' \otimes I_m)\,.\end{aligned}$$

Therefore the equality (16) is accomplished for all $A \in \mathcal{A}$ and $V \in \Theta$, which means that

$$P_A Ⓒ (P_{X\otimes I_m} V) = P_A Ⓒ (V P_{X\otimes I_m})$$

Then the equality (15) is obtained for all $A \in \mathcal{A}$ and $V \in \Theta$ using Lemma 1 in [3].

If the covariance operator V is of the form (4), then the condition (15) becomes

$$\begin{aligned}P_{X\otimes I_m} V &= (P_X \otimes I_m)[(XX') \otimes \Sigma_\lambda + I_p \otimes \Sigma_e] \\ &= (P_X XX') \otimes \Sigma_\lambda + P_X \otimes \Sigma_e \\ &= (XX' P_X) \otimes \Sigma_\lambda + P_X \otimes \Sigma_e \\ &= [(XX') \otimes \Sigma_\lambda + I_p \otimes \Sigma_e](P_X \otimes I_m) \\ &= V P_{X\otimes I_m}\,,\end{aligned}$$

because P_X is the orthogonal projection on the range of X.

Examples. 1. A particular form of the model (1) is the multivariate linear growth curve

$$Y = AB(X' \otimes I_m) + \Lambda(1_p \otimes I_m) + E \qquad (17)$$

where the within-individual design matrix X is partitioned as $(1_p\ Z)$ with its first column being a column of ones since X includes a constant term for each of the m variables. The matrix Z of order $p \times (q-1)$ is such that $1_p' Z = 0$.

The observations in (17) have the mean (2) and the covariance matrix (3) with

$$V = J_p \otimes \Sigma_\lambda + I_p \otimes \Sigma_e$$

where $J_p = 1_p 1_p'$.

Then the linear manifold Ω is invariant under Σ means that

$$\Sigma\mu = \mu V = AB(X' \otimes I_m)V = ABQ(X' \otimes I_m) \qquad (18)$$

if and only if there exists a matrix Q satisfying (10) for all $V \in \Theta$ and $\mu \in \Omega$. Such a matrix corresponding to the model (17) is $Q = R \otimes \Sigma_\lambda + I_q \otimes \Sigma_e$ with

$$R = \begin{pmatrix} p & 0 \\ 0 & 0 \end{pmatrix}$$

if and only if $1_p' Z = 0$.

Hence $BQ = \tilde{B} \in \mathcal{L}_{qm,r}$ means that (18) is an element of Ω for all $V \in \Theta$ and $\mu \in \Omega$. It can easily see that this condition stands independent on $A \in \mathcal{A}$ and that it can be replaced by the relation (9) with $\beta = Q\alpha$, which means $X\mathcal{X} = \mathcal{X}$ for all $V \in \Theta$.

Therefore the BLUE of μ exists in the model (17) and it is equal to the OPLSE if and only if X is invariant under all $V \in \Theta$ and this is equivalent to the condition for 1_p and Z to be linearly independent for all $A \in \mathcal{A}$.

2. A generalized growth-curve model considered in [25] is

$$Y = AB(X' \otimes I_m) + \Lambda(X' \otimes I_m) + T(W' \otimes I_m) + E \quad (19)$$

where W is a $p \times s$ design matrix of full column rank and T is an $n \times sm$ random matrix. Besides the assumptions of the model (1) it is supposed that the lines of T are independently and identically distributed with zero means and the same covariance matrix $I_p \otimes \Sigma_T$. They are also mutually independent on the random lines of Λ and E.

Then the expected value of Y in (19) is (2), an element of the linear manifold Ω given by (5), and the covariance matrix (3) with

$$V = (XX') \otimes \Sigma_\lambda + (WW') \otimes \Sigma_T + I_p \otimes \Sigma_e$$

The condition for the invariance of Ω becomes

$$\Sigma\mu = \mu V = AB(X' \otimes I_m)V = A\tilde{B}(X' \otimes I_m) \qquad (20)$$

if and only if $X'W = 0$, where $\tilde{B} = B[(X'X) \otimes \Sigma_\lambda + I_q \otimes \Sigma_e] \in \mathcal{L}_{qm,r}$. It can be easily seen that (20) is an element of Ω for all $V \in \Theta$ and $A \in \mathcal{A}$ if and only if

$X'W = 0$. Therefore the necessary and sufficient condition for the BLUE of μ to exist in the model (19) is that Ω is invariant under all $\Sigma \in \mathcal{S}$, which is equivalent to the invariance of $\mathcal{X}$ under all $V \in \Theta$ and this is the same as the condition for the equality (14). In the case of the model (19) the relation (14) holds if and only if X and W are linearly independent as it was already known.

It is also easy to see that $\tilde{B}$ can be written as BW which means that the element (20) lies in Ω is an equivalent condition of (10) and it is independent on $A \in \mathcal{A}$.

It follows that this results obtained for the family of the model (1) with a particular form (17) and a generalized form (19) are verified independently on the between-individuals matrix $A \in \mathcal{A}$.

The necessary and sufficient conditions in Theorems 1, 2, 3 are verified by the model (1), hence the BLUE (13) of μ exists and it is the OLSE (12). These two questions are equivalent in the multivariate growth-curve model (1) because of its special covariance structure.

Corollaries 1, 2, 3 assert that for the family of multivariate growth curve models (1) the necessary and sufficient conditions for the existence of $\widehat{\mu}_{BLUE}$ and its equality with $\widehat{\mu}_{OLSE}$ are independent on the between-individuals design matrix A and they have to be imposed only on the within - individual design matrix X. The special form of the orthogonal projection onto Ω allows these conclusions.

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