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On the equality of the ordinary least squares estimators and the best linear unbiased estimators in multivariate growth-curve models

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Abstract. It is well known that there were proved several necessary and sufficient conditions for the ordinary least squares estimators (OLSE) to be the best linear unbiased estimators (BLUE) of the fixed effects in general linear models. The purpose of this article is to verify one of these conditions given by Zyskind [39, 40]: there exists a matrix Q such that $\Omega X = XQ$, where X and Ω are the design matrix and the covariance matrix, respectively. It will be shown the accessibility of this condition in some multivariate growth-curve models, establishing the known result regarding the equality between OLSE and BLUE in this type of linear models.

Sobre la igualdad de los estimadores ordinarios de mínimos cuadrados y de los estimadores lineales no sesgados óptimos en modelos multivariantes de curvas de crecimiento.

Resumen. Es bien sabido que existen demostraciones de varias condiciones necesarias y suficientes para que los estimadores ordinarios de mínimos cuadrados (OLSE) sean los estimadores lineales insesgados óptimos (BLUE) de modelos lineales generales con efectos fijos. El propósito de este artículo es comprobar que una de esas condiciones dada por Zyskind [39, 40]: existe una matriz Q tal que $\Omega X = XQ$, donde X y Ω son la matriz de diseño y la matriz de covarianza, respectivamente. Se demostrará la accesibilidad de esta condición en algunos modelos multivariantes de curvas de crecimiento, estableciendo el resultado conocido teniendo en cuenta la igualdad entre OLSE y BLUE en este tipo de modelos lineales.

1 Introduction

The problem of the equality of the OLSE and the BLUE in linear models has a long tradition in statistics, starting perhaps with work of Anderson [1]. But the most important contribution to solve this problem belongs to Rao [31, 32, 33], and Zyskind [39, 40, 41]. Thus Zyskind [39] stated eight equivalent alternative conditions in the case of a positive definite covariance matrix in linear regression models. These conditions imply a relationship between the covariance matrix and the whole matrix of explanatory variables.

For the extended case when the covariance matrix is non-negative definite and the regressor matrix does not necessarily have full column rank, Rao [31] appears to be the first who derived the necessary and sufficient conditions and Zyskind [40] proved the first general theorem for OLSE to yield BLUE.

Seminal contributions in solving this problem were made by Watson [37, 38], Anderson [2], Searle [36], Durbin and Watson [17], Bloomfield and Watson [13]. Alternative proofs of some of the earlier result as

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well as their extensions were derived, using algebrical methods, by: Baksalary and Kala [4], Baksalary[5], Puntanen and Styan[29], McAleer [24], Qin and Lawless [30], Kurata and Kariya [22]. The results of this problem expressed in geometrical form were obtained by: Kruskal [21], Eaton [18], Haberman [19], Arnold [3]. Some alternative proofs using also a coordinate-free approach were given by Drygas [15, 16] and Beganu [10, 11].

For all model matrices having a fixed common linear part the problem of the equality between OLSE and BLUE was solved by McElroy [25], Zyskind [41], Balestra [7]. Milliken and Albohali [26] argued that McElroy's condition is sufficient but not necessary. A clarification of the issues involved in this debate was made by Baksalary and Eijnsbergen [6].

When the covariance matrix is unknown De Gruttola et al. [14] used a three-stage estimation procedure to obtain a generalized least squares estimator (GLSE) of the regression coefficients which is asymptotically efficient; Baltagi [8] derived a necessary and sufficient condition for two-stage and three-stage least squares estimators to be equivalent; Phillips and Park [27] studied an asymptotic equivalence of OLSE and GLSE; Khan and Powell [20] introduced a two-stage estimator of the regressors in linear censored regression models and proved that a small sample bias is in the opposite direction of the OLSE; Bates and DebRoy [9] used an iterative algorithm to estimate the parameters in multivariate mixed linear models, some of the intermediate calculations requiring GLSE; Biorn [12] provided that the GLSE can be interpreted as an weighted average of a group of estimators, where the weights are the inverses of their covariance matrices, and the results of the research work in this field can go on.

The purpose of this paper is to verify one of the necessary and sufficient conditions for OLSE to be BLUE given by Zyskind [39, 40] and to show its accessibility for some multivariate growth-curve models. This type of parametric models for repeated-measures data occupies a central role in the statistical literature on longitudinal studies, being available in significant fields. Therefore it may be useful to prove easier the equality between OLSE and BLUE of the fixed effects using this Zyskind's condition.

The paper is structured as follows. In Section 2 Zyskind's condition is presented in the general linear model. In Sections 3 and 4 Zyskind's condition will be verified using two multivariate growth-curve models with a fixed structure on the mean and differing numbers of multivariate random effects for each sampling unit. The previous results are applied in the particular case of the growth-curve model considered by Lange and Laird [23].

2 Zyskind's condition

Consider the general univariate linear model

$$y = X\beta + e \tag{1}$$

where y is an $n \times 1$ vector of observations, X is an $n \times k$ matrix of rank $r(X) = r \leq k$ of known real constants, β is a $k \times 1$ vector of unknown parameters and e is an $n \times 1$ vector of errors with zero mean and the covariance matrix Ω.

It is well known that the OLSE of $X\beta$ is any solution of the normal equations $X'X\beta = X'y$. If $r = k$, then the unique solution is

$$X\hat{\beta}_{\mathrm{OLSE}} = X(X'X)^{-1}X'y \tag{2}$$

where $P = X(X'X)^{-1}X'$ is the orthogonal projection on $\mathcal{C}(X)$, the columns space of X.

When Ω is positive definite, the BLUE of $X\beta$ in (1) is the solution of the generalized normal equations $X'\Omega^{-1}X\beta = X'\Omega^{-1}y$. Some authors refer to these estimators as the GLSE and others call them the weighted least squares estimators of $X\beta$. The BLUE of $X\beta$ is

$$X\hat{\beta}_{\mathrm{BLUE}} = X(X'\Omega^{-1}X)^{-1}X'\Omega^{-1}y \tag{3}$$

If $r < k$, any generalized inverse $(X'X)^{-}$ of $X'X$ and $(X'\Omega^{-1}X)^{-}$ of $X'\Omega^{-1}X$ will be used instead of $(X'X)^{-1}$ in (2) and $(X'\Omega^{-1}X)^{-1}$ in (3). In this case (Ω non-singular), Anderson [1] proved that

$$\hat{\beta}_{\mathrm{OLSE}} = \hat{\beta}_{\mathrm{BLUE}} \tag{4}$$

if $\mathcal{C}(X) = \mathcal{C}(Q_r)$, where Q_r is a matrix whose r columns are the r eigenvectors corresponding to r non-null eigenvalues of Ω.

Thus, the problem of the equality

$$X\hat{\beta}_{\text{OLSE}} = X\hat{\beta}_{\text{BLUE}} \tag{5}$$

may be replaced by (4). This replacement is also possible when the Moore-Penrose inverses $(X'X)^+$ and $(X'\Omega^{-1}X)^+$ are used in (2) and (3), respectively, instead of any generalised inverses.

When Ω is non-negative definite, then

$$X\hat{\beta}_{\text{BLUE}} = X(X'\Omega^- X)^{-1}X'\Omega^- y \tag{6}$$

if $r = k$ and the BLUE of $X\beta$ will be expressed by (6) with $(X'\Omega^- X)^-$ instead of $(X'\Omega^- X)^{-1}$ if $r < k$.

In order to show how the OLSE and the BLUE of $X\beta$ differ in general, using the relations (2) and (6), it can be written (see [4]) that

$$X\hat{\beta}_{\text{BLUE}} = X\hat{\beta}_{\text{OLSE}} - P\Omega M(M\Omega M)^+ y$$

where $M = I - P$.

Zyskind and Martin [42] established that the solution of the general normal equations $X'\Omega^+ X\beta = X'\Omega^+ y$ do not lead to BLUE of $X\beta$ and that the necessary and sufficient condition for

$$X\hat{\beta}_{\text{GLSE}} = X(X'\Omega^+ X)^+ X'\Omega^+ y$$

to equal $X\hat{\beta}_{\text{BLUE}}$ is $\mathcal{C}(X) \subset \mathcal{C}(\Omega)$. Kruskal [21] and Eaton [18] obtained the same condition in a coordinate-free aproach.

Baksalary and Kala [4], extending the former results, showed that if $X\hat{\beta}_{GLSE} = X\hat{\beta}_{\text{OLSE}}$, then they are both BLUE of $X\beta$.

But the first complete solution of (5) was derived by Rao [31] who gave an explicit representation of the set of all non-negative definite matrices Ω. Zyskind [40], extending the results stated in [39], proved eight necessary and sufficient conditions under which the OLSE is BLUE of $X\beta$. One of these conditions which follows to be used is:

A necessary and sufficient condition for OLSE *of β in model* (1) *to be* BLUE *is to exist a $k \times k$ matrix Q satisfying the relation*

$$\Omega X = XQ \tag{7}$$

when the covariance matrix Ω is non-negative definite.

The problem of the equalities (4) is treated in the same way for the multivariate linear regression models.

3 A multivariate growth curve model

Many longitudinal studies investigate changes over time in a characteristic (or more) which is measured repeatedly for each unit. A general family of multiple response models which includes the repeated-measurement and the growth curve models was considered by many authors (Potthoff and Roy [28]) and was generalized by Reinsel [34, 35]. Thus it is assumed that each of the m variables follows a response curve of the same linear type over the p occasions for each of the n individuals. Let y_k be an $mp \times 1$ observable random vector of the form

$$y_k = (X \otimes I_m)\operatorname{vec}\theta_k + (1_p \otimes I_m)\lambda_k + e_k \tag{8}$$

where X is a $p \times q$ known within-individual model matrix, θ_k is an $m \times q$ matrix of unknown parameters, λ_k is an $m \times 1$ vector of random effects associated with the kth individual and $e_k = (\varepsilon'_{1k} \ldots \varepsilon'_{pk})'$ is an $mp \times 1$ vector of errors, $k = 1, \ldots, n$. I_m is the identity matrix of order m, 1_p is a $p \times 1$ vector of ones and

"$\otimes$" is the Kronecher matrix product ($M \otimes N = (m_{ij}N)$). It is used the vec operator such that the columns of a matrix are rearranged one below another. Then $\operatorname{vec}\theta_k$ is an $mq \times 1$ vector of unknown parameters.

It is assumed that λ_k and ε_{jk} are independent and identical distributed random vectors with

$$E(\lambda_k) = 0, \qquad E(\varepsilon_{jk}) = 0$$

$$\operatorname{cov}(\lambda_k) = \Sigma_\lambda, \operatorname{cov}(\varepsilon_{jk}) = \Sigma_e, \qquad j = 1, \dots, p; \quad k = 1, \dots n.$$

Then the expected mean and the covariance matrix of y_k are

$$E(y_k) = (X \otimes I_m) \operatorname{vec} \theta_k \tag{9}$$

$$\operatorname{cov}(y_k) = J_p \otimes \Sigma_\lambda + I_p \otimes \Sigma_e = V, \qquad k = 1, \dots, n \tag{10}$$

where J_p is the $p \times p$ matrix of ones.

The repeated-measurement models alow for $(\operatorname{vec}\theta_1, \dots \operatorname{vec}\theta_n) = BA'$, where B is an $mq \times r$ matrix of unknown parameters and A is an $n \times r$ known between-individual model matrix.

Setting $Y' = (y_1 \dots y_n)$, $\Lambda' = (\lambda_1 \dots \lambda_n)$ and $E' = (e_1 \dots e_n)$, the model (8) can be written as

$$Y' = (X \otimes I_m)BA' + (1_p \otimes I_m)\Lambda' + E' \tag{11}$$

or, using the relation $\operatorname{vec}(ABC) = (C' \otimes A) \operatorname{vec} B$, as

$$y = (A \otimes X \otimes I_m)\beta + (I_n \otimes 1_p \otimes I_m)\lambda + e \tag{12}$$

where $y = \operatorname{vec} Y'$, $\beta = \operatorname{vec} B$, $\lambda = \operatorname{vec} \Lambda'$ and $e = \operatorname{vec} E'$. The relations (9) and (10) become

$$E(y) = (A \otimes X \otimes I_m)\beta$$

$$\operatorname{cov}(y) = I_n \otimes V = I_n \otimes J_p \otimes \Sigma_\lambda + I_n \otimes I_p \otimes \Sigma_e \tag{13}$$

Since the regression model (8) includes a constant term for each of m variables, it is assumed ([34]) that $X = (1_p \quad Z)$, where Z is a $p \times (q-1)$ matrix. It is also assumed without loss of generality that $r(X) = q$ and $r(A) = r$ and that Σ_λ and Σ_e are non-negative definite matrices.

The OLSE of β in model (12) is given by Reinsel [34] as

$$\hat{\beta}_{\text{OLSE}} = [(A'A)^{-1}A' \otimes (X'X)^{-1}X' \otimes I_m]y \tag{14}$$

or, equivalently, the OLSE of B in model (11) as

$$\hat{B}_{\text{OLSE}} = [(X'X)^{-1}X' \otimes I_m]Y'A(A'A)^{-1} \tag{15}$$

The BLUE of β in (12) and the BLUE of B in (11) will be

$$\hat{\beta}_{\text{BLUE}} = [(A'A)^{-1}A' \otimes ([(X' \otimes I_m)V^-(X \otimes I_m)]^{-1}(X' \otimes I_m)V^-)]y \tag{16}$$

$$\hat{B}_{\text{BLUE}} = [(X' \otimes I_m)V^-(X \otimes I_m)]^{-1}(X' \otimes I_m)V^-Y'A(A'A)^{-1} \tag{17}$$

where V is the covariance matrix (10).

Theorem 1 *The equation*

$$(I_N \otimes V)(A \otimes X \otimes I_m) = (A \otimes X \otimes I_m)Q \tag{18}$$

has the solution

$$Q = I_r \otimes (R \otimes \Sigma_\lambda + I_q \otimes \Sigma_e) \tag{19}$$

with

$$R = \begin{pmatrix} p & 0'_{q-1} \\ 0_{q-1} & 0_{q-1,q-1} \end{pmatrix} \tag{20}$$

if and only if Z is orthogonal to 1_p in model (12).

PROOF. Using the expression (13) and the properties of the Kronecker product ([33]), it can be written that

$$(I_n \otimes V)(A \otimes X \otimes I_m) = A \otimes (J_p X) \otimes \Sigma_\lambda + A \otimes X \otimes \Sigma_e$$

It follows that

$$J_p X = 1_p (p \;\; 0'_{q-1}) = X'R \tag{21}$$

if and only if $1'_p Z = 0$ with R given by (20). 0_{q-1} and $0_{q-1,q-1}$ are the null vector and the null matrix of corresponding orders.

Corollary 1 *The $qm \times qm$ matrix*

$$M = R \otimes \Sigma_\lambda + I_q \otimes \Sigma_e \tag{22}$$

with R given by (20) *verifies the relation*

$$V(X \otimes I_m)NA' = (X \otimes I_m)MNA' \tag{23}$$

for every $qm \times r$ matrix N if and only if $1'_p Z = 0$ in model (11).

PROOF. It follows from the relations (10) and (21) that

$$V(X \otimes I_m)NA' = [(J_p X) \otimes \Sigma_\lambda + X \otimes \Sigma_e]NA' = (X \otimes I_m)(R \otimes \Sigma_\lambda + I_q \otimes \Sigma_e)NA'$$

Corollary 2 *In the multivariate growth-curve models given by the matriceal form* (11) *or the vectorial form* (12)*, having the model matrix $X = (1_p \;\; Z)$ such that $1'_p Z = 0$, the* OLSE *of B or β are* BLUE.

PROOF. The relations (18) and (23) represent the necessary and sufficient condition (7) of Zyskind for verifying the equality (4) corresponding to models (12) and (11) (11), respectively. The OLSE and the BLUE of β and B are expressed in (14)—(17). ■

4 A generalized growth-curve model

A slightly more general growth-curve model of the matriceal form

$$Y' = (X \otimes I_m)BA' + (X \otimes I_m)\Lambda' + (W \otimes I_m)T' + E' \tag{24}$$

or the vectorial form

$$y = (A \otimes X \otimes I_m)\beta + (I_N \otimes X \otimes I_m)\lambda + (I_N \otimes W \otimes I_m)\tau + e \tag{25}$$

was considered by Reinsel [34, 35]. It is considered that W is a $p \times s$ matrix of known constants of full column rank, T is an $n \times ms$ matrix of random effects obtained by a similar procedure as Λ in model (11) and $\tau = \operatorname{vec} T'$. It is assumed that the matrices Λ', T' and E' are mutually independent and have random column vectors independently and identically distributed with zero means and the same covariance matrices $I_p \otimes \Sigma_\lambda$, $I_p \otimes \Sigma_\tau$ and $I_p \otimes \Sigma_e$, respectively. Under these assumptions y has the expected value given by (13) and the covariance matrix

$$\operatorname{cov}(y) = I_n \otimes [(XX') \otimes \Sigma_\lambda + (WW') \otimes \Sigma_\tau + I_p \otimes \Sigma_e] = I_n \otimes V \;, \tag{26}$$

Theorem 2 *The necessary and sufficient condition for the existence of an $rqm \times rqm$ matrix*

$$Q = I_r \otimes [(X'X) \otimes \Sigma_\lambda + I_q \otimes \Sigma_e] \tag{27}$$

verifying the relation (18) *is that W and X be orthogonal in model* (25).

PROOF. Replacing the covariance matrix given by (26) in the relation (18) it obtains that Q is given by (27) if and only if $W'X = 0$.

Corollary 3 *There exists a* $qm \times qm$ *matrix*

$$M = (XX') \otimes \Sigma_\lambda + I_q \otimes \Sigma_e \tag{28}$$

verifying the relation (23) *for every* $qm \times r$ *matrix* N *if and only if* W *is orthogonal to* X *in model* (24).

Corollary 4 *In the multivariate growth-curve models* (24) *and* (25) *the* OLSE *of* B *and* β*, respectively, are* BLUE *if and only if* W *and* X *are orthogonal.*

Example 1 *For* $m = 1$ *and the random components* Λ' *and* E'*, the model* (24) *becomes the balanced growth curve model saturated in the design matrix of the random effects considered by Lange and Laird* [23] *having the matriceal form*

$$Y' = XBA' + X\Lambda' + E' \tag{29}$$

The expected mean for this model will be $E(Y') = XBA'$ *or* $E(y) = (A \otimes X)\beta$ *and the covariance matrix will be*

$$\mathrm{cov}(y) = I_n \otimes (X\Sigma_\lambda X' + \sigma^2 I_p) = I_n \otimes V$$

Without loss of generality it is assumed that the columns of the within-individual model matrix X *constitute an orthonormal set, that is* $X'X = I_q$.

Under these assumptions, the condition (18) *written for* (29) *becomes*

$$(I_n \otimes V)(A \otimes X) = A \otimes (X\Sigma_\lambda X'X + \sigma^2 X) = (A \otimes X)[I_r \otimes (\Sigma_\lambda + \sigma^2 I_q)].$$

Thus, there exists an $rq \times rq$ *matrix* $Q = I_r \otimes (\Sigma_\lambda + \sigma^2 I_q)$*, which is a particular form of* (27) *(27).*

The similar condition (23) *will be satisfied by a* $q \times q$ *matrix* $M = \Sigma_\lambda + \sigma^2 I_q$*, which is the equivalent form of* (28).

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