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On equivalence problem in linear regression models. II. Unbiased estimation of
the covariance matrix scalar factor

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# ON EQUIVALENCE PROBLEM IN LINEAR REGRESSION MODELS

### Part II. UNBIASED ESTIMATION OF THE COVARIANCE MATRIX SCALAR FACTOR

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## INTRODUCTION

In Part I the problem of control and numerical stability of computation of the best linear unbiased estimation of the regression parameters was considered. The aim of this part is to solve an analogous problem in estimation of an unknown covariance matrix scalar factor.

Let us have the general regression model $(Y_{n,1}, X_{n,m}\beta_{m,1}, \sigma^2 V_{n,n})$ (see Part I). Let the random vector $Y$ have a normal distribution. In this case we can obtain the unbiased estimation of the unknown parameter $\sigma^2$ in several different ways.

a) In the "PANDORA-BOX" matrix

$$(1) \qquad \begin{pmatrix} V & X \\ X' & 0 \end{pmatrix}^- = \begin{pmatrix} C_1 & C_2 \\ C_3 & -C_4 \end{pmatrix}$$

it holds that

$$(2) \qquad \hat{\sigma}_1^2 = \frac{1}{R(V \vdots X) - R(X)} Y'C_1 Y = \frac{1}{Tr\, VC_1} Y'C_1 Y$$

is an unbiased estimation of $\sigma^2$. $R(V \vdots X)$ is the rank of the matrix $(V \vdots X)$, $Tr\, VC_1$ is the trace of the matrix $VC_1$ (The proof see in $[2]$ p. 298 and p. 294.)

b) If $(X')^-_{m(V)}$ is an arbitrary minimum $V$-seminorm $g$-inverse of the matrix $X'$ (transpose of the matrix $X$), $V^-$ is an arbitrary choice of the $g$-inverse of $V$ then

$$(3) \quad \hat{\sigma}_2^2 = \frac{1}{R(V \vdots X) - R(X)} (Y - X[(X')^-_{m(V)}]' Y)' V^- (Y - X[(X')^-_{m(V)}]' Y)$$

is an unbiased estimation of $\sigma^2$ (see $[3]$, p. 149).

c) The general model $(Y, X\beta, \sigma^2 V)$ can be transformed into a regular one $(Y_1 = F'(I - X(N'X)^- N') Y, P\gamma, \sigma^2 I)$, where N is a matrix of order $n \times (n - R)(X)$ with rank $n - R(X)$, so that $X'Z = 0$ holds, $V = JJ'$ (i.e. $R(V) = R(J)$ and J is of order $n \times R(V)$) and $F' = (J'J)^{-1} J'$. P is a matrix of full rank (for details see Part I), If the dimension of the vector $Y_1$ fulfils dim $Y_1 >$ dim $\gamma$, then

$$(4) \qquad \hat{\sigma}_3^2 = \frac{1}{\text{dim } Y_1 - \text{dim } \gamma} (Y_1 - P\hat{\gamma})' (Y_1 - P\hat{\gamma}) =$$

$$= \frac{1}{\text{dim } Y_1 - \text{dim } \gamma} \min_{\gamma} (Y_1 - P\gamma)' (Y_1 - P\gamma),$$

where $\hat{\gamma} = P'Y_1$, is an unbiased estimation of $\sigma^2$ (see [3], p. 141).

d) If $\hat{\beta}$ is the solution of the consistent system of normal equations .

$$(5) \qquad X'MX\hat{\beta} = X'MY$$

where

$$M = (V + XUX')^- + K ,$$

$$(6) \qquad R(X'MX) = R(X'), \quad \mu(V \vdots X) = \mu(V + XUX') = \mu(V + XU'X'),$$

$$VK'X = 0, \quad X'KX = 0,$$

then the BLUE $(p'\beta)^\frown$ of any estimable function $p'\beta$ is $p'\hat{\beta}$ (see [1] and [4]), $\mu(V \vdots X)$ is the vector space spanned by the columns of the matrix $(V \vdots X)$. Here a natural question arises, what are the necessary and sufficient conditions for the matrices U and K in order that

$$(7) \qquad \hat{\sigma}_4^2 = \frac{1}{R(V \vdots X) - R(X)} (Y - X\hat{\beta})' M(Y - X\hat{\beta})$$

might be a suitable unbiased estimation of $\sigma^2$.

Namely, the estimations (2), (3) and (4) are always unbiased and (7) is unbiased under some additional assumptions on the matrices U and K. From the view point of checking and numerical stability of computation procedures, a serious question is if and when these estimations are identical in almost every realization (see Part I).

We shall show that (2), (3) and (4) are identical in almost every realization and the necessary and sufficient conditions that (7) is the same unbiased estimation of $\sigma^2$ in almost every realization as (2), (3) and (4) are (6) and $Z'V(K + K') VZ = 0$, where Z is a matrix of order $n \times (n - R(X))$ with rank $n - R(X)$, such that $X'Z = 0$ holds.

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**Lemma 1.** *In the regression model* $(\xi,\, A\delta,\, \sigma^2 I)$, *where the random vector $\xi$ has a normal distribution with the mean value* $\mathbf{E}(\xi) = A\delta$ *and the covariance matrix* $\sigma^2 I$,

$$\frac{1}{\dim \xi - \mathbf{R}(A)}\, \xi'\big(I - A(A'A)^- A'\big)\,\xi$$

*is an unbiased estimation of* $\sigma^2$, *it has* $\big(\sigma^2/(\dim \xi - \mathbf{R}(A))\big)\chi^2$ *distribution with* $\dim \xi - \mathbf{R}(A)$ *degrees of freedom and does not depend on the choice of* $(A'A)^-$.

The proof is in [3] p. 142 and Lemma 2.2.6.

Let us have the general model $(Y,\, X\beta,\, \sigma^2 V)$. If we take an arbitrary but fixed $(N'X)^-$, then the random vector $Y_1 = F'(I - X(N'X)^- N')\, Y$ has a normal distribution with the mean value $P\Lambda Q'\eta,\, \eta \in \mathscr{R}^m$. $P$, $\Lambda$ and $Q$ are matrices of full rank satisfying

$$F'X\big(I - (N'X)^- N'X\big) = P\Lambda Q'\,,$$

$P'P = Q'Q = I$, $\Lambda$ is a diagonal matrix (see Part I). The covariance matrix of the vector $Y_1$ is $\sigma^2 I$. Lemma 1 implies that the random variable

$$(8) \qquad \hat{\sigma}^2 = \frac{1}{\dim Y_1 - \mathbf{R}\big(F'X(I - (N'X)^- N'X)\big)}\ \cdot$$

$$\cdot\ Y_1'\big\{I - P\Lambda Q'\big[(P\Lambda Q')'\,(P\Lambda Q')\big]\,Q\Lambda P'\big\}\, Y_1 =$$

$$= \frac{1}{\dim Y_1 - \mathbf{R}\big(F'X(I - (N'X)^- N'X)\big)}\, Y_1'\,\{I - PP'\}\, Y_1$$

is an unbiased estimation of $\sigma^2$ and has $\big(1/(\dim Y_1 - R(F'X(I - (N'X)^- N'X)))\big)\chi^2$ distribution.

**Lemma 2.** *For*

$$\tilde{\beta} = \big\{(N'X)^- N' + (I - (N'X)^- N'X)\,Q\Lambda^{-1}P'F'(I - X(N'X)^- N')\big\}\, Y$$

*it holds with probability* 1:

$$\min_{\beta:\, N'X\beta = N'Y} (F'Y - F'X\beta)'\,(F'Y - F'X\beta) = (Y - X\tilde{\beta})'\, FF'(Y - X\tilde{\beta})\,.$$

Proof. First we shall show that $\tilde{\beta}$ and a suitable $\lambda$ solve the equations

$$(9) \qquad X'FF'X\tilde{\beta} + X'N\lambda = X'FF'Y$$

$$N'X\tilde{\beta} = N'Y\,.$$

From Lemma 1 Part I we see that it holds $Y = Xa + Vb,\ a \in \mathscr{R}^m,\ b \in \mathscr{R}^n$ with

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probability 1. From the proof of Lemma 4 in Part I we conclude that

$$(N'X)^- N' + (I - (N'X)^- N'X) Q\Lambda^{-1}P'F'(I - X(N'X)^- N')$$

is one choice of $[(X')^-_{m(V)}]'$ and we easily see that $\tilde{\beta}$ solves the second equation in (9). Further,

$$X'FF'X\tilde{\beta} + X'N\lambda =$$
$$= X'FF'X\{(N'X)^- N' + (I - (N'X)^- N'X) Q\Lambda^{-1}P'F'(I - X(N'X)^- N')\}\ .$$
$$.(Xa + Vb) + X'N\lambda = X'FF'Xa + X'FF'X(I - (N'X)^- N'X) Q\Lambda^{-1}P'F'Vb +$$
$$+ X'N\lambda = X'FF'Y - X'F(F' - F'X(I - (N'X)^- N'X) Q\Lambda^{-1}P'F') Vb +$$
$$+ X'N\lambda = X'FF'Y - X'F(I - P\Lambda Q'Q\Lambda^{-1}P') F'Vb + X'N\lambda = X'FF'Y -$$
$$- X'F(I - PP') F'Vb + X'N\lambda\ .$$

From the equation

$$(I - (N'X)^- N'X)' X'F(I - PP') F'V = Q\Lambda P'(I - PP') F'V = 0$$

we see that

(10) $\quad \mu(X'F(I - PP') F'V) = \mu(X'FF'[I - X(I - (N'X)^- N'X) Q\Lambda^{-1}P'F']V) \subset$
$$\subset Ker\{(I - (N'X)^- N'X)'\} = \mu(X'N)\ ,$$

where

$$Ker\{(I - (N'X)^- N'X)'\} = \{y : (I - (N'X)^- N'X)'\, y = 0\}\ .$$

The relation (10) shows that to every $b \in \mathscr{R}^n$ there exists a $\lambda \in \mathscr{R}^{n-R(V)}$ such that the equation $X'FF'X\tilde{\beta} + X'N\lambda = X'FF'Y$ holds. Therefore $\tilde{\beta}$ and $\lambda$ are solutions of (9).

Let now $\beta^*$ be an arbitrary vector such that $N'X\beta^* = N'Y$ is true. Then

$$(Y - X\beta^*)'\, FF'(Y - X\beta^*) - (Y - X\tilde{\beta})'\, FF'(Y - X\tilde{\beta}) =$$
$$= -2(\beta^*)'{}_j\, X'FF'Y + (\beta^*)'\, X'FF'X\beta^* + 2\tilde{\beta}'X'FF'Y - \tilde{\beta}'X'FF'X\tilde{\beta} =$$
$$= -2(\beta^*)'X'FF'Y + (\beta^*)'\, X'FF'X\beta^* + \tilde{\beta}'X'FF'X\tilde{\beta} +$$
$$+ 2(\beta^*)'\, X'N\lambda = (\beta^* - \tilde{\beta})'\, X'FF'X(\beta^* - \tilde{\beta}) \geqq 0\ .$$

The proof is complete.

**Lemma 3.** *For an arbitrary choice of* $V^-$ *and* $(X'^-_{m(V)})$ *it holds with probability* 1:

$$(Y - X\tilde{\beta})'\, FF'(Y - X\tilde{\beta}) = (Y - X\tilde{\beta})'\, V^-(Y - X\tilde{\beta}) =$$
$$= (Y - X[(X')^-_{m(V)}]'\, Y)'\, V^-(Y - X[(X')^-_{m(V)}]'\, Y)\ .$$

Proof. According to Lemma 1, Lemma 4 and Theorem 1 in Part I

$$Y - X\tilde{\beta} = Xa + Vb - X[(X')^-_{m(V)}]'\, (Xa + Vb) = (I - X[(X')^-_{m(V)}]')\, Vb$$

with probability 1, and this equation does not depend on the choice of $(X')^-_{m(V)}$.
Hence an arbitrary matrix $(X')^-_{m(V)}$ fulfils

(11)    $(Y - X[(X')^-_{m(V)}]' Y)' V^-(Y - X[(X')^-_{m(V)}]' Y) = (Y - X\tilde{\beta})' V^-(Y - X\tilde{\beta}).$

But $Y - X\tilde{\beta} \in \mu(V)$ with probability 1 and (11) does not depend on the choice of $V^-$.
One choice of $V^-$ is FF' and the proof is complete.

**Lemma 4.**

$$\min_{\beta : N'X\beta = N'Y} (F'Y - F'X\beta)' (F'Y - F'X\beta) =$$

$$= Y_1'\{I - P\Lambda Q'(Q\Lambda P'P\Lambda Q')^- Q\Lambda P'\} Y_1 = Y_1'\{I - PP'\} Y_1 .$$

Proof. According to [3] p. 24 we have

$$\min_{\beta : N'X\beta = N'Y} (F'Y - F'X\beta)' (F'Y - F'X\beta) =$$

$$= \min_{\delta} (F'Y - F'X[(N'X)^- N'Y + (I - (N'X)^- N'X) \delta])' (F'Y - $$

$$- F'X[(N'X)^- N'Y + (I - (N'X)^- N'X)\delta]) =$$

$$= \min_{\delta} (F'(I - X(N'X)^- N') Y - P\Lambda Q'\delta)' (F'(I - X(N'X)^- N') Y - P\Lambda Q'\delta) =$$

$$= (Y_1 - P\Lambda Q'(P\Lambda Q')^-_{l(1)} Y_1)' (Y_1 - P\Lambda Q'(P\Lambda Q')^-_{l(1)} Y_1) =$$

$$= \{(I - P\Lambda Q'(Q\Lambda P'P\Lambda Q')^- Q\Lambda P') Y_1\}' .$$

$$. \{(I - P\Lambda Q'(Q\Lambda P'P\Lambda Q')^- Q\Lambda P') Y_1\} =$$

$$= Y'\{I - P\Lambda Q'(Q\Lambda P'P\Lambda Q')^- Q\Lambda P'\} Y_1$$

from the definition of the least-squares inverses $(P\Lambda Q')^-_{l(1)}$ and their properties (see
[2] (1c. 5.3)). The proof is complete.

**Lemma 5.**

$$\boldsymbol{R}(V) - \boldsymbol{R}(F'X(I - (N'X)^- N'X)) = \boldsymbol{R}(V \vdots X) - \boldsymbol{R}(X) .$$

Proof. It is easy to see (e.g. (1.b 6) in [2]) that

$$\boldsymbol{R}(F'X(I - (N'X)^- N'X)) = \boldsymbol{R}\left(\begin{pmatrix} F' \\ N' \end{pmatrix} X\right) - \boldsymbol{R}(N'X) =$$

$$= \boldsymbol{R}(X) - \boldsymbol{R}(N'X) = \boldsymbol{R}(X) - \boldsymbol{R}\begin{pmatrix} X' \\ V \end{pmatrix} + \boldsymbol{R}(V) =$$

$$= \boldsymbol{R}(X) - \boldsymbol{R}(V \vdots X) + \boldsymbol{R}(V)$$

and we have

$$R(V) - R(N'X(I - (F'X)^- N'X)) = R(V \vdots X) - R(X).$$

The lemma is proved.

We have

$$\dim \gamma = R(F'X(I - (N'X)^- N'X))$$

for $\gamma$ in c) which yields the following result:

**Corollary 1.**

$$\hat{\sigma}_2^2 = \frac{1}{R(V \vdots X) - R(X)} (Y - X[(X')_{m(V)}^-]' Y)' V^- (Y - X[(X')_{m(V)}^-]' Y) =$$

$$= \frac{1}{\dim Y_1 - R(F'X(I - (N'X)^- N'X))} Y_1'\{I - P\Lambda Q'(Q\Lambda P'P\Lambda Q')^- Q\Lambda P'\} Y_1 =$$

$$= \hat{\sigma}^2 = \frac{1}{\dim Y_1 - \dim \gamma} Y_1' (I - PP') Y_1 = \hat{\sigma}_3^2$$

*holds with probability* 1.

The corollary is evident if we mention that

$$(Q\Lambda P'P\Lambda Q')^- = (Q\Lambda\Lambda Q')^- = Q\Lambda^{-1}\Lambda^{-1}Q'.$$

**Lemma 6.** *If* $C_1$ *is defined in* (1), *then*

$$(Y - X[(X')_{m(V)}^-]' Y)' V^- (Y - X[(X')_{m(V)}^-]' Y) = Y'C_1 Y$$

*is true with probability* 1.

The proof follows from the properties of the matrix (1), see [2] 4i.

**Corollary 2.** *It is true that*

$$\hat{\sigma}_2^2 = \hat{\sigma}_3^2 = \hat{\sigma}_1^2 = \hat{\sigma}^2$$

*with probability* 1 *and we proved the equivalence of estimations* (2), (3) *and* (4) *in realizations.*

Let us return to the problem d). We want the estimation (7) to be numerically equivalent with the estimations (2), (3) and (4) with probability 1.

**Lemma 7.** *An arbitrary matrix* U *with*

$$\mu(V + XUX') = \mu(V + XU'X') = \mu(V \vdots X)$$

*satisfies the relation*

$$(Y - X[(X')^-_{m(V)}]' Y)' V^-(Y - X[(X')^-_{m(V)}]' Y) =$$

$$= (Y - X[(X')^-_{m(V)}]' Y)' (V + XUX')^- (Y - X[(X')^-_{m(V)}]' Y)$$

*for any choice of* $(V + XUX')^-$ *with probability* 1.

The proof is easily obtained (if we notice that $Y = Xa + Vb = (V + XUX') u$ with probability 1) from the properties of $(X')^-_{m(V)}$ (see Part I).

**Lemma 8.** *The relation*

$$(Y - X[(X')^-_{m(V)}]' Y)' M(Y - X[(X')^-_{m(V)}]' Y) =$$

$$= (Y - X[(X')^-_{m(V)}]' Y)' V^-(Y - X[(X')^-_{m(V)}]' Y)$$

*holds with probability* 1 *iff*

$$(Y - X[(X')^-_{m(V}]' Y)' K(Y - X[(X')^-_{m(V)}]' Y) = 0 ,$$

*where* M *and* K *are defined in* (6).

The proof is an easy consequence of the definition of the matrix M and Lemma 7.

As $Y = Xa + Vb$ holds with probability 1, we get for the matrix K from Lemma 8, (6) and from the properties of $(X')^-_{m(V)}$ (see Part I) the condition

(12) $$b'(VKV - VKV(X')^-_{m(V)} X') b = 0$$

for every $b \in \mathcal{R}^n$.

In order to find a necessary and sufficient condition for the matrix K to fulfil (12) we need another lemma.

**Lemma 9.**

$$u'Au = 0 \quad for\ every \quad u \quad iff \quad A + A' = 0 .$$

The proof is easy and is omitted.

In this way we have obtained for the matrix K from (12) the n.a.s. condition

$$VKV - VKV(X')^-_{m(V)} X' + VK'V - X[(X')^-_{m(V)}]' VK'V = 0 ,$$

or, equivalently,

(13) $$(I - X[(X')^-_{m(V)}]') V(K + K') V(I - (X')^-_{m(V)} X') = 0 .$$

**Lemma 10.** *Let* Z *be a matrix of order* $n \times (n - \mathbf{R}(X))$ *with rank* $n - \mathbf{R}(X)$ *such that* $X'Z = 0$, *then*

$$Z(Z'Z)^{-1} Z' = (I - (X')^-_{m(V)}X')$$

*for any choice of* $(X')^-_{m(V)}$.

Proof. An arbitrary element u fulfils

$$Z(Z'Z)^{-1} Z'u = Z(Z'Z)^{-1} Z'(P_{\mu(Z)}u + P_{KerZ'}u) =$$

$$= Z(Z'Z)^{-1} Z'Zv = Zv$$

where $P_{\mu(Z)}$ is the projection operator onto $\mu(Z)$.

$$X'(I - (X')^-_{m(V)} X') = 0 \quad \text{implies} \quad \mu(I - (X')^-_{m(V)} X') \in \mu(Z).$$

$$\left. \begin{array}{l} R(Z) = n - R(X) \\ R(I - (X')^-_{m(V)} X') = n - R(X) \end{array} \right\} \Rightarrow \mu(I - (X')^-_{m(V)} X') = \mu(Z)$$

and thus

$$Ker \, Z' = Ker(I - (X')^-_{m(V)} X').$$

We have the identities

$$(I - (X')^-_{m(V)} X') u = (I - (X')^-_{m(V)} X') (P_{\mu(Z)}u + P_{KerZ'}u) =$$

$$= (I - (X')^-_{m(V)} X') Zv + (I - (X')^-_{m(V)} X') P_{Ker(I-(X')^-_{m(v)}X')} u = Zv,$$

because of the relation $X'Z = 0$. The proof is complete.

**Lemma 11.** *The relation*

$$(Y - X[(X')^-_{m(V)}]' Y)' M(Y - X[(X')^-_{m(V)}]' Y) =$$

$$= (Y - X[(X')^-_{m(V)}]' Y)' V^-(Y - X[(X')^-_{m(V)}]' Y)$$

*holds with probability* 1 *iff*

(14) $$Z'V(K + K') VZ = 0.$$

Proof. From (13) and Lemma 10 we have

$$Z(Z'Z)^{-1} Z'V(K + K') VZ(Z'Z)^{-1} Z' = 0,$$

which is equivalent with (14). The lemma is proved.

**Corollary 3.** *The n.a.s. condition for* $p'\hat{\beta}$ *to be the* BLUE *for any estimable function* $p'\beta$ *and*

$$\hat{\sigma}^2_4 = \hat{\sigma}^2_3 = \hat{\sigma}^2_2 = \hat{\sigma}^2_1 = \hat{\sigma}^2$$

*with probability* 1, *where* $\hat{\beta}$ *is the solution of* (5), *is that* (6) *and* (14) *hold.*

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## CONCLUSIONS

The aim of this part was to show the numerical equivalence of the basic estimation algorithms for the covariance matrix scalar factor. The main results are Corollaries 1, 2 and 3.

*References*

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Súhrn

## PROBLÉM EKVIVALENCIE V LINEÁRNYCH REGRESNÝCH MODELOCH

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V prípade všeobecného regresného modelu, tj. ak ani matica plánu, ani kovariančná matica náhodného vektora nie sú plnej hodnosti, existuje niekoľko rôznych spôsobov určenia nevychýleného a združene efektívneho odhadu odhadnuteľneho lineárneho funkcionálu neznámych regresných parametrov a tiež nevychýleného odhadu neznámeho skalárneho faktora kovariančnej matice. V prvej časti práce sa ukázalo, že všetky dané odhady lineárneho funkcionálu sú numericky tie isté skoro iste, a v druhej časti sa zase ukázalo, že všetky dané odhady skalárneho faktora kovariančnej matice za určitých podmienok sú numericky totožné skoro iste.

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