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Natural estimation of variances in a general finite discrete spectrum linear regression model

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Abstract The method of "natural" estimation of variances in a general (orthogonal or nonorthogonal) finite discrete spectrum linear regression model of time series is suggested. Using geometrical language of the theory of projectors a form and properties of the estimators are investigated. Obtained results show that in describing the first and second moment properties of the new estimators the central role plays a matrix known in linear algebra as the Schur complement. Illustrative examples with particular regressors demonstrate direct applications of the results.

Keywords Time series · Finite discrete spectrum linear regression model · Natural estimators of variance components · Orthogonal and oblique projectors · The Schur complement

1 Introduction

In recent articles (Štulajter 2003; Štulajter and Witkovský 2004; Štulajter 2007) authors have introduced and investigated a time series model called *the finite discrete spectrum linear regression model* or shortly FDSLRM, which represents time series modeling and predicting by linear regression models (see Brockwell and Davis 1991; Christensen 1991, 2002; Štulajter 2002)—the alternative approach to the most popular and well-known Box–Jenkins methodology (e.g. Box et al. 1994).

The class of FDSLRM models whose mean values are given by linear regression and error terms are characterized by a purely finite discrete spectrum and white noise, offers applications in a wide range of real situations. In practice we usually need to

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estimate not only mean value parameters, but also unknown parameters of the FDSLRM covariance function. One solution of this problem was just given in Štulajter and Witkovský (2004) who used the double ordinary least squares estimator (DOOLSE) and obtained invariant unbiased, not consistent quadratic estimators.

The used approach, however, works only for the orthogonal version of the FDSLRM and in some cases it gives negative estimates. There are also such cases that we have to use a numerical nonlinear constrain optimization procedure to compute the DOOLSE estimates. In general it means that we have no explicit expression for estimators, which causes a difficult theoretical study of their properties.

Because of these reasons we suggest in Sect. 2 of the article an alternative method of estimating unknown variance parameters of the covariance function, called by us "natural" estimation, appropriate for the FDSLRM with and without the assumption of orthogonality and leading to estimates, which are always non-negative (from the given parametric space). Moreover the method is based on the least square approach as DOOLSE so estimating does not require the normality assumption as it is in case of ML, REML or MIVQUE estimation (Searle et al. 1992; Christensen 2002). In Sect. 3 using theory of projectors, summarized, e.g. in recent works of Ben-Israel and Greville (2003) or Galántai (2003), we obtain the first and second moment properties of estimators. Final Sect. 4 includes illustrative examples, in which we apply developed results.

In the rest of the introduction we establish notation and recapitulate used model and basic results from Štulajter (2003) (or Štulajter and Witkovský 2004) providing a starting point and assumptions for our considerations.

A model of time series $X(.)$ is said to be *the finite discrete spectrum linear regression model* (FDSLRM), if $X(.)$ satisfies

$$X(t) = \sum_{i=1}^{k} \beta_i f_i(t) + \sum_{j=1}^{l} Y_j v_j(t) + w(t); \; t = 1, 2, \ldots, \tag{1.1}$$

where

$\beta = (\beta_1, \beta_2, \ldots, \beta_k)' \in \mathbb{E}^k$ is a vector of unknown regression parameters;
$Y = (Y_1, Y_2, \ldots, Y_l)'$ is a $l \times 1$ random vector with zero mean value, $E[Y] = 0$, and with covariance matrix $Cov(Y) = diag(\sigma_j^2)$ of size $l \times l$, where unknown variances $\sigma_j^2 \geq 0$ for all $j = 1, 2, \ldots, l$;
$f_i(.)$; $i = 1, 2, \ldots, k$ and $v_j(.)$; $j = 1, 2, \ldots, l$ are known real functions defined on $\mathbb{E}$;
$w(.)$ is white noise time series with the variance $D[w(t)] = \sigma^2 > 0$ and it is uncorrelated with Y.

We denote the unknown variance parameters of Y and $w(.)$, which are also variance parameters of the FDSLRM, by $\nu = (\sigma^2, \sigma_1^2, \ldots, \sigma_l^2)'$. Under the FDSLRM assumptions direct computation applied to the definition of the time series covariance function $R(s,t)$ yields its expression in the form $R_\nu(s,t) = \sigma^2 \delta_{s,t} + \sum_{j=1}^{l} \sigma_j^2 v_j(s) v_j(t)$; $s, t = 1, 2, \ldots$ with the parameter ν belonging to the parametric space $\Upsilon = (0, \infty) \times \langle 0, \infty)^l$.

The basic result dealing with any finite observation of the FDSLRM time series—random vector $X = (X(1), \ldots, X(n))'$—says that the observation X satisfies the following linear regression model (also called the FDSLRM model):

$$X = F\beta + \varepsilon, E(\varepsilon) = 0, Cov(\varepsilon) = \sigma^2 I_n + \sum_{j=1}^{l} \sigma_j^2 V_j \text{ is a p.d. matrix,} \tag{1.2}$$

where

$F = (f_1\ f_2\ \ldots\ f_k) \in \mathbb{E}^{n\times k}$ is the design matrix of the model with columns $f_i = (f_i(1), \ldots, f_i(n))'$; $i = 1, 2, \ldots, k$;
$V_j = v_j v_j' \in \mathbb{E}^{n\times n}$; $v_j = (v_j(1), v_j(2), \ldots, v_j(n))'$; $j = 1, 2, \ldots, l$ are matrices describing the structure of covariance matrix $Cov(\varepsilon) \equiv \Sigma_\nu$.

The FDSLRM model (1.2) is said to be *orthogonal*, if $f_i \perp v_j$ for all $i = 1, 2, \ldots, k$; $j = 1, 2, \ldots, l$ and $v_i \perp v_j$ for all $i, j = 1, 2, \ldots, l, i \neq j$. In this article we do not assume validity of the orthogonality conditions what will be also reminded by calling the model *a general*(*or nonorthogonal*) FDSLRM.

Model (1.2) is equivalent to a model belonging to the class of linear mixed models (see, e.g. McCulloch and Searle 2001; Christensen 2002):[1]

$$X = F\beta + VY + w, E(w) = 0, Cov(w) = \sigma^2 I_n, Cov(Y, w) = 0, \tag{1.3}$$

where $V = (v_1\ v_2\ \ldots\ v_l) \in \mathbb{E}^{n\times l}$ and random vector $w = (w(1), \ldots, w(n))'$ is a finite observation of white noise $w(.)$. Symbols $F, \beta, Y, w(.)$ and v_j; $j = 1, 2, \ldots, l$ have the same meaning as above.

Since the observation of the FDSLRM is a special case of the linear mixed model, the problem of estimating ν is related to the problem of estimating variance-covariance components in linear mixed models studied besides Štulajter and Witkovský (2004), e.g. for more general cases in Rao and Kleffe (1988), Volaufová and Witkovský (1991) or Searle et al. (1992).

We shall assume that both matrices $F \in \mathbb{E}^{n\times k}$ and $V \in \mathbb{E}^{n\times l}$ are of full column rank,[2] i.e. $r(F, V) = k + l$ and number $k + l + 1$ of unknown parameters β and ν, which arise in the FDSLRM (1.1), is smaller than length n of a realization $x = (x_1, x_2, \ldots, x_n) \in \mathbb{E}^n$ of finite observation X.

Finally we shall employ the following notation (Galántai 2003) resulting from using theory of projectors: $P_{\mathscr{N}} \equiv$ *the orthogonal projector onto some subspace* $\mathscr{N}$; $P_{\mathscr{N}^\perp} \equiv M_{\mathscr{N}} \equiv$ *the orthogonal projector onto the orthogonal complement of* $\mathscr{N}$; $P_{\mathscr{N},\mathscr{O}} \equiv$ *the oblique projector onto* $\mathscr{N}$ *along* $\mathscr{O}$; $\mathscr{L}(H) = \{Hx | x \in \mathbb{E}^n\} \equiv$ *the column space of* $H \in \mathbb{E}^{m\times n}$; $\mathcal{N}(H) = \{x \in \mathbb{E}^n | Hx = 0\} \equiv$ *the null space of* $H \in \mathbb{E}^{m\times n}$.

[1] In this case unobservable vector β is frequently called a vector of "fixed effects" and Y is an unobservable vector of "random effects".

[2] To have no problems in distinguishing between a matrix product (FV) and $\begin{pmatrix}F & V\end{pmatrix}$ as matrix F augmented by V, we will frequently write the matrix $\begin{pmatrix}F & V\end{pmatrix}$ as $(F,\ V)$.

2 "Natural" variance component estimation in the FDSLRM

2.1 Definition of "natural" estimators

Variances of the FDSLRM $\sigma_j^2 = Cov(Y_j) = E(Y_j^2)$; $j = 1, 2, \ldots, l$, so that if components Y_j were known, a "natural estimator" of σ_j^2 would be just Y_j^2. These unobservable "natural estimators" and their name are identical with those used in MINQUE estimating (Rao and Kleffe 1988; Searle et al. 1992; Christensen 2002).

Although Y is a random vector, according to McCulloch and Searle (2001) it is convenient to consider the linear regression model conditional on unobservable realizations $y \in \mathbb{E}^l$ of Y. In such models mean values are $E(X|Y = y) = F\beta + Vy$ and realization y of Y can be understood as other unknown mean value parameters of model (1.3). From this viewpoint FDSLRM model (1.3) is nothing else than a regression model, linear with respect to unknown regression parameters $(\beta, y)' \in \mathbb{E}^{k+l}$ and with covariance matrix $Cov(X|Y = y) = Cov(w) = \sigma^2 I_n$—in the theory of linear models known as the classical linear regression model (LRM).

In this (and any) considered classical LRM the standard unbiased estimator of σ^2 is given (see, e.g. Christensen 2002) by the sum of squares for residuals of the ordinary least squares method divided by the degrees of freedom.[3] Since the ordinary least squares method also provides an estimator for regression parameters β and y, then according to the above-mentioned idea of unobservable natural estimators a real estimator for σ_j^2 should be square of a given component y_j of the estimator of y.

These considerations motivate the following definition. Let us consider for a FDSLRM observation X of time series $X(.)$ the following classical linear regression model

$$X = \begin{pmatrix} F, & V \end{pmatrix} \begin{pmatrix} \beta \\ y \end{pmatrix} + w; \; E(w) = 0, \; Cov(w) = E(ww') = \sigma^2 I_n, \tag{2.1}$$

where the known $n \times (k + l)$ design matrix $(F, \; V) = (f_1 \; f_2 \; \ldots \; f_k \; v_1 \; v_2 \; \ldots \; v_l)$ is of full column rank $(k + l)$ and $y \in \mathbb{E}^l$ is an unknown realization of random vector Y. Then estimators $\widetilde{\nu}(X) = (\widetilde{\sigma}^2(X), \widetilde{\sigma}_1^2(X), \ldots, \widetilde{\sigma}_l^2(X))'$ of ν are said to be *observable natural estimators* or shortly *natural estimators*, if

$$\widetilde{\sigma}^2(X) = \tfrac{1}{n-k-l}[X - F\widetilde{\beta}(X) - V\widetilde{y}(X)]'[X - F\widetilde{\beta}(X) - V\widetilde{y}(X)], \tag{2.2}$$

$$\widetilde{\sigma}_j^2(X) = \widetilde{y}_j^2(X), \; j = 1, 2, \ldots, l, \tag{2.3}$$

where $(\widetilde{\beta}(X), \widetilde{y}(X))' = (\widetilde{\beta}_1(X), \ldots, \widetilde{\beta}_k(X), \widetilde{y}_1(X), \ldots, \widetilde{y}_l(X))'$ is the ordinary least square estimator of $(\beta, y)' \in \mathbb{E}^{k+l}$.

[3] This estimator can be also obtained through the double least squares principle (Štulajter 2002). Therefore it is also called the double ordinary least squares estimator (DOOLSE) for a classical LRM.

From projection theory we know that the ordinary least square estimator $(\widetilde{\beta}(X), \widetilde{y}(X))'$ of $(\beta, y)'$ for linear regression model (2.1) is given by the equation:

$$\begin{pmatrix} \widetilde{\beta}(X) \\ \widetilde{y}(X) \end{pmatrix} = \begin{pmatrix} F'F & F'V \\ V'F & V'V \end{pmatrix}^{-1} \begin{pmatrix} F'X \\ V'X \end{pmatrix}, \tag{2.4}$$

where the $(k+l) \times (k+l)$ Gram matrix $G = \begin{pmatrix} F'F & F'V \\ V'F & V'V \end{pmatrix}$ is of full rank, since $r(G) = r[(F, V)'(F, V)] = r(F, V) = k + l$.

If (F, V) is of full column rank, then F must be too, so making use of the so-called Banachiewicz formula for the inverse of a partitioned (block) matrix,[4] see e.g. Zhang et al. (2005), we can write

$$G^{-1} = \begin{pmatrix} * & * \\ -W^{-1}(V'F)(F'F)^{-1} & W^{-1} \end{pmatrix}, \tag{2.5}$$

where symbol * denotes blocks not needed in deriving $\widetilde{y}(X)$ and where $W = V'V - V'F(F'F)^{-1}F'V \in \mathbb{E}^{l \times l}$ is called the Schur complement of $F'F$ in G. Substituting (2.5) to (2.4) and rearranging, we finally get the following form of estimator $\widetilde{y}(X)$ of y

$$\widetilde{y}(X) = W^{-1}V'(I - F(F'F)^{-1}F')X. \tag{2.6}$$

2.2 Geometrical interpretation of natural estimators

Now we use the geometrical language of projection theory for describing definition and properties of natural estimators. Such intermediate step provides us a powerful tool in easier establishing and understanding new features of given concepts.

The orthogonal projector $P_{\mathscr{L}^{\perp}(F)} \equiv M_F = I - F(F'F)^{-1}F'$ offers the following simplification of (2.6):

$$\widetilde{y}(X) = TX;\, T \equiv W^{-1}V'M_F \in \mathbb{E}^{l \times n}, \tag{2.7}$$

where the Schur complement $W = V'M_F V$. Since every orthogonal projector M_F is a symmetric matrix, $W \in \mathbb{E}^{l \times l}$ has to be also symmetric.

Our natural estimators of ν can be effectively expressed by means of projectors:

$\widetilde{\sigma}^2(X) = \frac{1}{n-k-l}\, \|MX\|^2$, where M is $P_{\mathscr{L}^{\perp}(F,\, V)}$.
$\widetilde{\sigma}_j^2(X) = \widetilde{y}_j^{\,2}(X);\ j = 1, 2, \ldots, l$, where $V\widetilde{y}(X) = P_{\mathscr{L}(V),\, \mathscr{L}^{\perp}(M_F V)}X$.

The first expression for $\widetilde{\sigma}^2(X)$ is the standard result of the unbiased variance estimation in classical linear regression models (Štulajter 2002). Concerning $\widetilde{\sigma}_j^2(X)$, if H denotes matrix VT, then it is obvious from properties of V and from expression (2.7) for T that $H^2 = H$, $\mathscr{L}(H) = \mathscr{L}(V)$, $\mathscr{N}(H) = \mathscr{N}(T) = \mathscr{N}(V'M_F) = \mathscr{L}^{\perp}(M_F V)$.

[4] There exist two standard forms of inverses for given block matrix, which are mathematically equivalent. We have chosen the form providing simpler algebraic expressions.

Then from basic properties of oblique projectors we know that every idempotent matrix H is the oblique projector $P_{\mathscr{L}(H),\,\mathscr{N}(H)}$, which means that $H = P_{\mathscr{L}(V),\,\mathscr{L}^{\perp}(M_F V)}$.

3 Statistical properties of natural estimators

3.1 First and second moment properties

As we mentioned above, the expressions of natural estimators through projectors give us a powerful tool in understanding and elegant proving properties of matrices T and M, which determine statistical properties of the estimators. It is easy to show next lemma:

Lemma 3.1 (basic properties of T and M)

(i) $TT' = W^{-1}$ *and* $r(T) = l$
(ii) $TF = 0$, $TV = I_l$ *and* $(VT)^2 = VT$
(iii) $T\Sigma_\nu T' = \sigma^2 W^{-1} + diag(\sigma_j^2)$
(iv) $[M_F(VT)]' = M_F(VT)$
(v) $M^2 = M$, $M' = M$, $tr(M) = n - k - l$
(vi) $M\,(F\;\;V) = 0$ *and* $TM = 0$
(vii) $M\Sigma_\nu = \sigma^2 M$
(viii) $M = M_F - M_F VT$

Proof (i) Employing (2.7), $M_F^2 = M_F$, $M_F' = M_F$ and symmetry of $W = V'M_F V$ we can write $TT' = W^{-1}V'M_F(W^{-1}V'M_F)' = W^{-1}$. Since $r(T) = r(TT')$, we conclude that $r(T) = r(W^{-1}) = l$.

(ii) According to the standard properties of oblique projectors (Galántai 2003) projector $P_{\mathscr{L}(V),\,\mathscr{L}^{\perp}(M_F V)} = VT$ immediately gives $VTv_j = v_j$ and $VTf_i = 0$, where v_j and f_i are columns of V and F. It implies $VTV = V$, $VTF = 0$. Hence first two properties of (ii) are results of multiplying the equalities on the left by a left inverse to the full column rank V. The last property is simply a restatement of projector idempotentness.

(iii) Applying (i), (ii) and the expression for Σ_ν from (1.2)

$$T\Sigma_\nu T' = \sigma^2 TT' + \sum_{j=1}^{l} \sigma_j^2 T v_j\, v_j' T' = \sigma^2 W^{-1} + \sum_{j=1}^{l} \sigma_j^2 e_j\, e_j',$$

where e_j denotes the jth unit vector with unity for its jth element and zeros elsewhere. Since the last term is only another form of $diag(\sigma_j^2)$, (iii) is valid.

(iv) This property can be reached by a direct routine computation.

In a very similar way using properties of orthogonal projectors we can prove the basic properties (v)–(viii) dealing with matrix M. □

The natural estimators of ν can be written as quadratic forms

$\widetilde{\sigma}^2(X) = \frac{1}{n-k-l}(MX)'(MX) = \frac{1}{n-k-l}X'MX$,
$\widetilde{\sigma}_j^2(X) = (t_j'X)^2 = X't_j t_j'X$, $j = 1, 2, \ldots, l$, where t_j' are rows of T,

so results $MF = 0$ and $TF = 0$ from Lemma 3.1 lead to conclusion that natural estimators are invariant quadratic estimators.[5]

In the following theorem we summarize mean and covariance characteristics of natural estimators.

Theorem 3.1 *Natural estimators of* ν *have the following properties:*

(i) $E_\nu[\widetilde{\sigma}^2(X)] = \sigma^2$ *and* $E_\nu[\widetilde{\sigma}_j^2(X)] = \sigma_j^2 + \sigma^2(W^{-1})_{jj}$; $j = 1, 2, \ldots, l$.

If $X \sim N_n(F\beta, \Sigma)$*, then*

(ii) $D_\nu[\widetilde{\sigma}^2(X)] = \frac{2\sigma^4}{n-k-l}$ *and* $Cov_\nu[\widetilde{\sigma}^2(X), \widetilde{\sigma}_j^2(X)] = 0$; $j = 1, 2, \ldots, l$,

(iii) $D_\nu[\widetilde{\sigma}_j^2(X)] = 2[\sigma_j^2 + \sigma^2(W^{-1})_{jj}]^2$; $j = 1, 2, \ldots, l$,

(iv) $Cov_\nu[\widetilde{\sigma}_i^2(X), \widetilde{\sigma}_j^2(X)] = 2[\sigma^2(W^{-1})_{ij}]^2$; $i, j = 1, 2, \ldots, l, i \neq j$.

(v) $\mathrm{MSE}_\nu[\widetilde{\sigma}_j^2(X)] = 2[\sigma_j^2 + \sigma^2(W^{-1})_{jj}]^2 + \sigma^4(W^{-1})_{jj}^2$; $j = 1, 2, \ldots, l$.

Proof Since used arguments are very similar in proofs of items (i)–(iv) we show only proofs of (i) and (iv). Applying previous results with the aid of well-known expressions for mean values and covariances of invariant quadratic estimators (see, e.g. Christensen 2002) $E_\nu(X'AX) = tr(A\Sigma_\nu)$ and if $X \sim N(F\beta, \Sigma_\nu)$, then $Cov_\nu(X'AX, X'BX) = 2tr(A\Sigma_\nu B\Sigma_\nu)$, we find

(i)

$$\begin{aligned} E_\nu[\widetilde{\sigma}_j^2(X)] &= tr(t_j t_j' \Sigma_\nu) = tr(t_j' \Sigma_\nu t_j) = t_j' \Sigma_\nu t_j \\ &= (T\Sigma_\nu T')_{jj} = \sigma_j^2 + \sigma^2(W^{-1})_{jj} \\ E_\nu[\widetilde{\sigma}^2(X)] &= \frac{1}{n-k-l} tr(M\Sigma_\nu) = \frac{\sigma^2}{n-k-l} tr(M) = \sigma^2 \end{aligned}$$

(iv)

$$\begin{aligned} Cov_\nu[\widetilde{\sigma}_i^2(X), \widetilde{\sigma}_j^2(X)] &= 2tr(t_i t_i' \Sigma_\nu t_j t_j' \Sigma_\nu) = 2tr(t_i' \Sigma_\nu t_j t_j' \Sigma_\nu t_i) \\ &= 2(T\Sigma_\nu T')_{ij}(T\Sigma_\nu T')_{ji} = 2(\sigma^2(W^{-1})_{ij})^2. \end{aligned}$$

The last assertion (v) is a trivial consequence of (i), (iii) and the well-known general expression $\mathrm{MSE}(\widetilde{\sigma}_j^2) = D(\widetilde{\sigma}_j^2) + [E(\widetilde{\sigma}_j^2) - \sigma_j^2]^2$ for the mean squared error (MSE) defined as $E[\widetilde{\sigma}_j^2 - \sigma_j^2]^2$. □

Obtained results show that unlike modified DOOLSE estimators used in orthogonal FDSLRM's, our natural estimators $\widetilde{\nu}(X) = (\widetilde{\sigma}^2(X), \widetilde{\sigma}_1^2(X), \ldots, \widetilde{\sigma}_l^2(X))'$ of ν with the exception $\widetilde{\sigma}^2(X)$ are *biased* and *not consistent* and a bias is determined by diagonal elements of the inverse of the Schur complement $W = V'V - V'F(F'F)^{-1}F'V = (V'M_F V) \in \mathbb{E}^{l \times l}$ of $F'F$ in Gram matrix $G = \begin{pmatrix} F'F & F'V \\ V'F & V'V \end{pmatrix}$ for linear regression model

[5] We recall that if X satisfies a linear regression model with $E_\beta(X) = F\beta$ as it is in case of the FDSLRM observation, then quadratic form $X'AX$ is called *invariant quadratic estimator* (with respect to β), if $AF = 0$, which means that such quadratic form does not depend on the mean value parameter β. Many authors (e.g. Searle et al. 1992; Christensen 2002) also call such estimator the *translation invariant* estimator.

(2.1). The consistent and unbiased estimator is only estimator $\widetilde{\sigma}^2(X)$ of σ^2, which is also uncorrelated with remaining estimators.

Generally it is clear that if we have only data x, one realization of a finite length n of a time series $X(.)$ given by the FDSLRM, then for every $j = 1, 2, \ldots, l$ we have only one realization y_j of the random variable Y_j, whose square in practice is never equal to σ_j^2, so it is impossible to find a consistent estimator of the unknown variance $\sigma_j^2 = E_\nu[Y_j^2]$ based only on one value (estimate) of the random variable Y_j. The same reason causes that in an orthogonal FDSLRM the DOOLSE $\hat{\nu}(X)$ used by Štulajter and Witkovský (2004) is also not a consistent estimator of ν. In general, in any FDSLRM there is no consistent estimator of the variances parameter ν.

From the viewpoint of the criteria-based methodology of quadratic estimators, described, e.g. in Searle et al. (1992), which is based on three main criteria—unbiasedness, invariance, minimum variance (or mean squared error)—our natural estimators $\widetilde{\sigma}_j^2(X)$; $j = 1, \ldots, l$ belong to the LaMotte class C_2 of invariant quadratic estimators. It is not difficult to see that our natural estimators are not the best in C_2 with respect to the minimum MSE criterion,[6] because we can consider estimators $\hat{\sigma}_j^2(X) = \widetilde{\sigma}_j^2(X) - (W^{-1})_{jj}\widetilde{\sigma}^2(X)$, which according to results of Lemma 3.1 and Theorem 3.1 are invariant and unbiased with $\mathrm{MSE}[\hat{\sigma}_j^2(X)] = D[\widetilde{\sigma}_j^2(X)] + 2\sigma^4(W^{-1})_{jj}^2/(n-k-l)$ and which clearly have MSE's equal to MSE's of corresponding $\widetilde{\sigma}_j^2(X)$ for $n = k+l-2$ and smaller MSE's for $n > k + l + 2$.

Because modified estimators $\hat{\sigma}_j^2(X)$ are simultaneously in the LaMotte class C_4 of invariant unbiased quadratic estimators, our natural estimators must have bigger MSE's then the well-known MINQUE at $\nu = (\sigma^2, \sigma_1^2, \ldots, \sigma_l^2)$—the best estimators in the LaMotte class C_4.

However, since computation of MINQUE estimators involves some pre-assigned value ν_0 of ν, which in practice is again never equal to the unknown ν, MINQUE are best at ν_0 and not necessarily best at ν. In such case for general FDSLRM our natural estimators could have smaller MSE's than MINQUE for ν_0, but this question is not yet resolved and now it is an open problem. Moreover our natural estimators have much simpler form and way of computation (giving always non-negative estimates) than MINQUE.

Finally it is worthwhile to notice that although the mentioned modified estimators $\hat{\sigma}_j^2(X)$ possess unbiasedness, from our perspective they do not become very important, since they do not guarantee non-negativity of estimates (similarly like MINQUE; or Štulajter–Witkovský's DOOLSE estimators).

3.2 Further asymptotic properties

Now we will find an appropriate condition of asymptotic unbiasedness. Let symbol X_n denote the finite observation X of time series $X(.)$, if that observation has size $n \times 1$.

[6] We remind that an estimator $\overset{*}{\sigma}{}_j^2(X)$ of σ_j^2 is called the best at ν in some class C, if it has the least MSE among all estimators of σ_j^2 from C (see also LaMotte 1973).

Then natural estimators of ν, matrices F, V, W and G also depend on n, so that we will use the more specific notation $\widetilde{\nu}(X) = \widetilde{\nu}(X_n)$, $F = F_n$, $V = V_n$, $W = W_n$, $G = G_n$.

If we apply the concept of the order $O(1/n)$ of a real matrix sequence[7] to the sequence of inverses of the Schur complements W_n and combine it with the well-known fact for any matrix sequence $\{A_n\}$: $\lim_{n\to\infty} A_n = 0 \in \mathbb{E}^{r\times s}$, if $A_n = O(1/n)$, then Theorem 3.1 yields the following result showing a sufficiency for asymptotic unbiasedness of $\sigma_j^2(X_n)$ and corresponding asymptotic second-order properties in case of normality of observation X_n.

Theorem 3.2 *Let us consider a general FDSLRM*

$$X_n = F_n\beta + \varepsilon_n,\ E(\varepsilon_n) = 0,\ Cov_\nu(\varepsilon_n) = \Sigma_n = \sigma^2 I + \sum_{j=1}^{l} \sigma_j^2 v_{n,j} v_{n,j}',$$

where $v_{n,j}$; $j = 1, 2, \ldots, l$ are columns of V_n and $\begin{pmatrix} F_n & V_n \end{pmatrix} \in \mathbb{E}^{n\times(k+l)}$ are of full rank. Let $W_n^{-1} = O(1/n)$, where $W_n \in \mathbb{E}^{l\times l}$ are Schur complements of $(F_n'F_n)$ in the $(k+l)\times(k+l)$ partitioned Gram matrices $G_n = \begin{pmatrix} F_n'F_n & F_n'V_n \\ V_n'F_n & V_n'V_n \end{pmatrix}$. Then natural estimators $\widetilde{\sigma}_j^2(X_n)$ of variances σ_j^2; $j = 1, 2, \ldots, l$ are:

(i) *asymptotically unbiased, i.e.* $\lim_{n\to\infty} E[\widetilde{\sigma}_j^2(X_n)] = \sigma_j^2$.

If $X_n \sim N_n(F_n\beta, \Sigma_n)$, then the estimators are also

(i) *mutually asymptotically uncorrelated, i.e.* $\lim_{n\to\infty} Cov[\widetilde{\sigma}_i^2(X_n), \widetilde{\sigma}_j^2(X_n)] = 0$ *for $i \neq j$; $i, j = 1, 2, \ldots, l$*

(ii) *with asymptotic dispersions $2\sigma_j^4$, i.e.* $\lim_{n\to\infty} D[\widetilde{\sigma}_j^2(X_n)] = 2\sigma_j^4$.

4 Illustrations

In the following we briefly illustrate theoretical results obtained in previous sections. Our concern is primarily to show different forms of Schur complements which play the central role in establishing properties of natural estimators.

Example 4.1 Let $X(.)$ be a time series given by the model

$$X(t) = \beta_1 + Y_1 t + w(t);\ t = 1, 2, \ldots$$

It means that the FDSLRM has the mean value as an unknown constant and the errors are given by a random linear trend plus a white noise term.

The corresponding model of FDSLRM observation (1.2) has the form $X = F\beta + \varepsilon$; $E[\varepsilon] = 0$, $Cov_\nu(X) = \sigma^2 I + \sigma_1^2 v_1 v_1'$, where $F = (1, 1, \ldots, 1)' \equiv j_n$, $V = v_1 = (1, 2, \ldots, n)'$. Then we get $M_F = I - F(F'F)^{-1}F = I_n - \frac{1}{n}J_n = C_n$,

[7] A sequence $\{A_n\}$ of $r \times s$ matrices is said to be of the order $O(1/n)$, if for any fixed pair of i and $j (i = 1, .., r;\ j = 1, \ldots, s)$ a real sequence $\left\{\left|(A_n)_{ij}/(1/n)\right|\right\}$ formed by matrix elements $(A_n)_{ij}$ is bounded. In such case we write $A_n = O(1/n)$.

where $J_n = j_n j_n'$ is a matrix whose every element is unity and C_n is the well-known *centering matrix*.[8]

After that a routine computation with the aid of the properties of C_n leads to $W_n = v_1' v_1 - n\bar{v}_1^2 = (n^3 - n)/12$, $T = t_1' = W_n^{-1}(v_1' - \bar{v}_1 j_n')$, $M = M_F - M_F V T = C_n - W_n^{-1}(v_1 - \bar{v}_1 j_n)(v_1' - \bar{v}_1 j_n')$, where $\bar{v}_1 = 1/n \sum_{t=1}^{n} t = n(n+1)/2$ and $v_1' v_1 = \|v_1\|^2 = \sum_{t=1}^{n} t^2$. Inverses $W_n^{-1} = 12/(n^3 - n) = O(1/n)$, therefore $\widetilde{\sigma}_1^2(X)$ is an asymptotically unbiased estimator with asymptotic covariance $2\sigma_1^4$. The $\widetilde{\sigma}_1^2(X)$ is given by

$$\widetilde{\sigma}_1^2(X) = \left(\tfrac{12}{n^3-n}\right)^2 \sum_{s=1}^{n}\sum_{t=1}^{n} \left(s - \tfrac{n+1}{2}\right)\left(t - \tfrac{n+1}{2}\right) X(s)X(t)$$

and is uncorrelated with the consistent unbiased estimator $\widetilde{\sigma}^2(X)$ with $D_\nu[\widetilde{\sigma}^2(X)] = \frac{2\sigma^4}{n-2}$, whose explicit form after calculating elements of M is

$$\widetilde{\sigma}^2(X) = \tfrac{1}{n-2}\left(\sum_{t=1}^{n} X(t)^2 - \sum_{s=1}^{n}\sum_{t=1}^{n}\left[\tfrac{1}{n} + \tfrac{12}{n^3-n}\left(s - \tfrac{n+1}{2}\right)\left(t - \tfrac{n+1}{2}\right)\right] X(s)X(t)\right).$$

Example 4.2 Let $X(.)$ be a time series given by the model

$$X(t) = \beta_1 + \beta_2 t + Y_1 \cos\lambda t + Y_2 \sin\lambda t + w(t);\ t = 1, 2, \ldots,$$

where $\lambda \in \langle 0, \pi\rangle$ is some non-fourier frequency and Y_1, Y_2 are uncorrelated random variables with zero mean values and variances $\sigma_j^2 = D[Y_j]$; $j = 1, 2$. Since in this case we have

$$F = (f_1\ f_2) = \begin{pmatrix} 1 & 1 & \ldots & 1 \\ 1 & 2 & \ldots & n \end{pmatrix}',$$

$$V = (v_1\ v_2) = \begin{pmatrix} \cos\lambda & \cos 2\lambda & \ldots & \cos n\lambda \\ \sin\lambda & \sin 2\lambda & \ldots & \sin n\lambda \end{pmatrix}',$$

the orthogonal projection matrix M_F onto $\mathscr{L}^\perp(F)$ is identical with orthogonal projection matrix M onto $\mathscr{L}^\perp(F, V)$ in the previous example. The only difference are other symbols. The role of column v_1 takes column f_2, so

$$M_F = C_n - (f_2' f_2 - n\bar{f}_2^2)(f_2 - \bar{f}_2 j_n)(f_2' - \bar{f}_2 j_n').$$

[8] The centering matrix has these elementary properties: $C_n' = C_n$, $C_n^2 = C_n$, $C_n J_n = J_n C_n = 0$, $C_n x = x - \bar{x} j_n$, $x' C_n y = x'y - n\bar{x}\bar{y}$; $x, y \in E^n$.

This expression yields to 2×2 inverse of the Schur complement W_n^{-1} given by expression

$$W_n^{-1} = \frac{1}{D_n} \begin{pmatrix} (W_n)_{22} & -(W_n)_{12} \\ -(W_n)_{12} & (W_n)_{11} \end{pmatrix}; \, D_n = (W_n)_{11}(W_n)_{22} - (W_n)_{12}^2,$$

where

$$(W_n)_{11} = \sum_{t=1}^{n} \cos^2 \lambda t - \tfrac{1}{n} \left(\sum_{t=1}^{n} \cos \lambda t \right)^2 - \tfrac{12}{n^3-n} \left[\sum_{t=1}^{n} \left(t - \tfrac{n+1}{2}\right) \cos \lambda t \right]^2,$$

$$(W_n)_{22} = \sum_{t=1}^{n} \sin^2 \lambda t - \tfrac{1}{n} \left(\sum_{t=1}^{n} \sin \lambda t \right)^2 - \tfrac{12}{n^3-n} \left[\sum_{t=1}^{n} \left(t - \tfrac{n+1}{2}\right) \sin \lambda t \right]^2,$$

$$(W_n)_{12} = \sum_{t=1}^{n} \cos \lambda t \sin \lambda t - \tfrac{1}{n} \sum_{t=1}^{n} \cos \lambda t \sum_{t=1}^{n} \sin \lambda t -$$

$$- \tfrac{12}{n^3-n} \sum_{t=1}^{n} \left(t - \tfrac{n+1}{2}\right) \cos \lambda t \, \cdot \sum_{t=1}^{n} \left(t - \tfrac{n+1}{2}\right) \sin \lambda t.$$

By boundedness of trigonometric functions and the well-known trigonometric identities we can derive for W_n elements that $(W_n)_{11} = O(n)$, $(W_n)_{22} = O(n)$, $(W_n)_{12} = O(1)$, $D_n = O(n^2)$, which means that matrix sequence $\left\{W_n^{-1}\right\}$ is of the order $O(1/n)$, so our natural estimators $\widetilde{\sigma}_j^2(X)$; $j = 1, 2$ are again asymptotically unbiased with asymptotic dispersions $2\sigma_j^2$. They also become mutually asymptotically uncorrelated.

Remark 4.1 Finally we remark that our sufficient condition for asymptotic unbiasedness holds in many other types of FDSLRM. In orthogonal FDSLRM's it is equivalent with condition: $\left\| v_j \right\|^2$ is of $O(n)$ for all j, and it is fulfilled e.g. in the very useful FDSLRM with harmonic regressors containing Fourier frequencies (see the model in Štulajter 2007). The fact that the considered condition does not always hold in every FDSLRM can be demonstrated e.g. in the model

$$X(t) = \beta_1 + \beta_2 \ln t + Y_1 \exp(-\gamma_1 t) + Y_2 \exp(-\gamma_2 t) + w(t); \, t = 1, 2, \ldots, n$$

with $\gamma_1, \gamma_2 \in (0, \infty)$, $\gamma_1 \neq \gamma_2$, where applying the same argument and way of calculations as in Example 4.2, we can prove that W_n^{-1} is of the order $O(1)$.

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