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Corrections of Estimators in Linearized Models *

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Abstract

Nonlinear regression models have been frequently linearized, since standard estimators in linear models are simple. However these estimators in linearized models are more or less influenced by a nonlinearity of the model. Relatively simple corrections suppresing this influence in the case that the nonlinearity is low are presented in the paper.

Key words: Nonlinear regression model, Bates and Watts measures of nonlinearity, linearization.

1991 Mathematics Subject Classification: 62J05, 62F10

1 Introduction

Let **Y** be an *n*-dimensional random vector with the mean value $E(\mathbf{Y}|\boldsymbol{\beta}) = \mathbf{f}(\boldsymbol{\beta})$, $\boldsymbol{\beta} \in \mathbb{R}^k$ (k-dimensional linear real space) and with the covariance matrix $\boldsymbol{\Sigma}$; the vector function $\mathbf{f}(\boldsymbol{\beta}) = (f_1(\boldsymbol{\beta}), \dots, f_n(\boldsymbol{\beta}))', \boldsymbol{\beta} \in \mathbb{R}^k$, possesses continuous second derivatives. Let such an approximate value $\boldsymbol{\beta}_0$ of the actual value $\boldsymbol{\beta}^*$ of the parameter $\boldsymbol{\beta}$ be given that

$$\mathbf{f}(\boldsymbol{\beta}^*) = \mathbf{f}_0 + \mathbf{F}\delta\boldsymbol{\beta} + (1/2)\boldsymbol{\kappa}_{\delta\beta}$$
(1.1)

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is sufficiently good approximation of the actual value $f(\beta^*)$; here

$$\beta^* = \beta_0 + \delta\beta, \quad \mathbf{f}_0 = \mathbf{f}(\beta_0),$$
$$\{\mathbf{F}\}_{i,j} = \partial f_i(\beta) / \partial \beta_j |_{\beta = \beta_0}, \quad i = 1, \dots, n, \quad j = 1, \dots, k,$$
$$\kappa_{\delta\beta} = (\delta\beta' \mathbf{H}_1 \delta\beta, \dots, \delta\beta' \mathbf{H}_n \delta\beta)',$$

and

$$\mathbf{H}_i = \partial^2 f_i(\boldsymbol{\beta}) / (\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}')|_{\boldsymbol{\beta} = \boldsymbol{\beta}_0}, \quad i = 1, \dots, n.$$

If Y is normally distributed, the linearized model is

$$\mathbf{Y} - \mathbf{f}_0 \sim N_n(\mathbf{F}\delta\boldsymbol{\beta}, \boldsymbol{\Sigma}), \quad \delta\boldsymbol{\beta} \in R^k.$$
(1.2)

Of course, this model is not totally adequate to reality. Nevertheless it has been used frequently in practice. The BLUE (best linear unbiased estimators) of β is influenced by the neglected terms in the Taylor series (1.1) and the same is valid for the estimator $\hat{\sigma}^2$ of the parameter σ^2 in the case $\Sigma = \sigma^2 \mathbf{V}$, where \mathbf{V} is a given matrix.

How to correct estimators in the linearized model or how to decise whether these corrections are necessary is the aim of the paper.

The paper is based mainly on [1], [2], [3], [4], [5], [6], [7] and [9].

Assumption Let the rank $r(\mathbf{F})$ of the matrix \mathbf{F} be k < n and let the matrix Σ and \mathbf{V} , respectively, be positive definite.

2 Auxiliary statements

The sequence of the following lemmas is either commonly known or it can be easily proved. That is why they are given without proofs.

Lemma 2.1 The BLUE of β in (1.2) is

$$\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}_0 + (\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F})^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(\mathbf{Y} - \mathbf{f}_0) = \boldsymbol{\beta}_0 + (\mathbf{F}'\mathbf{V}^{-1}\mathbf{F})^{-1}\mathbf{F}'\mathbf{V}^{-1}(\mathbf{Y} - \mathbf{f}_0)$$

and its covariance matrix is

$$\operatorname{Var}(\hat{\boldsymbol{\beta}}) = (\mathbf{F}' \boldsymbol{\Sigma}^{-1} \mathbf{F})^{-1} = \sigma^2 (\mathbf{F}' \mathbf{V}^{-1} \mathbf{F})^{-1}.$$

Let \mathbf{A}^+ denote the Moore-Penrose generalized inverse of the matrix \mathbf{A} ; i.e.

$$\mathbf{A} = \mathbf{A}\mathbf{A}^{+}\mathbf{A}, \quad \mathbf{A}^{+}\mathbf{A}\mathbf{A}^{+} = \mathbf{A}^{+}, \quad \mathbf{A}\mathbf{A}^{+} = (\mathbf{A}\mathbf{A}^{+})', \quad \mathbf{A}^{+}\mathbf{A} = (\mathbf{A}^{+}\mathbf{A})'$$

(in more detail cf. [8]).

Lemma 2.2 If $\Sigma = \sigma^2 V$, where V is a given matrix, then the best unbiased estimator of σ^2 in (1.2) is

$$\hat{\sigma}^2 = (\mathbf{Y} - \mathbf{f}_0)'(\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ (\mathbf{Y} - \mathbf{f}_0)/(n-k),$$

where $\mathbf{M}_F = \mathbf{I} - \mathbf{F}\mathbf{F}^+$.

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Lemma 2.3 The estimator $\hat{\sigma}^2$ is under the model (1.2) distributed as

$$\sigma^2 \chi^2_{n-k}(0)/(n-k),$$

where $\chi^2_{n-k}(0)$ is the random variable possessing the central chi-square distribution with n-k degrees of freedom.

Lemma 2.4 Let $\chi_f^2(\delta)$ be the random variable possessing the noncentral chisquare distribution with f degrees of freedom and with the parameter noncentrality equal to δ . Then

$$E(\chi_f^2(\delta)) = f + \delta, \quad \operatorname{Var}(\chi_f^2(\delta)) = 2f + 4\delta.$$

Lemma 2.5 Let $\mathbf{Y} \sim N_k(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and let $\mathbf{A} = \mathbf{A}'$ be such a matrix that $\mathbf{Y}' \mathbf{A} \mathbf{Y} \sim \chi_f^2(\delta)$. Then $\delta = \boldsymbol{\mu}' \mathbf{A} \boldsymbol{\mu}$.

Lemma 2.6 Let $\mathbf{Y} \sim N_k(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and let $\mathbf{A} = \mathbf{A}'$ and $\mathbf{B} = \mathbf{B}'$, respectively, be $k \times k$ matrices and \mathbf{a} a k-dimensional vector, then

$$cov(\mathbf{a'Y}, \mathbf{Y'AY}) = 2\mathbf{a'\Sigma}\mathbf{A}\boldsymbol{\mu},$$

$$cov(\mathbf{Y'AY}, \mathbf{Y'BY}) = 2Tr(\mathbf{A\Sigma}\mathbf{B\Sigma}) + 4\boldsymbol{\mu'}\mathbf{A\Sigma}\mathbf{B}\boldsymbol{\mu},$$

$$Var(\mathbf{a'Y} + \mathbf{Y'AY}) = \mathbf{a'\Sigma}\mathbf{a} + 4\mathbf{a'\Sigma}\mathbf{A}\boldsymbol{\mu} + 2Tr(\mathbf{A\Sigma}\mathbf{B\Sigma}) + 4\boldsymbol{\mu'}\mathbf{A\Sigma}\mathbf{B}\boldsymbol{\mu}.$$

In the following $\mathbf{C} = \mathbf{F}' \boldsymbol{\Sigma}^{-1} \mathbf{F}$ and $\mathbf{C}_0 = \mathbf{F}' \mathbf{V}^{-1} \mathbf{F}$.

Definition 2.7 The Bates and Watts [1] parametric measure of a nonlinearity in the model (1.1) at the point β_0 is

$$K^{(par)}(\boldsymbol{\beta}_0) = \sup\left\{\frac{\sqrt{\boldsymbol{\kappa}_{\delta\beta}'(\mathbf{P}_F^{\Sigma^{-1}})'\boldsymbol{\Sigma}^{-1}\mathbf{P}_F^{\Sigma^{-1}}\boldsymbol{\kappa}_{\delta\beta}}}{\mathbf{s}'\mathbf{C}\mathbf{s}} : \mathbf{s} \in R^k\right\}.$$

Since $(\mathbf{P}_F^{\Sigma^{-1}})' \mathbf{\Sigma}^{-1} \mathbf{P}_F^{\Sigma^{-1}} = \mathbf{\Sigma}^{-1} \mathbf{F} \mathbf{C}^{-1} \mathbf{F}' \mathbf{\Sigma}^{-1} = (1/\sigma^2) \mathbf{V}^{-1} \mathbf{F} \mathbf{C}_0^{-1} \mathbf{F}' \mathbf{V}^{-1}$ we are

$$K^{(par)}(\boldsymbol{\beta}_{0}) = \sigma sup \left\{ \frac{\sqrt{\boldsymbol{\kappa}_{s}' \mathbf{V}^{-1} \mathbf{F} \mathbf{C}_{0}^{-1} \mathbf{F}' \mathbf{V}^{-1} \boldsymbol{\kappa}_{s}}}{\mathbf{s}' \mathbf{C}_{0} \mathbf{s}} : \mathbf{s} \in \mathbb{R}^{k} \right\}$$
$$= \sigma K_{0}^{(par)}(\boldsymbol{\beta}_{0}).$$

The Bates and Watts intrinsic measure of a nonlinearity in the model (1.1) at the point β_0 is

$$K^{(int)}(\boldsymbol{\beta}_0) = \sup\left\{\frac{\sqrt{\boldsymbol{\kappa}_{\delta\beta}'(\mathbf{M}_F^{\Sigma^{-1}})'\boldsymbol{\Sigma}^{-1}\mathbf{M}_F^{\Sigma^{-1}}\boldsymbol{\kappa}_{\delta\beta}}}{\mathbf{s}'\mathbf{C}\mathbf{s}} : \mathbf{s} \in \mathbb{R}^k\right\}.$$

Since

$$(\mathbf{M}_F^{\Sigma^{-1}})' \Sigma^{-1} \mathbf{M}_F^{\Sigma^{-1}} = (\mathbf{M}_F \Sigma \mathbf{M}_F)^+, \Sigma = \sigma^2 \mathbf{V}$$

and

$$(\mathbf{M}_F \mathbf{\Sigma} \mathbf{M}_F)^+ = (1/\sigma^2)(\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+,$$

we have

$$K^{(int)}(\boldsymbol{\beta}_0) = \sigma sup \left\{ \frac{\sqrt{\boldsymbol{\kappa}_s'(\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \boldsymbol{\kappa}_s}}{\mathbf{s}' \mathbf{C}_0 \mathbf{s}} : \mathbf{s} \in R^k \right\} = \sigma K_0^{(int)}(\boldsymbol{\beta}_0).$$

3 Estimator of β

The estimator $\hat{\beta}$ from Lemma 2.1 is not unbiased under the model (1.1). Its bias is obviously

$$\mathbf{b} = E(\hat{\boldsymbol{\beta}}) - \boldsymbol{\beta} = E(\delta\hat{\boldsymbol{\beta}}) - \delta\boldsymbol{\beta} = \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(1/2)\boldsymbol{\kappa}_{\delta\beta} = \mathbf{C}_0^{-1}\mathbf{F}'\mathbf{V}^{-1}(1/2)\boldsymbol{\kappa}_{\delta\beta}$$

(i.e. the bias is the quantity of the second order in $\delta\beta$).

It seems to be the most natural to correct the estimator $\delta \hat{\beta}$ by a random vector $-\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(1/2)\hat{\kappa}_{\delta\beta}$, where $\hat{\kappa}_{\delta\beta}$ is a simple unbiased estimator of $\kappa_{\delta\beta}$.

Lemma 3.1

(i)
$$E(\boldsymbol{\kappa}_{\hat{\delta\beta}}) = \boldsymbol{\kappa}_{\delta\beta} + 4\Delta \mathbf{b} + \boldsymbol{\kappa}_{b} + \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}^{-1}) \end{pmatrix},$$

where

$$\boldsymbol{\Delta} = (1/2) \begin{pmatrix} \delta \boldsymbol{\beta}' \mathbf{H}_1 \\ \vdots \\ \delta \boldsymbol{\beta}' \mathbf{H}_n \end{pmatrix} \quad and \quad \mathbf{b} = \mathbf{C}^{-1} \mathbf{F}' \boldsymbol{\Sigma}^{-1} (1/2) \boldsymbol{\kappa}_{\delta \boldsymbol{\beta}}.$$

(*ii*)
$$\operatorname{Var}(\boldsymbol{\kappa}_{\hat{\boldsymbol{\delta}}\hat{\boldsymbol{\theta}}}) = 2\mathbf{S}_{C^{-1}} + 4\mathbf{W},$$

where

$$\{ \mathbf{S}_{C^{-1}} \}_{i,j} = Tr(\mathbf{H}_i \mathbf{C}^{-1} \mathbf{H}_j \mathbf{C}^{-1}), \quad i, j = 1, \dots, n, \\ \{ \mathbf{W} \}_{i,j} = \delta \boldsymbol{\beta}' \mathbf{H}_i \mathbf{C}^{-1} \mathbf{H}_j \delta \boldsymbol{\beta}, \quad i, j = 1, \dots, n.$$

Proof (i) is a direct consequence of the equality

$$E(\delta\hat{\boldsymbol{\beta}}'\mathbf{H}_{i}\delta\hat{\boldsymbol{\beta}}) = E(\delta\hat{\boldsymbol{\beta}}')\mathbf{H}_{i}E(\delta\hat{\boldsymbol{\beta}}) + Tr[\mathbf{H}_{i}\operatorname{Var}(\delta\hat{\boldsymbol{\beta}})]$$

= $(\delta\boldsymbol{\beta} + \mathbf{b})'\mathbf{H}_{i}(\delta\boldsymbol{\beta} + \mathbf{b}) + Tr(\mathbf{H}_{i}\mathbf{C}^{-1}).$

(ii) follows from Lemma 2.6.

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Remark 3.2 If $\hat{\kappa}_{\delta\beta}$ is chosen in the form

$$\hat{\boldsymbol{\kappa}}_{\delta\beta} = \boldsymbol{\kappa}_{\delta\hat{\beta}} - \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}^{-1}) \end{pmatrix},$$

it is unbiased when the term $4\Delta \mathbf{b}$ (of the third order in $\delta\beta$) and the term κ_b (of the fourth order in $\delta\beta$) are neglected. Since $\hat{\kappa}_{\delta\beta}$ is simple, it seems to be reasonable to use it for a correction.

In [5] and attempt was made to find the locally best quadratic estimator of β . Its form is not so simple as the estimator

$$\delta \tilde{\boldsymbol{\beta}} = \delta \hat{\boldsymbol{\beta}} - (1/2) \mathbf{C}^{-1} \mathbf{F}' \boldsymbol{\Sigma}^{-1} \left[\boldsymbol{\kappa}_{\delta \hat{\boldsymbol{\beta}}} - \begin{pmatrix} Tr(\mathbf{H}_{1} \mathbf{C}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n} \mathbf{C}^{-1}) \end{pmatrix} \right]$$
(3.1)

and the difference of the covariance matrices seems not to be essentially different from the zero matrix (in more detail cf. [5]).

Theorem 3.3 The mean value of the estimator (3.1) is

$$E(\delta \tilde{\boldsymbol{\beta}}) = \delta \boldsymbol{\beta} - (1/2) \mathbf{C}^{-1} \mathbf{F}' \mathbf{\Sigma}^{-1} (4 \Delta \mathbf{b} + \boldsymbol{\kappa}_b)$$

(i.e. the bias is of the third order in $\delta\beta$) and its covariance matrix is

$$\begin{aligned} \operatorname{Var}(\delta\tilde{\boldsymbol{\beta}}) &= \mathbf{C}^{-1} + (1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{S}_{C^{-1}}\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} \\ &- \mathbf{C}^{-1}(\mathbf{H}_{1}\delta\boldsymbol{\beta},\ldots,\mathbf{H}_{n}\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} \\ &- \mathbf{C}^{-1}(\mathbf{H}_{1}\mathbf{b},\ldots,\mathbf{H}_{n}\mathbf{b})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} \\ &- \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}2\boldsymbol{\Delta}\mathbf{C}^{-1} - \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1} \begin{pmatrix} \mathbf{b}'\mathbf{H}_{1} \\ \vdots \\ \mathbf{b}'\mathbf{H}_{n} \end{pmatrix} \mathbf{C}^{-1} \\ &+ \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{W}\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}. \end{aligned}$$

Proof Ther first statement is a direct consequence of Lemma 3.1 and Remark 3.2. As far as the second statement is concerned, it follows from the relationships.

$$\begin{aligned} \operatorname{Var}(\delta\beta) &= \operatorname{Var}(\delta\beta) \\ &+ \operatorname{cov}\left(\delta\hat{\beta}, -(1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\left[\boldsymbol{\kappa}_{\delta\hat{\beta}} - \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}^{-1} \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}^{-1}) \end{pmatrix}\right]\right) \\ &+ \operatorname{cov}\left(-(1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\left[\boldsymbol{\kappa}_{\delta\hat{\beta}} - \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}^{-1} \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}^{-1}) \end{pmatrix}\right], \delta\hat{\beta} \right) \end{aligned}$$

+ Var
$$\left(-(1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1} \left[\boldsymbol{\kappa}_{\delta\hat{\beta}} - \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}^{-1}) \end{pmatrix} \right] \right),$$

where $\operatorname{Var}(\delta \hat{\boldsymbol{\beta}}) = \mathbf{C}^{-1}$.

With respect to Lemma 2.6

$$\operatorname{cov}(\delta\hat{\boldsymbol{\beta}},\delta\hat{\boldsymbol{\beta}}'\mathbf{H}_i\delta\hat{\boldsymbol{\beta}}) = 2\mathbf{C}^{-1}\mathbf{H}_i E(\delta\hat{\boldsymbol{\beta}}) = 2\mathbf{C}^{-1}\mathbf{H}_i\delta\boldsymbol{\beta} + 2\mathbf{C}^{-1}\mathbf{H}_i\mathbf{b}$$

and thus

$$\operatorname{cov}\left(\delta\hat{\boldsymbol{\beta}}, -(1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\left[\boldsymbol{\kappa}_{\delta\hat{\boldsymbol{\beta}}} - \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}^{-1} \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}^{-1}) \end{pmatrix}\right]\right)$$
$$= -\mathbf{C}^{-1}(\mathbf{H}_{1}\delta\boldsymbol{\beta}, \dots, \mathbf{H}_{n}\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} - \mathbf{C}^{-1}(\mathbf{H}_{1}\mathbf{b}, \dots, \mathbf{H}_{n}\mathbf{b})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}$$
$$= -2\mathbf{C}^{-1}\boldsymbol{\Delta}'\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} - \mathbf{C}^{-1}(\mathbf{H}_{1}\mathbf{b}, \dots, \mathbf{H}_{n}\mathbf{b})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}.$$

With respect to Lemma 3.1

$$\begin{aligned} \operatorname{Var}[-(1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\kappa}_{\delta\hat{\beta}}] &= \\ &= (1/4)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\operatorname{Var}(\boldsymbol{\kappa}_{\delta\hat{\beta}})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} \\ &= (1/4)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(2\mathbf{S}_{C^{-1}}+4\mathbf{W})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} \\ &= (1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{S}_{C^{-1}}\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} + \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{W}\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} \qquad \Box \end{aligned}$$

The effect of the correction of $\hat{\beta}$ can be judget by a comparison of the mean square error characteristics, i.e.

$$MSE(\hat{\boldsymbol{\beta}}) = \operatorname{Var}(\hat{\boldsymbol{\beta}}) + \mathbf{b}\mathbf{b}' = \mathbf{C}^{-1} + (1/4)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\kappa}_{\delta\beta}\boldsymbol{\kappa}_{\delta\beta}'\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}$$

and

$$\begin{split} MSE(\delta\tilde{\boldsymbol{\beta}}) &= \operatorname{Var}(\tilde{\boldsymbol{\beta}}) + [E(\tilde{\boldsymbol{\beta}}) - \boldsymbol{\beta}][E(\tilde{\boldsymbol{\beta}}) - \boldsymbol{\beta}]'\\ &= \mathbf{C}^{-1} + (1/2)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{S}_{C^{-1}}\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}\\ &- 2\mathbf{C}^{-1}\boldsymbol{\Delta}'\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} - 2\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\Delta}\mathbf{C}^{-1}\\ &- \mathbf{C}^{-1}(\mathbf{H}_{1}\mathbf{b}, \dots, \mathbf{H}_{n}\mathbf{b})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1} - \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\begin{pmatrix}\mathbf{b}'\mathbf{H}_{1}\\ \vdots\\ \mathbf{b}'\mathbf{H}_{n}\end{pmatrix}\mathbf{C}^{-1}\\ &+ \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{W}\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}\\ &+ (1/4)\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(4\boldsymbol{\Delta}\mathbf{b} + \boldsymbol{\kappa}_{b})(4\mathbf{b}'\boldsymbol{\Delta}' + \boldsymbol{\kappa}_{b}')\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}. \end{split}$$

If the a priori information on $\delta\beta = \beta^* - \beta_0$ satisfies criteria given in Section 5, then we can expect

$$\forall \{\mathbf{h} \in R^k\} MSE(\mathbf{h}'\hat{\boldsymbol{\beta}}) < MSE(\mathbf{h}'\hat{\boldsymbol{\beta}}).$$

Even this statement is not proved, it has been verified in each numerically calculated case (cf. also the example in Section 5).

Corrections of estimators in linearized models

4 Estimator of σ^2

Let Σ be of the form $\Sigma = \sigma^2 \mathbf{V}$. The estimator

$$\hat{\sigma}^2 = (\mathbf{Y} - \mathbf{f}_0)' (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ (\mathbf{Y} - \mathbf{f}_0)/(n-k)$$

from Lemma 2.2 is biased under the model (1.1).

Lemma 4.1 Under the model (1.1)

$$\hat{\sigma}^2 \sim \sigma^2 \chi^2_{n-k}(\delta)/(n-k),$$

where

$$\delta = \left(\frac{1}{2}\boldsymbol{\kappa}_{\delta\beta}\right)' (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \left(\frac{1}{2}\boldsymbol{\kappa}_{\delta\beta}\right) / \sigma^2.$$

Proof It is a direct consequence of Lemma 2.5.

Corollary 4.2 The bias of the estimator $\hat{\sigma}^2$ is

$$E(\hat{\sigma}^2) - \sigma^2 = rac{1}{4(n-k)} \kappa_{\deltaeta}' (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \kappa_{\deltaeta}.$$

The bias is of the fourth order (in $\delta\beta$) and tends to 0 if $n \to \infty$. However situations can occur when it is not negligible.

Lemma 4.3 If

$$\delta \boldsymbol{\beta}' \mathbf{C}_0 \delta \boldsymbol{\beta} \le \varepsilon \frac{2\sqrt{n-k}}{K_0^{(int)}} \sigma, \tag{4.1}$$

then

$$\frac{E(\hat{\sigma}^2) - \sigma^2}{\sigma^2} \leq \varepsilon^2$$

Proof The implication is a direct consequence of the definition of the bias $E(\hat{\sigma}^2) - \sigma^2$ and Corollary 4.2;

$$E(\hat{\sigma}^2) - \sigma^2 = \frac{1}{4(n-k)} \kappa'_{\delta\beta} (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \kappa_{\delta\beta}$$

$$\leq \frac{1}{4(n-k)} (\delta\beta' \mathbf{C}_0 \delta\beta)^2 (K_0^{(int)} \sigma)^2 \leq \varepsilon^2 \sigma^2$$

$$\Rightarrow \delta\beta' \mathbf{C}_0 \delta\beta \leq \varepsilon \frac{2\sqrt{n-k\sigma}}{K_0^{(int)}} \Rightarrow E(\hat{\sigma}^2) - \sigma^2 \leq \varepsilon^2 \sigma^2.$$

If (4.1) cannot be satisfied, we can try to correct the bias. The most simple way is to use the statistic $\hat{\kappa}_{\delta\beta}$ from Remark 3.2.

In the following σ is assumed to be the same order as $\delta\beta$ (e.g. $\sigma^4\delta\beta$ is of the fifth order).

 $\mathbf{Lemma} \ \mathbf{4.4}$

(i)

$$E\left(\kappa_{\delta\beta}'(\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+}\kappa_{\delta\beta}'\right) = \left[\kappa_{\delta\beta} + 4\Delta\mathbf{b} + \kappa_{b} + \sigma^{2} \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}_{0}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}_{0}^{-1}) \end{pmatrix} \right]' (\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+} \times \left[\kappa_{\delta\beta} + 4\Delta\mathbf{b} + \kappa_{b} + \sigma^{2} \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}_{0}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}_{0}^{-1}) \end{pmatrix} \right] + Tr\left[(\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+}\operatorname{Var}(\kappa_{\delta\beta})\right] = \kappa_{\delta\beta}'(\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+}\kappa_{\delta\beta} + Tr\left[(\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+}2\sigma^{4}\mathbf{S}_{C_{0}^{-1}} + 4\sigma^{2}\mathbf{W}_{0}\right] + 5th order terms$$

. **

(here $\{\mathbf{W}_0\}_{i,j} = \delta \boldsymbol{\beta}' \mathbf{H}_i \mathbf{C}_0^{-1} \mathbf{H}_j \delta \boldsymbol{\beta}, \ i, j = 1, \dots, n$). (ii)

$$E(\hat{\sigma}^2) = \sigma^2 + \frac{1}{4(n-k)} \kappa'_{\delta\beta} (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \kappa_{\delta\beta};$$

$$Var(\hat{\sigma}^2) = \frac{2\sigma^4}{n-k} + 5th \text{ order terms};$$

$$E(\hat{\sigma}^4) = \sigma^4 + \frac{2\sigma^4}{n-k} + 5th \text{ order terms}$$

Proof (i) is a consequence of Lemma 2.6 and (ii) is a consequence of Lemmas 4.1. and 2.4. $\hfill \Box$

The estimator of the bias

$$d=rac{1}{4(n-k)}oldsymbol{\kappa}_{\deltaeta}'(\mathbf{M}_F\mathbf{V}\mathbf{M}_F)^+oldsymbol{\kappa}_{\deltaeta}$$

will be considered in the form

$$\hat{d} = A - \hat{B},$$

where A is a random variable with the property E(A) = d + B and \hat{B} is an estimator of B.

Let

$$A = \frac{1}{4(n-k)} \left[\kappa_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} \right]' (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \\ \times \left[\kappa_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} \right]$$

and

$$B = \frac{1}{4(n-k)} Tr \left\{ (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \operatorname{Var} \left[\boldsymbol{\kappa}_{\delta \hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} \right] \right\}.$$

In order to correct the estimator $\hat{\sigma}^2$ until the fourth order, it is necessary to prove that the mean value of A is correct until the fourth order (in $\delta\beta$) and in the second step to estimate the quantity B until the fourth order (in $\delta\beta$).

Since $\delta \hat{\beta}$ and $\hat{\sigma}^2$ are stochastically independent random variables and on the basis of Lemma 3.1, we have

$$\operatorname{Var} \begin{bmatrix} \kappa_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} \end{bmatrix} = \\ = 2\sigma^4 \mathbf{S}_{C_0^{-1}} + 4\sigma^2 \mathbf{W}_0 + \operatorname{Var}(\hat{\sigma}^2) \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} (Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}), \dots, Tr(\mathbf{H}_n \mathbf{C}_0^{-1})) .$$

With respect to Lemma 2.4 and Lemma 4.1 $\operatorname{Var}(\hat{\sigma}^2) = 2\sigma^4/(n-k) + \dots$ and $E(\hat{\sigma}^4) = \sigma^4 + 2\sigma^4/(n-k) + \dots$ Thus

$$E\left[\frac{2\hat{\sigma}^4}{n-k}\left(1-\frac{2}{n-k}\right)\right] = \frac{2\sigma^4}{n-k} - \frac{8\sigma^4}{(n-k)^3} + \dots$$

In the following the term $8\sigma^4/(n-k)^3$ is neglected and thus we obtain

$$\begin{aligned} \operatorname{Var} \left[\boldsymbol{\kappa}_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_1^{-1}) \end{pmatrix} \right] = \\ &= E \left\{ 2\hat{\sigma}^4 \left(1 - \frac{2}{n-k} \right) \mathbf{S}_{C_0^{-1}} + 4\hat{\sigma}^2 \mathbf{W}_0 + \frac{2\hat{\sigma}^4}{n-k} \left(1 - \frac{2}{n-k} \right) \\ &\times \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} (Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}), \dots, Tr(\mathbf{H}_n \mathbf{C}_0^{-1})) \right\} + 5\text{th order terms} \end{aligned}$$

Thus \hat{B} can be taken in the form

$$\hat{B} = \frac{1}{4(n-k)} Tr\left\{ (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \left[2\hat{\sigma}^4 \left(1 - \frac{2}{n-k} \right) \mathbf{S}_{C_0^{-1}} + 4\hat{\sigma}^2 \mathbf{W}_0 + \frac{2\hat{\sigma}^4}{n-k} \left(1 - \frac{2}{n-k} \right) \left(\frac{Tr(\mathbf{H}_1 \mathbf{C}_0^{-1})}{\vdots} \right) (Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}), \dots, Tr(\mathbf{H}_n \mathbf{C}_0^{-1})) \right] \right\}$$

Further

$$\begin{split} E(A) &= \frac{1}{4(n-k)} E\left\{ \begin{bmatrix} \kappa_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1\mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n\mathbf{C}_0^{-1}) \end{pmatrix} \end{bmatrix}' (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \\ &\times \begin{bmatrix} \kappa_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1\mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n\mathbf{C}_0^{-1}) \end{pmatrix} \end{bmatrix} \right\} \\ &= \frac{1}{4(n-k)} \begin{bmatrix} E(\kappa_{\delta\hat{\beta}}) - E(\hat{\sigma}^2) \begin{pmatrix} Tr(\mathbf{H}_1\mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n\mathbf{C}_0^{-1}) \end{pmatrix} \end{bmatrix}' (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \\ &\times \begin{bmatrix} E(\kappa_{\delta\hat{\beta}}) - E(\hat{\sigma}^2) \begin{pmatrix} Tr(\mathbf{H}_1\mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n\mathbf{C}_0^{-1}) \end{pmatrix} \end{bmatrix} \\ &+ \frac{1}{4(n-k)} Tr \left\{ (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \operatorname{Var} \begin{bmatrix} \kappa_{\delta\hat{\beta}} - \hat{\sigma}^2 \begin{pmatrix} Tr(\mathbf{H}_1\mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n\mathbf{C}_0^{-1}) \end{pmatrix} \end{bmatrix} \right\}. \end{split}$$

Thus with respect to Lemma 3.1 (i)

$$E(A) - B =$$

$$= \frac{1}{4(n-k)} \left[\kappa_{\delta\beta} + 4\Delta \mathbf{b} + \kappa_b - \frac{1}{4(n-k)} \kappa'_{\delta\beta} (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ + \kappa_{\delta\beta} \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} \right]'$$

$$\times (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \left[\kappa_{\delta\beta} + 4\Delta \mathbf{b} + \kappa_b - \frac{1}{4(n-k)} \kappa'_{\delta\beta} (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ + \kappa_{\delta\beta} \begin{pmatrix} Tr(\mathbf{H}_1 \mathbf{C}_0^{-1}) \\ \vdots \\ Tr(\mathbf{H}_n \mathbf{C}_0^{-1}) \end{pmatrix} \right]$$

$$= \frac{1}{4(n-k)} \kappa'_{\delta\beta} (\mathbf{M}_F \mathbf{V} \mathbf{M}_F)^+ \kappa_{\delta\beta} + 5\text{th order terms}$$

and the following theorem is proved.

Theorem 4.5 The estimator

$$\tilde{\sigma}^{2} = \hat{\sigma}^{2} - \left[\boldsymbol{\kappa}_{\delta\hat{\beta}} - \hat{\sigma}^{2} \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}_{0}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}_{0}^{-1}) \end{pmatrix} \right]' (\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+} \left[\boldsymbol{\kappa}_{\delta\hat{\beta}} - \hat{\sigma}^{2} \begin{pmatrix} Tr(\mathbf{H}_{1}\mathbf{C}_{0}^{-1}) \\ \vdots \\ Tr(\mathbf{H}_{n}\mathbf{C}_{0}^{-1}) \end{pmatrix} \right] \\ + \frac{1}{4(n-k)} Tr \left\{ (\mathbf{M}_{F}\mathbf{V}\mathbf{M}_{F})^{+} \left[2\hat{\sigma}^{4} \left(1 - \frac{2}{n-k} \right) \mathbf{S}_{C_{0}^{-1}} + 4\hat{\sigma}^{2}\mathbf{W}_{0} \right] \right\}$$

Corrections of estimators in linearized models

$$+\frac{2\hat{\sigma}^4}{n-k}\begin{pmatrix}Tr(\mathbf{H}_1\mathbf{C}_0^{-1})\\\vdots\\Tr(\mathbf{H}_n\mathbf{C}_0^{-1})\end{pmatrix}(Tr(\mathbf{H}_1\mathbf{C}_0^{-1}),\ldots,Tr(\mathbf{H}_n\mathbf{C}_0^{-1}))\right]\bigg\}$$

is of the property

 $E(\tilde{\sigma}^2) = \sigma^2 + 5th \text{ order terms.}$

Even Theorem 4.5 gives the correction for standardly used estimator $\hat{\sigma}^2$, its structure is detering. The esimator $\tilde{\sigma}^2$ is of a little chance to be used in practice. Therefore it is necessary to check whether the correction is necessary (cf. Lemma 4.3 and the following section).

5 A low nonlinearity

In [4] it was proved (the linearization region with respect to the bias)

$$\delta \boldsymbol{\beta}' \mathbf{C} \delta \boldsymbol{\beta} \leq \frac{2c_b}{K^{(par)}} \Rightarrow \forall \{ \mathbf{h} \in R^k \} | E[\widehat{\mathbf{h}' \boldsymbol{\beta}}(\mathbf{Y}, \mathbf{0}) | \boldsymbol{\beta}] - \mathbf{h}' \boldsymbol{\beta} | \leq c_b \sqrt{\mathbf{h}' \mathbf{C}^{-1} \mathbf{h}}$$

(here $\widehat{\mathbf{h}'\beta}(\mathbf{Y},\mathbf{0}) = \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(\mathbf{Y}-\mathbf{f}_0)$). Thus it is desirable to have a situation characterized by the inequality

$$\frac{2c_b}{K^{(par)}} \gg \chi_k^2(0, 1-\alpha),$$

for sufficiently small α . This implies the suitable values of $K^{(par)}$, i.e.

$$K^{(par)} \ll \frac{2c_b}{\chi_k^2(0,1-\alpha)}.$$

For $c_b = 1$ cf. Table 5.1

Table 5.1									
k	2	5	10	20	30				
$\boxed{\frac{2}{\chi^2_k(0,0.95)}}$	0.334	0.180	0.109	0.064	0.046				

Further (the linearization region with respect to a testing the hypothesis "data fit the model (1.2)") in [4] it was proved

$$\delta \boldsymbol{\beta}' \mathbf{C} \delta \boldsymbol{\beta} \leq \frac{2\sqrt{\delta_{crit}}}{K^{(int)}}$$

$$\Rightarrow P\left\{ [\mathbf{Y} - \mathbf{f}_0 - \mathbf{F} \widehat{\delta \boldsymbol{\beta}}(\mathbf{Y}, \mathbf{0})]' \mathbf{C} [\mathbf{Y} - \mathbf{f}_0 - \mathbf{F} \widehat{\delta \boldsymbol{\beta}}(\mathbf{Y}, \mathbf{0})] \geq \chi_k^2(0, 1 - \alpha) \right\} \leq \alpha + \varepsilon,$$

where

$$P\{\chi_k^2(\delta_{crit}) \ge \chi_k^2(0, 1-\alpha)\} = \alpha + \varepsilon.$$

For $1 - \alpha = 0.975$ and $\varepsilon = 0.025$ cf. Table 5.2

Table 5.2

k	2	5	10	20	30
$\boxed{\frac{2\sqrt{\delta_{crit}}}{\chi^2_k(0,0.975)}}$	0.191	0.140	0.108	0.079	0.063

If the model (1.1) does not exceed values given in tables 5.1. and 5.2 respectively, then it can be considered as a model with a low nonlinearity at β_0 , i.e. we can use the model (1.2) without any deterioration of the estimators of β .

If (cf. Lemma 4.3) in addition

$$\sqrt{\delta_{crit}} \ll \sqrt{n-k\varepsilon\sigma},$$

then the model enables us to estimate in the standard way also the parameter σ^2 .

Example 5.1 Let $Y \sim N_1(2\delta\beta + (1/2)0.1\delta\beta^2, \sigma^2 = 0.1^2)$ (i.e. $\beta_0 = 0$). Thus $F = 2, C = 400, H = 0.1, \kappa_{\delta\beta} = 0.1\delta\beta^2, C^{-1} = \sigma^2(F'F)^{-1} = 0.0025, \sqrt{\operatorname{Var}(\hat{\beta})} = 0.05, b = C^{-1}F'\Sigma^{-1}(1/2)\kappa_{\delta\beta} = 0.025\delta\beta^2$ and $K^{(par)} = \frac{1}{400}, K^{(int)} = 0.$

 $MSE(\hat{\beta}) = 0.0025 + 0.000625\delta\beta^4,$

 $MSE(\tilde{\beta}) = 0.0025 - 0.00000005\delta\beta + 0.00000619\delta\beta^2.$

If $\delta\beta = 1$, then $MSE(\hat{\beta}) = 0.0031$ and $MSE(\tilde{\beta}) = 0.0025$, i.e.

$$[MSE(\hat{\beta})/MSE(\hat{\beta})] = 1.24.$$

If $\delta\beta = -2$, then $MSE(\hat{\beta}) = 0.0125$ and $MSE(\tilde{\beta}) = 0.0025$, i.e.

$$[MSE(\hat{\beta})/MSE(\hat{\beta})] = 5.$$

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