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Lubomír Kubáček; Eva Tesaříková

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Estimation of Dispersion in Nonlinear Regression Models with Constraints *

Lubomír KUBÁČEK [1], Eva TESAŘÍKOVÁ [2]

[1] *Department of Mathematical Analysis and Applications of Mathematics*
Faculty of Science, Palacký University
Tomkova 40, 779 00 Olomouc, Czech Republic
e-mail: kubacekl@aix.upol.cz

[2] *Department of Algebra and Geometry, Faculty of Science, Palacký University*
Tomkova 40, 779 00 Olomouc, Czech Republic
e-mail: tesariko@aix.upol.cz

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Abstract

Dispersion of measurement results is an important parameter that enables us not only to characterize not only accuracy of measurement but enables us also to construct confidence regions and to test statistical hypotheses. In nonlinear regression model the estimator of dispersion is influenced by a curvature of the manifold of the mean value of the observation vector. The aim of the paper is to find the way how to determine a tolerable level of this curvature.

Key words: Nonlinear regression model, linearization, estimation of dispersion.

2000 Mathematics Subject Classification: 62J05, 62F10

1 Introduction

The frequently used model in regression analysis is $\mathbf{Y} \sim N_n(\mathbf{f}(\boldsymbol{\beta}), \sigma^2\mathbf{V})$, $\boldsymbol{\beta} \in R^k$ (k-dimesional Euclidean space), where $\mathbf{Y}$ is an n-dimensional normally distributed observation vector, $\mathbf{f}(\boldsymbol{\beta})$ is its mean value, $\boldsymbol{\beta}$ is an unknown k-dimensional parameter, σ^2 is an unknown scalar parameter, $\sigma^2 \in (0, \infty)$, and $\mathbf{V}$ is a known $n \times n$ positive semidefinite matrix.

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Sometimes the parameter $\boldsymbol{\beta}$ must satisfy a constraint $\mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}$.

The following text is devoted to the problem of determining of a tolerable level of a model curvature

$$\mathbf{Y} \sim N_n(\mathbf{f}(\boldsymbol{\beta}), \sigma^2\mathbf{V}), \quad \mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}, \tag{1}$$

how this curvature can be defined and how to use this measure of nonlinearity to a determination of a linearization region. This region will be defined as a set of such shifts of the parameter $\boldsymbol{\beta}$ arround the chosen value $\boldsymbol{\beta}_0$ which does not cause any essential deterioration of a quality of the estimator of σ^2 in the case that the actual value $\boldsymbol{\beta}^*$ of the parameter $\boldsymbol{\beta}$ is equal to $\boldsymbol{\beta}_0$.

2 Notation and auxiliary statement

Let in the model (1) the function $\mathbf{f}(\cdot)$ and $\mathbf{g}(\cdot)$ can be approximed as

$$\mathbf{f}(\boldsymbol{\beta}) = \mathbf{f}_0 + \mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) \quad \text{and} \quad \mathbf{g}(\boldsymbol{\beta}) = \mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}),$$

where

$$\begin{aligned}
\mathbf{f}_0 &= \mathbf{f}(\boldsymbol{\beta}_0), \quad \mathbf{F} = \partial\mathbf{f}(\mathbf{u})/\partial\mathbf{u}'|_{u=\beta_0}, \quad \delta\boldsymbol{\beta} = \boldsymbol{\beta} - \boldsymbol{\beta}_0,\\
\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) &= \Big(\kappa_1(\delta\boldsymbol{\beta}), \dots, \kappa_n(\delta\boldsymbol{\beta})\Big)',\\
\kappa_i(\delta\boldsymbol{\beta}) &= \delta\boldsymbol{\beta}'\mathbf{F}_i\delta\boldsymbol{\beta}, \quad i = 1, \dots, n,\\
\mathbf{F}_i &= \partial^2 f_i(\mathbf{u})/\partial\mathbf{u}\partial\mathbf{u}'|_{u=\beta_0}, \quad i = 1, \dots, n,\\
\mathbf{G} &= \partial\mathbf{g}(\mathbf{u})/\partial\mathbf{u}'|_{u=\beta_0},\\
\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) &= \Big(\gamma_1(\delta\boldsymbol{\beta}), \dots, \gamma_q(\delta\boldsymbol{\beta})\Big)',\\
\gamma_i(\delta\boldsymbol{\beta}) &= \delta\boldsymbol{\beta}'\mathbf{G}_i\delta\boldsymbol{\beta}, \quad i = 1, \dots, q,\\
\mathbf{G}_i &= \partial^2 g_i(\mathbf{u})/\partial\mathbf{u}\partial\mathbf{u}'|_{u=\beta_0}, \quad i = 1, \dots, q.
\end{aligned}$$

The model

$$\mathbf{Y} - \mathbf{f}_0 \sim N_n(\mathbf{F}\delta\boldsymbol{\beta}, \sigma^2\mathbf{V}), \quad \mathbf{G}\delta\boldsymbol{\beta} = \mathbf{0} \tag{2}$$

is a linearized version of the model (1) and

$$\mathbf{Y} - \mathbf{f}_0 \sim N_n\Big(\mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}), \sigma^2\mathbf{V}\Big), \quad \mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0} \tag{3}$$

is a quadratic version of the model (1).

Assumption In the following text it is assumed that it is valid

$$r(\mathbf{F}_{n,k}) = k < n \quad \text{and} \quad r(\mathbf{G}_{q,k}) = q < k,$$

respectively, for the ranks of the matrices $\mathbf{F}$ and $\mathbf{G}$, respectively, and that the matrix $\mathbf{V}$ is positive definite.

Lemma 2.1 *The best quadratic estimator $\hat{\sigma}^2$ of the parameter σ^2 in the model (2) is*

$$\hat{\sigma}^2 = (\mathbf{Y} - \mathbf{f}_0)'\Big(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\Big)^+(\mathbf{Y} - \mathbf{f}_0)/(n + q - k) \tag{4}$$

and $\hat{\sigma}^2 \sim \sigma^2\chi^2_{n+q-k}(0)/(n+q-k)$.

Here $\mathbf{M}_{G'} = \mathbf{I} - \mathbf{G}'(\mathbf{G}\mathbf{G}')^-\mathbf{G}, (\mathbf{G}'\mathbf{G})^-$ is any g-inverse of the matrix $\mathbf{G}\mathbf{G}'$, the symbol

$$\Big(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\Big)^+$$

means the Moore–Penrose g-inverse of the matrix $\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}$ (cf. [5]) and $\chi^2_{n+q-k}(0)$ is the random variable with the central chi-square distribution with $n + q - k$ degrees of freedom.

Proof Cf. e.g. in [3].

3 Measure of nonlinearity

Lemma 3.1 *The estimator (4) in the model (3) is of the property*

$$(\mathbf{Y} - \mathbf{f}_0)'\Big(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\Big)^+(\mathbf{Y} - \mathbf{f}_0)/(n + q - k) \sim \sigma^2\frac{\chi^2_{n+q-k}(\delta)}{n+q-k},$$

where $\delta = \frac{1}{4\sigma^2}\boxed{1}'\Big(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\Big)^+\boxed{1}$,

$$\boxed{1} = \boldsymbol{\kappa}(\delta\boldsymbol{\beta}) - \mathbf{F}\mathbf{G}'(\mathbf{G}\mathbf{G}')^-\boldsymbol{\gamma}(\delta\boldsymbol{\beta}).$$

Proof It is sufficient to prove the equality

$$E(\mathbf{Y} - \mathbf{f}_0) = \mathbf{F}\mathbf{M}_{G'}\delta\boldsymbol{\beta} + \frac{1}{2}\Big[\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) - \mathbf{F}\mathbf{G}'(\mathbf{G}\mathbf{G}')^-\boldsymbol{\gamma}(\delta\boldsymbol{\beta})\Big].$$

Since

$$E(\mathbf{Y} - \mathbf{f}_0) = \mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) = \mathbf{F}\mathbf{M}_{G'}\delta\boldsymbol{\beta} - \mathbf{F}\mathbf{G}'(\mathbf{G}\mathbf{G}')^-\mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) =$$
$$= \mathbf{F}\mathbf{M}_{G'}\delta\boldsymbol{\beta} + \frac{1}{2}\Big[\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) - \mathbf{F}\mathbf{G}'(\mathbf{G}\mathbf{G}')^-\boldsymbol{\gamma}(\delta\boldsymbol{\beta})\Big],$$

the statement is proved. □

Corollary 3.2 *Since $E[\chi^2_f(\delta)] = f + \delta$, the estimator (4) is biased and*

$$E(\hat{\sigma}^2) - \sigma^2 = \frac{1}{4(n+q-k)}\boxed{1}'\Big(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\Big)^+\boxed{1}.$$

Now an analogy of the intrinsic curvature of the Bates and Watts [1] can be defined.

Definition 3.3 The quantity

$$K_{0,I}^{int}(\boldsymbol{\beta}_0) = \sup\left\{ \frac{\sqrt{\boxed{1}'\left(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\right)^{+}\boxed{1}}}{\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q} \right\},$$

where

$$\begin{aligned} \boxed{1} &= \boldsymbol{\kappa}(\mathbf{K}_G\delta\mathbf{s}) - \mathbf{F}\mathbf{G}^{-}\gamma(\mathbf{K}_G\delta\mathbf{s}), \\ \mathcal{M}(\mathbf{K}_G) &= \mathcal{M}(\mathbf{M}_{G'}), \quad \mathbf{K}_G \text{ is } k\times(k-q) \text{ matrix}, \\ \mathbf{C}_0 &= \mathbf{F}'\mathbf{V}^{-1}\mathbf{F}, \end{aligned}$$

is intrinsic curvature at the point $\boldsymbol{\beta}_0$ for the model with constraints $\mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}$.

Remark 3.4 The Bates and Watts [1] intrinsic curvature for a regular model without constraints $\mathbf{Y} \sim N_n(\mathbf{f}(\boldsymbol{\beta}), \boldsymbol{\Sigma}), \boldsymbol{\beta} \in R^k$, is defined as

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

where $\mathbf{M}_F^{\Sigma^{-1}} = \mathbf{I} - \mathbf{F}(\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F})^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}$.

The model (3) can be reparametrized in the following way.

$$\boldsymbol{\beta} = \boldsymbol{\beta}_0 + \mathbf{K}_G\delta\mathbf{s} - \frac{1}{2}\mathbf{G}^{-}\boldsymbol{\gamma}(\mathbf{K}_G\delta\mathbf{s}) + \text{ terms of the higher order},$$

$$\mathbf{Y} - \mathbf{f}_0 \sim N_n\Big(\mathbf{F}\mathbf{K}_G\delta\mathbf{s} - \frac{1}{2}\mathbf{F}\mathbf{G}^{-}\boldsymbol{\gamma}(\mathbf{K}_G\delta\mathbf{s}) + \frac{1}{2}\boldsymbol{\kappa}(\mathbf{K}_G\delta\mathbf{s}), \sigma^2\mathbf{V}\Big).$$

Now, if the scheme

$$\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) \to \boldsymbol{\kappa}(\mathbf{K}_G\delta\mathbf{s}) - \mathbf{F}\mathbf{G}^{-}\boldsymbol{\gamma}(\mathbf{K}_G\delta\mathbf{s}), \quad \mathbf{M}_F \to \mathbf{M}_{FM_{G'}},$$

$$\left(\mathbf{M}_F^{\Sigma^{-1}}\right)'\boldsymbol{\Sigma}^{-1}\mathbf{M}_F^{\Sigma^{-1}} = \left(\mathbf{M}_F\boldsymbol{\Sigma}\mathbf{M}_F\right)^{+} \to \left(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{F_{G'}}\right)^{+}$$

and the relationship

$$\delta\mathbf{s}'\mathbf{K}_G'\mathbf{F}'\mathbf{V}^{-1}\mathbf{F}\mathbf{K}_G\delta\mathbf{s} = \delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s},$$

is taken into account, the expression for $K_{0,I}^{int}(\boldsymbol{\beta}_0)$ is obtained and its geometrical meaning can be seen.

Remark 3.5 If the model is linear, i.e. $\mathbf{Y} \sim N_n(\mathbf{F}\boldsymbol{\beta}, \sigma^2\mathbf{V})$, however the constraints $\mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}$ are nonlinear, then $K_{0,I}^{int}(\boldsymbol{\beta}_0)$ is equal to

$$K_{0,I}^{int}(\boldsymbol{\beta}_0) = \sup\left\{ \frac{\sqrt{\boldsymbol{\gamma}'(\mathbf{K}_G\delta\mathbf{s})\left(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\right)^{+}\boldsymbol{\gamma}(\mathbf{K}_G\delta\mathbf{s})}}{\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q} \right\}.$$

The curvature of the manifold $\{\boldsymbol{\beta} : \mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}\}$ at the point $\boldsymbol{\beta}_0$ can be characterized as follows.

The parameter $\delta\boldsymbol{\beta}$ can be expressed as

$$\delta\boldsymbol{\beta} = \mathbf{K}_G\delta\mathbf{s} - \frac{1}{2}\mathbf{G}^{-}\boldsymbol{\gamma}(\mathbf{K}_G\delta\mathbf{s}) + \dots$$

The natural norm in the parametric space R^k can be assumed as

$$\|\delta\boldsymbol{\beta}\| = \sqrt{\delta\boldsymbol{\beta}\mathbf{F}'(\sigma^2\mathbf{V})^{-1}\mathbf{F}\delta\boldsymbol{\beta}},$$

since it is the Mahalanobis norm introduced by the estimator

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

Thus the quantity $\sigma C_0^{constr}(\boldsymbol{\beta}_0)$, where

$$C_0^{constr}(\boldsymbol{\beta}_0) = \sup\left\{\frac{\sqrt{\boxed{2}'\mathbf{C}_0\boxed{2}}}{\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q}\right\},$$

$$\boxed{2} = \mathbf{M}_{M_{G'}}^{C_0}\mathbf{G}'(\mathbf{G}\mathbf{G}')^{-1}\boldsymbol{\gamma}(\mathbf{K}_G\delta\mathbf{s}),$$

can be considered as the intrinsic curvature of the constraints $\mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}$. However

$$(\mathbf{G}\mathbf{G}')^{-1}\mathbf{G}\left(\mathbf{M}_{M_{G'}}^{C_0}\right)'\mathbf{C}_0\mathbf{M}_{M_{G'}}^{C_0}\mathbf{G}'(\mathbf{G}\mathbf{G}')^{-1} =$$
$$= (\mathbf{G}\mathbf{G}')^{-1}\mathbf{G}\left\{\mathbf{I} - \left[\mathbf{C}_0^{-1} - \mathbf{C}_0^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}_0^{-1}\right]\mathbf{C}_0\right\}'$$
$$\times \mathbf{C}_0\left\{\mathbf{I} - \left[\mathbf{C}_0^{-1} - \mathbf{C}_0^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}_0^{-1}\right]\mathbf{C}_0\right\}\mathbf{G}'(\mathbf{G}\mathbf{G}')^{-1} = (\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}$$

and

$$(\mathbf{G}\mathbf{G}')^{-1}\mathbf{G}\mathbf{F}'\left(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\right)^{+}\mathbf{F}\mathbf{G}'(\mathbf{G}\mathbf{G}')^{-1} =$$
$$= (\mathbf{G}\mathbf{G}')^{-1}\mathbf{G}\mathbf{F}'\left\{\mathbf{V}^{-1} - \mathbf{V}^{-1}\mathbf{F}\mathbf{M}_{G'}\left[\mathbf{M}_{G'}\mathbf{F}'\mathbf{V}^{-1}\mathbf{F}\mathbf{M}_{G'}\right]^{+} \times \mathbf{M}_{G'}\mathbf{F}'\mathbf{V}^{-1}\right\}\mathbf{F}\mathbf{G}'(\mathbf{G}\mathbf{G}')^{-1}$$
$$= (\mathbf{G}\mathbf{G}')^{-1}\mathbf{G}\left\{\mathbf{C}_0 - \mathbf{C}_0\left[\mathbf{C}_0^{-1} - \mathbf{C}_0^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}_0^{-1}\right]\mathbf{C}_0\right\}\mathbf{G}'(\mathbf{G}\mathbf{G}')^{-1}$$
$$= (\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}.$$

Thus under the condition $\boldsymbol{\kappa}(\cdot) = \mathbf{0}$,

$$K_{0,I}^{int}(\boldsymbol{\beta}_0) = C_0^{constr}(\boldsymbol{\beta}_0).$$

Remark 3.6 If the model is nonlinear, i.e. $\mathbf{Y} \sim N_n(\mathbf{f}(\boldsymbol{\beta}), \sigma^2\mathbf{V})$, however the constraints are linear, i.e. $\mathbf{G}\delta\boldsymbol{\beta} = \mathbf{0}$, then $K_{0,I}^{int}(\boldsymbol{\beta}_0)$ is equal to

$$K_{0,I}^{int}(\boldsymbol{\beta}_0) = \sup\left\{\frac{\sqrt{\boldsymbol{\kappa}'(\mathbf{K}_G\delta\mathbf{s})\left(\mathbf{M}_{FM_{G'}}^{V^{-1}}\right)'\mathbf{V}^{-1}\mathbf{M}_{FM_{G'}}^{V^{-1}}\boldsymbol{\kappa}(\mathbf{K}_G\delta\mathbf{s})}}{\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q}\right\}.$$

Since

$$\left(\mathbf{M}_{FM_{G'}}^{V^{-1}}\right)'\mathbf{V}^{-1}\mathbf{M}_{FM_{G'}}^{V^{-1}} =$$
$$= \left(\mathbf{M}_{F}^{V^{-1}}\right)'\mathbf{V}^{-1}\mathbf{M}_{F}^{V^{-1}} + \mathbf{V}^{-1}\mathbf{F}\mathbf{C}_0\mathbf{G}'(\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}_0^{-1}\mathbf{F}'\mathbf{V}^{-1},$$

it can be written

$$K_{0,I}^{int}(\boldsymbol{\beta}_0) \le K_0^{int}(\boldsymbol{\beta}_0),$$

in the case $\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0}$, with respect to Remark 3.4. Here $K_0^{int}(\boldsymbol{\beta}_0) = K^{int}(\boldsymbol{\beta}_0)$ for $\sigma = 1$.

4 Linearization region

Definition 4.1 The ε-linearization region (at the point $\boldsymbol{\beta}_0$) for an estimation of the parameter σ^2 is

$$\mathcal{L}_\sigma = \left\{\boldsymbol{\beta}_0 + \delta\boldsymbol{\beta} : \delta\boldsymbol{\beta} = \mathbf{K}_G\delta\mathbf{s}, E(\hat{\sigma}^2) - \sigma^2 < \varepsilon^2\sigma^2\right\}.$$

Theorem 4.2 *The ε-linearization region from Definition 4.1 is*

$$\mathcal{L}_\sigma = \left\{\boldsymbol{\beta}_0 + \delta\boldsymbol{\beta} : \delta\boldsymbol{\beta} = \mathbf{K}_G\delta\mathbf{s}, \delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s} \le \frac{2\sigma\varepsilon\sqrt{n+q-k}}{K_{0,I}^{int}(\boldsymbol{\beta}_0)}\right\}.$$

Proof The relationships

$$E(\hat{\sigma}^2) - \sigma^2 = \frac{1}{4(n+q-k)}\boxed{1}'\left(\mathbf{M}_{FM_{G'}}\mathbf{V}\mathbf{M}_{FM_{G'}}\right)^+\boxed{1} \le$$
$$\le \frac{1}{4(n+q-k)}\left(\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s}\right)^2\left(K_{0,I}^{int}(\boldsymbol{\beta}_0)\right)^2$$

are implied by a comparison of the bias from Corollary 3.2 and Definition 3.3. Thus

$$E(\hat{\sigma}^2) - \sigma^2 \le \frac{1}{4(n+q-k)}\left(\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s}\right)^2\left(K_{0,I}^{int}(\boldsymbol{\beta}_0)\right)^2 \le \sigma^2\varepsilon^2$$
$$\Leftrightarrow \delta\mathbf{s}\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s} \le \frac{2\sigma\varepsilon\sqrt{n+q-k}}{K_{0,I}^{int}(\boldsymbol{\beta}_0)}. \qquad \square$$

Remark 4.3 The actual value $\boldsymbol{\beta}^*$ of the parameter $\boldsymbol{\beta}$ is unknown. However some information on $\boldsymbol{\beta}^*$ is given by the estimator

$$\hat{\hat{\boldsymbol{\beta}}} = \boldsymbol{\beta}_0 + \left\{\mathbf{I} - \mathbf{C}_0^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}\right)\hat{\boldsymbol{\beta}},$$

where $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}_0 + (\mathbf{F}'\mathbf{V}^{-1}\mathbf{F})^{-1}\mathbf{F}'\mathbf{V}^{-1}(\mathbf{Y} - \mathbf{f}_0)$ and by the confidence region

$$\mathcal{E}_\beta = \left\{\boldsymbol{\beta}_0 + \mathbf{K}_G\mathbf{u} : (\mathbf{u} - \delta\hat{\hat{\boldsymbol{\beta}}})'\mathbf{C}_0(\mathbf{u} - \delta\hat{\hat{\boldsymbol{\beta}}}) \le (k-q)\hat{\sigma}^2 F_{k-q,n+q-k}(1-\alpha)\right\}.$$

(The equalities

$$\mathrm{Var}(\hat{\hat{\boldsymbol{\beta}}}) = \sigma^2[\mathbf{C}_0 - \mathbf{C}_0\mathbf{G}'(\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}^{-1}]$$

and

$$[\mathbf{C}_0 - \mathbf{C}_0\mathbf{G}'(\mathbf{G}\mathbf{C}_0^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}^{-1}]^+ = \mathbf{C}_0$$

are utilized.)

Remark 4.4 With respect to Theorem 4.2 and the expression for the $(1-\alpha)$-confidence ellispoid, it is clear that the values of the semiaxes of the ellipsoid depend on σ linearly, however the semiaxes of $\mathcal{L}_\sigma$ depend linearly on $\sqrt{\sigma}$. Thus the inclusion $\mathcal{E}_\beta \subset \mathcal{L}_\sigma$ can be attain by a smaller σ. It can be established by a proper design of experiment.

Remark 4.5 If $\mathcal{E}_\beta$ is significantly smaller than $\mathcal{L}_\sigma$ and $\mathcal{E}_\beta \subset \mathcal{L}_\sigma$, we can estimate parameter σ^2 by (4) and we can be sure that $E(\hat{\sigma}^2) - \sigma^2 < \varepsilon^2\sigma^2$.

Let $b(\hat{\sigma}^2) = E(\hat{\sigma}^2) - \sigma^2$ and $b(\hat{\sigma}) = E(\hat{\sigma}) - \sigma$. Then the approximation

$$b(\hat{\sigma}) \approx \sigma\frac{b(\hat{\sigma}^2)}{2} \leq \sigma\frac{\varepsilon^2}{2}$$

can be used. Thus, from the viewpoint of practice it seems to be important the validity of the following implication

$$\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}_0\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\sigma\varepsilon\sqrt{n+q-k}}{K_{0,I}^{int}(\boldsymbol{\beta}_0)} \Rightarrow b(\hat{\sigma}) \leq \sigma\frac{\varepsilon^2}{2}\,.$$

5 Numerical example

In [4] the problem of linearization of the model with constraints with respect to the estimation of the parameter $\boldsymbol{\beta}$ was solved. The numerical example given there was chosen as follows.

$$\{\mathbf{f}\}_i(\boldsymbol{\beta}) = f_i(\boldsymbol{\beta}) = \begin{cases} l_1(x_i,\beta_1) = x_i\beta_1, & x_i \leq 5, \\ l_2(x_i,\beta_2,\beta_3) = \beta_1\exp(\beta_3 x_i), & x_i \geq 5 \end{cases}$$

and

$$g(\beta_1,\beta_2,\beta_3) = 5\beta_1 - \beta_2\exp(5\beta_3).$$

Measurement regarding this model was calculated at the points $x = 1,2,3,6,7,8$ and $\mathrm{Var}(\mathbf{Y}) = \sigma^2\mathbf{I}$. In [4] it is shown that for $\sigma = 0.5$ the model cannot be linearized with respect to the estimation of $\boldsymbol{\beta}$. The value of the parameter σ must be smaller than 0.01 in order for the linearization be admissible.

Quite different situation occurs in this example in the case that the estimator of σ^2 is under consideration. With the help of [7] we obtain the following results. Analogously as in [4], let the functions $\mathbf{f}(\cdot)$ and $g(\cdot)$ be those given at the beginning of the section, $x = 1, 2, 3, 6, 7, 8$, $\mathrm{Var}(\mathbf{Y}) = \sigma^2\mathbf{I}$ and

$$\beta_1 = 1.473, \beta_2 = 33, \beta_3 = -0.29999, \alpha = 0.05, \varepsilon = 0.1, \sigma = 0.5.$$

Then the figures 1, 2 and 3 show that the $(1-\alpha)$-confidence ellipsoid is included into $\mathcal{L}_\sigma$ and the same is valid also for $\sigma = 1$; cf. figures 4,5,6.

$\sigma = 0.5$

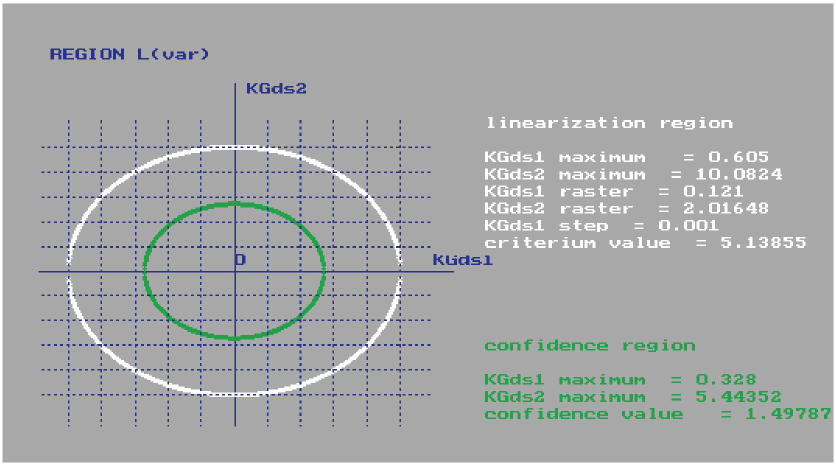

Figure 1 The sections of the confidence ellipsoid and the linearization region $\mathcal{L}_\sigma$ by the axes β_1 and β_2.

$\sigma = 0.5$

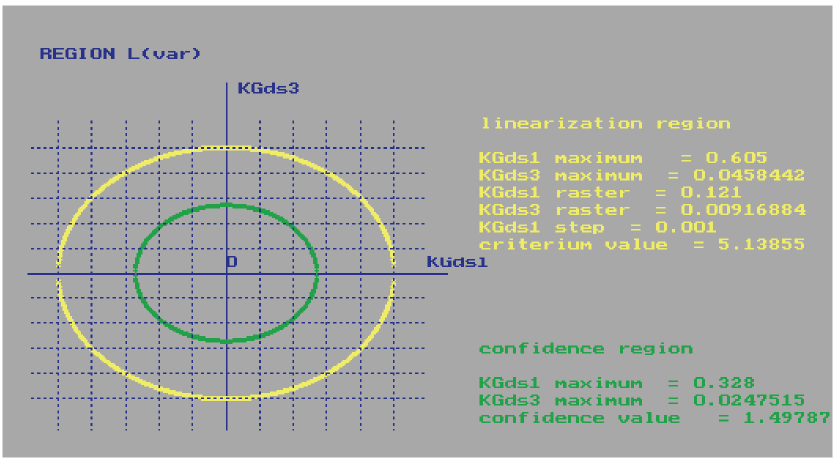

Figure 2 The sections of the confidence ellipsoid and the linearization region $\mathcal{L}_\sigma$ by the axes β_1 and β_3.

$\sigma = 0.5$

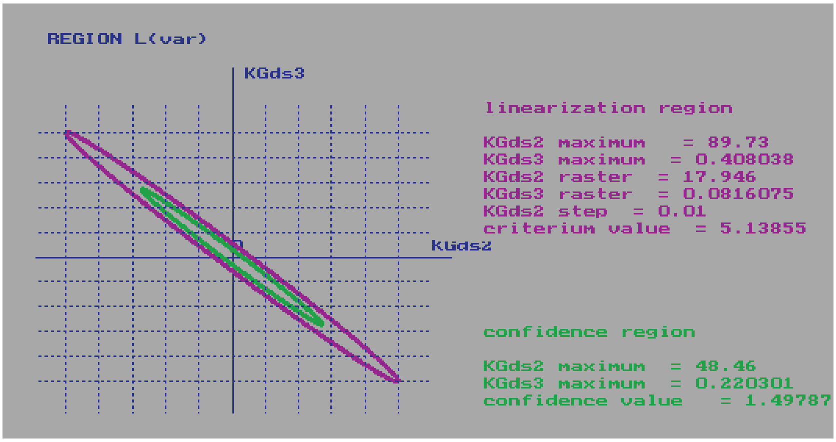

Figure 3 The sections of the confidence ellipsoid and the linearization region $\mathcal{L}_\sigma$ by the axes β_2 and β_3.

$\sigma = 1$

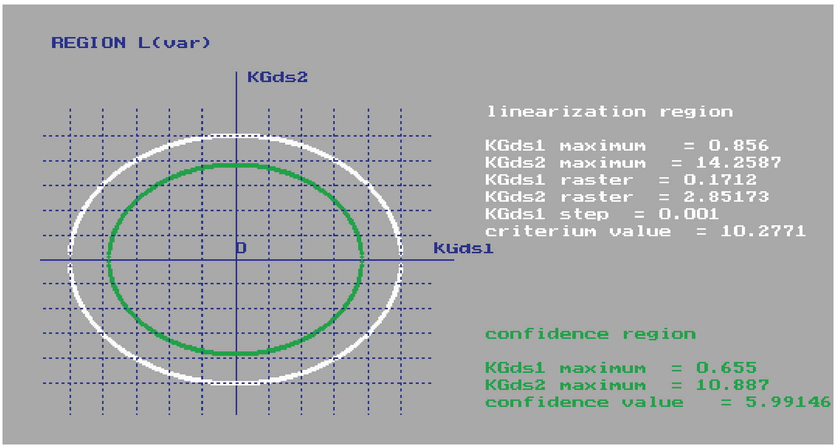

Figure 4 The sections of the confidence ellipsoid and the linearization region $\mathcal{L}_\sigma$ by the axes β_1 and β_2.

$\sigma = 1$

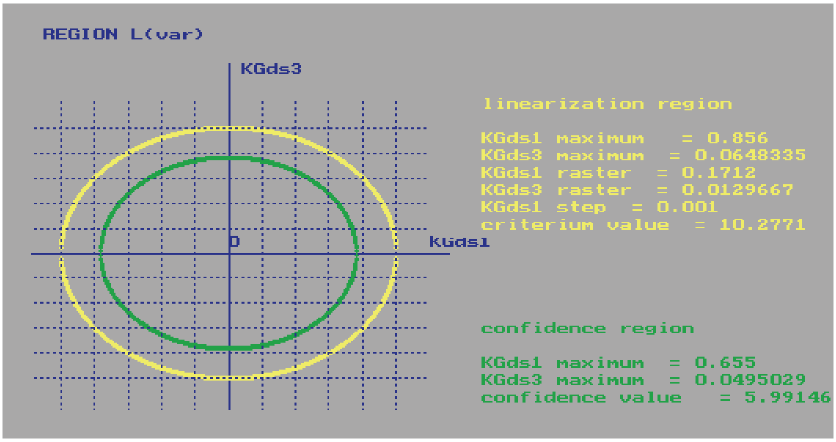

Figure 5 The sections of the confidence ellipsoid and the linearization region $\mathcal{L}_\sigma$ by the axes β_1 and β_3.

$\sigma = 1$

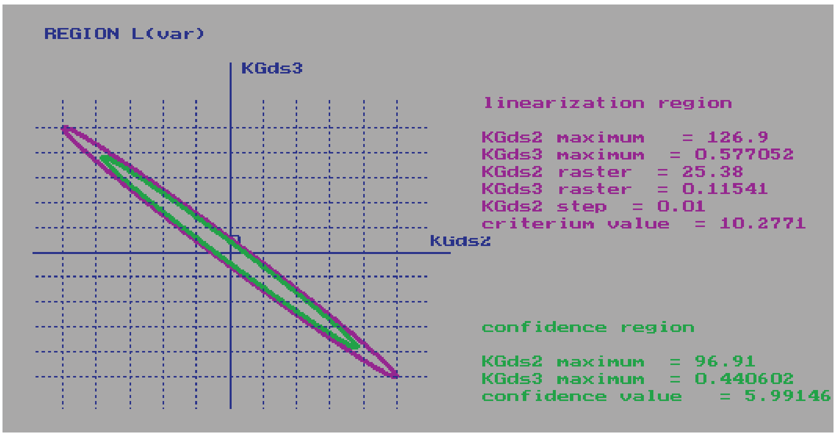

Figure 6 The sections of the confidence ellipsoid and the linearization region $\mathcal{L}_\sigma$ by the axes β_2 and β_3.

The empirical probabilty density function is given at figure 7 for $\sigma = 0.5$

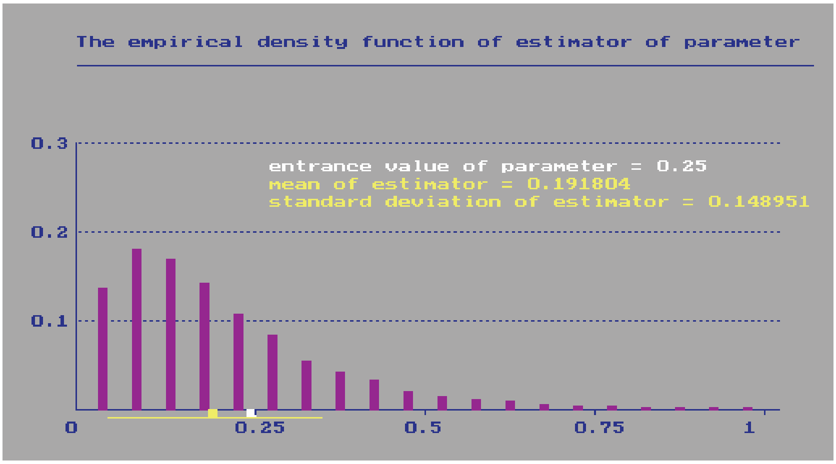

Figure 7 The empirical density function of the estimator $\hat{\sigma}^2$ (4) for $\sigma = 0.5$

The linearization is possible if the value of $K_{0,I}^{int}(\boldsymbol{\beta})$ is sufficiently small with respect to the quantile $F_{k-q,n+q-k}(1-\alpha)$ (cf. Remark 4.3). Therefore table 1 gives the different values of the parameter $\boldsymbol{\beta}$ for our example and table 2 gives the corresponding values $K_{0,I}^{int}(\boldsymbol{\beta})$; the values signed by the star are too large for the linearization of the model with respect to estimation of σ^2 if $\sigma = 0.5$.

β_1	$\beta_2(\beta_3 = -1)$	$\beta_2(\beta_3 = -0.5)$	$\beta_2(\beta_3 = 0.5)$	$\beta_2(\beta_3 = 1)$
0.5	371.032 898	30.456 235	0.205 212	0.016 845
1.0	742.065 796	60.912 470	0.410 425	0.033 690
1.5	1 113.098 693	91.368 705	0.615 637	0.050 535
2.0	1 484.131 591	121.824 940	0.820 850	0.067 379
2.5	1 855.164 488	152.281 174	1.026 062	0.084 224

Table 1 The values of the parameter $\boldsymbol{\beta}$ for Table 2

β_1	$\beta_3 = -1$	$\beta_3 = -0.5$	$\beta_3 = 0.5$	$\beta_3 = 1$
0.5	0.172199*	0.138345*	0.049 621	0.022 430
1.0	0.086 301	0.069 146	0.024 779	0.011 198
1.5	0.056 943	0.045 983	0.016 533	0.007 457
2.0	0.043 192	0.034 565	0.012 372	0.005 568
2.5	0.034 546	0.027 661	0.009 908	0.004 437

Table 2 The values of $K_{0,I}^{int}(\boldsymbol{\beta})$ for $\boldsymbol{\beta}$ given in Table 1

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