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Confidence Regions in Nonlinear Models with Constraints *

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Abstract

There are some difficulties in a construction of confidence regions in nonlinear models with constraints. Even the exact algorithm (in the case of normality) can be derived, the numerical calculation is rather tedious. Thus if a simple algorithm can be find it will be preferred in practice. The aim of the paper is to find a simple criterion which enables us to decide whether it is possible to use algorithms used in linear models.

Key words: Nonlinear model, model with constraints, confidence region, measures of nonlinearity.

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1 Introduction

In order to be sure that a simple approximation of an exact confidence region in a nonlinear model is good for practical purposes it is necessary to find a suitable criterion. This is the aim of the paper.

The solution is based on the idea that the nonlinear model can be characterized as quadratic in a sufficient neighbourhood of the actual value of the parameter and on a utilization of suitable measures of nonlinearity.

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2 Notation and auxiliary statements

Let $\mathbf{f}(\boldsymbol{\beta})$ be an n-dimensional vector function which can be developed at the point $\boldsymbol{\beta}_0$ in the Taylor series $\mathbf{f}(\boldsymbol{\beta}) = \mathbf{f}(\boldsymbol{\beta}_0) + \mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$, $\delta\boldsymbol{\beta} = \boldsymbol{\beta} - \boldsymbol{\beta}_0$, on the domain given by the set $\{\boldsymbol{\beta} : \mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}\}$.

Let

$$\mathbf{Y} \sim N_n\left(\mathbf{f}_0 + \mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}), \boldsymbol{\Sigma}\right), \quad \mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0}, \tag{1}$$

where $\mathbf{Y}$ is an n-dimensional random vector (observation vector),

$$\begin{aligned}
\mathbf{f}_0 &= \mathbf{f}(\boldsymbol{\beta}_0), \quad \mathbf{F} = \partial\mathbf{f}(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0', \\
\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) &= (\kappa_1(\delta\boldsymbol{\beta}), \ldots, \kappa_n(\delta\boldsymbol{\beta}))', \\
\kappa_i(\delta\boldsymbol{\beta}) &= \delta\boldsymbol{\beta}'\mathbf{F}_i\delta\boldsymbol{\beta}, \quad i = 1, \ldots, n, \\
\mathbf{F}_i &= \partial^2 f_i(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0\partial\boldsymbol{\beta}_0', \\
\mathbf{f}(\boldsymbol{\beta}_0) &= (f_1(\boldsymbol{\beta}_0), \ldots, f_n(\boldsymbol{\beta}_0))', \quad \mathbf{G} = \partial\mathbf{g}(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0', \\
\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) &= (\gamma_1(\delta\boldsymbol{\beta}), \ldots, \gamma_q(\delta\boldsymbol{\beta}))', \\
\gamma_i(\delta\boldsymbol{\beta}) &= \delta\boldsymbol{\beta}'\mathbf{G}_i\delta\boldsymbol{\beta}, \quad \mathbf{G}_i = \partial^2 g_i(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0\partial\boldsymbol{\beta}_0', \quad i = 1, \ldots, q, \\
\mathbf{g}(\boldsymbol{\beta}_0) &= (g_1(\boldsymbol{\beta}_0), \ldots, g_q(\boldsymbol{\beta}_0))'.
\end{aligned}$$

Sufficiently good approximation of the mean value of the observation vector $\mathbf{Y}$ is $\mathbf{f}_0 + \mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$ and analogously a good approximation of the constraints $\mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}$ is $\mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0}$. The covariance matrix of $\mathbf{Y}$ is $\boldsymbol{\Sigma}$, which it is assumed to be known.

In the following it is assumed that the ranks of the matrices $\mathbf{F}$ and $\mathbf{G}$, respectively, satisfy the conditions

$$r(\mathbf{F}) = k < n, \; r(\mathbf{G}) = q < k \quad \text{and} \quad \boldsymbol{\Sigma} \text{ is positive definite (p.d.).}$$

The linear version of the model (1) is

$$\mathbf{Y} \sim N_n(\mathbf{f}_0 + \mathbf{F}\delta\boldsymbol{\beta}, \boldsymbol{\Sigma}), \quad \mathbf{G}\delta\boldsymbol{\beta} = \mathbf{0}. \tag{2}$$

Lemma 2.1 *The best linear unbiased eastimator (BLUE) of the parameter $\boldsymbol{\beta}$ in the model (2) is*

$$\hat{\hat{\boldsymbol{\beta}}} = \boldsymbol{\beta}_0 + \widehat{\widehat{\delta\boldsymbol{\beta}}} = \boldsymbol{\beta}_0 + [\mathbf{I} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}]\widehat{\delta\boldsymbol{\beta}} = \boldsymbol{\beta}_0 + \mathbf{P}^C_{\mathcal{K}er(G)}\widehat{\delta\boldsymbol{\beta}},$$

where $\widehat{\delta\boldsymbol{\beta}} = \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}(\mathbf{Y} - \mathbf{f}_0)$ (the BLUE in the model (2) without constraints). Here $\mathbf{C} = \mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F}$ and the symbol $\mathbf{P}^C_{\mathcal{K}er(G)}$ means the projection matrix in the norm $\|\mathbf{x}\| = \sqrt{\mathbf{x}'\mathbf{C}\mathbf{x}}, \mathbf{x} \in R^k$ (k-dimesional Euclidean space) on the subspace $\mathcal{K}er(\mathbf{G}) = \{\mathbf{u} : \mathbf{G}\mathbf{u} = \mathbf{0}\}$.

Further

$$\mathrm{Var}(\hat{\hat{\boldsymbol{\beta}}}) = \mathbf{C}^{-1} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}^{-1}.$$

Proof cf. [4].

Lemma 2.2 *One version of the g-inverse (cf. [6]) of the matrix* $\operatorname{Var}(\hat{\hat{\boldsymbol{\beta}}})$ *is* $\mathbf{C}$.

Proof It is a direct consequence of the definition of g-inverse. □

Lemma 2.3 *The* $(1-\alpha)$*-confidence ellipsoid for the parameter* $\boldsymbol{\beta}$ *in the model (2) is*

$$\mathcal{E}_{1-\alpha} = \left\{\mathbf{u} : \mathbf{u} \in R^k, \mathbf{u} = \hat{\hat{\boldsymbol{\beta}}} + \mathbf{k}, \mathbf{k} \in \mathcal{K}er(\mathbf{G}), \mathbf{k}'\mathbf{C}\mathbf{k} \leq \chi^2_{k-q}(1-\alpha)\right\}, \tag{3}$$

where $\chi^2_{k-q}(1-\alpha)$ *is* $(1-\alpha)$*-quantile of the chi-square distribution with* $k-q$ *degrees of freedom.*

Proof cf. [4].

3 Measures of nonlinearity

Lemma 3.1 *The BLUE of the parameter* $\boldsymbol{\beta}$ *in the model (2) is biased in the model (1) and its bias is*

$$E(\widehat{\widehat{\delta\boldsymbol{\beta}}}) - \delta\boldsymbol{\beta} = \mathbf{M}^C_{C^{-1}G'}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) + \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}),$$

where

$$\mathbf{M}^C_{C^{-1}G'} = \mathbf{I} - \mathbf{P}^C_{C^{-1}G'} = \mathbf{I} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}.$$

Proof

$$\begin{aligned}
E(\widehat{\widehat{\delta\boldsymbol{\beta}}}) &= \mathbf{M}^C_{C^{-1}G'}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\left[\mathbf{F}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right]\\
&= \delta\boldsymbol{\beta} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}\delta\boldsymbol{\beta} + \mathbf{M}^C_{C^{-1}G'}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\\
&= \delta\boldsymbol{\beta} + \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) + \mathbf{M}^C_{C^{-1}G'}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}).
\end{aligned}$$

□

Definition 3.2 Let (cf. also [3] and [4])

$$C^{(par)}_{I,\delta\beta} = \sup\left\{\frac{2\sqrt{\mathbf{b}'(\mathbf{K}_G\delta\mathbf{s})\mathbf{C}\mathbf{b}(\mathbf{K}_G\delta\mathbf{s})}}{\delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q}\right\},$$

where $\mathbf{b}(\delta\boldsymbol{\beta}) = E(\widehat{\widehat{\delta\boldsymbol{\beta}}}) - \delta\boldsymbol{\beta}$ and $\mathbf{K}_G$ is $k \times (k-q)$ matrix with the property $\mathcal{M}(\mathbf{K}_G) = \mathcal{K}er(\mathbf{G})$.

It is to be remarked that $\mathbf{K}_G\delta\mathbf{s}$ is linear approximation of the shift $\delta\boldsymbol{\beta}$.

Theorem 3.3 *If*

$$\delta\mathbf{s}'\mathbf{K}_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\varepsilon}{C^{(par)}_{I,\delta\beta}},$$

then

$$\forall\{\mathbf{h} \in R^k\}|\mathbf{h}'\mathbf{b}(\delta\beta)| \leq \varepsilon\sqrt{\mathbf{h}'\mathbf{C}^{-1}\mathbf{h}}.$$

Proof The definition of the quantity $C^{(par)}_{I,\delta\beta}$ implies

$$2\sqrt{\mathbf{b}(\delta\beta)'\mathbf{C}\mathbf{b}(\delta\beta)} \leq C^{(par)}_{I,\delta\beta}\delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s}.$$

Thus if $\delta\mathbf{s}'\mathbf{K}_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\varepsilon}{C^{(par)}_{I,\delta\beta}}$, then

$$\sqrt{\mathbf{b}'(\delta\beta)\mathbf{C}\mathbf{b}(\delta\beta)} \leq \varepsilon \Leftrightarrow \forall\{\mathbf{h} \in R^k\}|\mathbf{h}'\mathbf{b}(\delta\beta)| \leq \varepsilon\sqrt{\mathbf{h}'\mathbf{C}^{-1}\mathbf{h}}.$$

The last equivalence is implied by the Scheffé theorem [7]. □

The nonlinearity of the constraints $\mathbf{g}(\beta) = \mathbf{0}$ can be, at least partially, characterized by its curvature. If

$$\mathbf{G}\delta\beta + \frac{1}{2}\gamma(\delta\beta) = \mathbf{0}, \tag{4}$$

then $\delta\beta = \mathbf{K}_G\delta\mathbf{s} + \frac{1}{2}\mathbf{G}^-\gamma(\mathbf{K}_G\delta\mathbf{s})$ characterizes the solution of the equation (4) up to quadratic terms. In the model (2) the natural norm of the parametric space R^k is given by the relation $\|\mathbf{u}\| = \sqrt{\mathbf{u}'\mathbf{C}\mathbf{u}}$, where $\mathbf{C} = \mathbf{F}'\mathbf{\Sigma}^{-1}\mathbf{F}$ (cf. also Lemma 1.1). Thus a definition of the curvature of the constraints can be given as follows.

Definition 3.4 Let $\mathbf{G}\delta\beta + \frac{1}{2}\gamma(\delta\beta) = \mathbf{0}$. Then

$$C^{(constr)} = \sup\left\{\frac{\sqrt{\gamma'(\mathbf{K}_g\delta\mathbf{s})(\mathbf{G}^-)'(\mathbf{P}^C_{C^{-1}G'})'\mathbf{C}\mathbf{P}^C_{C^{-1}G'}\mathbf{G}^-\gamma(\mathbf{K}_G\delta\mathbf{s})}}{\delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q}\right\}$$

is the intrinsic curvature of the constraints (at the point β_0).

Remark 3.5 The definition of $C^{(constr)}$ does not depend on a choice of the g-inverse $\mathbf{G}^-$ of the matrix $\mathbf{G}$. It is implied by the following

$$\gamma'(\delta\beta)(\mathbf{G}^-)'(\mathbf{P}^C_{C^{-1}G'})'\mathbf{C}\mathbf{P}^C_{C^{-1}G'}\mathbf{G}^-\gamma(\delta\beta) = \\ = \gamma'(\delta\beta)(\mathbf{G}^-)'\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{G}^-\gamma(\delta\beta)$$

and

$$\mathbf{G}\delta\beta = -\frac{1}{2}\gamma(\delta\beta) \Rightarrow \gamma(\delta\beta) \subset \mathcal{M}(\mathbf{G}) \Rightarrow \mathbf{G}\mathbf{G}^-\gamma(\delta\beta) = \gamma(\delta\beta).$$

Thus

$$C^{(constr)} = \sup\left\{\frac{\sqrt{\gamma'(\mathbf{K}_g\delta\mathbf{s})(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\gamma(\mathbf{K}_G\delta\mathbf{s})}}{\delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s}} : \delta\mathbf{s} \in R^{k-q}\right\}.$$

Corollary 3.6 *If* $\mathbf{h} \in \mathcal{M}[(\mathbf{M}^{C}_{C^{-1}G'})']$, *then the bias of the estimator* $\widehat{\widehat{\mathbf{h}'\delta\boldsymbol{\beta}}}$ *in the model (1) is* $\mathbf{h}'\mathbf{b}(\delta\boldsymbol{\beta}) = \mathbf{h}'\mathbf{M}^{C}_{C^{-1}G'}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$ *and thus it does not depend on the curvature* $C^{(constr)}$.

If $\mathbf{h} \in \mathcal{M}[(\mathbf{P}^{C}_{C^{-1}G'})']$, *then the bias is* $\mathbf{h}'\mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta})$ *and thus the bias is influenced by the curvature of the constraints only.*

Remark 3.7 The quantity $\mathbf{h}'\mathbf{C}^{-1}\mathbf{h}$ is the variance of the estimator $\mathbf{h}'\widehat{\delta\boldsymbol{\beta}}$ of the function $\mathbf{h}'\delta\boldsymbol{\beta}, \delta\boldsymbol{\beta} \in R^k$, in the model $\mathbf{Y} \sim N_n(\mathbf{f}_0 + \mathbf{F}\delta\boldsymbol{\beta}, \boldsymbol{\Sigma})$ without constraints on the parameter $\delta\boldsymbol{\beta}$. In the model (2) this function can be written as $\mathbf{h}'\mathbf{K}_G\delta\mathbf{s}$, $\delta\mathbf{s} \in R^{k-q}$, and the variance of its estimator is

$$\mathrm{Var}(\widehat{\widehat{\delta\boldsymbol{\beta}}}) = \mathbf{h}'[\mathbf{C}^{-1} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}^{-1}]\mathbf{h} \leq \mathbf{h}'\mathbf{C}^{-1}\mathbf{h}.$$

The equality

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

is valid iff $\mathbf{h} \in \mathcal{M}\left[\left(\mathbf{M}^{C}_{C^{-1}G'}\right)'\right]$. In this case

$$|\mathbf{h}'\mathbf{b}(\delta\boldsymbol{\beta})| = |\mathbf{h}'[\mathbf{I} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}]\mathbf{F}'\boldsymbol{\Sigma}^{-1}\tfrac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})|$$

and the curvature of the constraints $\mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0}$ has no influence on the bias $\mathbf{h}'\mathbf{b}(\delta\boldsymbol{\beta})$.

If $\mathbf{h} \in \mathcal{M}\left[\left(\mathbf{P}^{C}_{C^{-1}G'}\right)'\right]$, then $\mathrm{Var}(\mathbf{h}'\widehat{\widehat{\delta\boldsymbol{\beta}}}) = 0$; however the bias of the estimator $\widehat{\widehat{\mathbf{h}'\delta\boldsymbol{\beta}}}$ is

$$|\mathbf{h}'\mathbf{b}(\delta\boldsymbol{\beta})| = |\mathbf{h}'\mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\tfrac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta})|.$$

Thus the bias is influenced by the curvature of the constraints only. In this case the bias cannot be dominated by the variance, however it can be dominated by the quantity $\mathbf{h}'\mathbf{C}^{-1}\mathbf{h}$ (the variance of the estimator in linear model without constraints).

Therefore from the viewpoint of practice it seems to be suitable to define the linearization region for the bias of the estimator $\hat{\hat{\boldsymbol{\beta}}}$ as a set

$$\left\{\delta\boldsymbol{\beta} : \delta\boldsymbol{\beta} = \mathbf{K}_G\delta\mathbf{s}, \delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\varepsilon}{C^{(par)}_{I,\delta\beta}}\right\}.$$

If the model (1) is reparametrized as $\delta\boldsymbol{\beta} = \mathbf{K}_G\delta\mathbf{s}$, then we can define another measure of nonlinearity.

Definition 3.8 The Bates and Watts parametric measure of nonlinearity of the new model is

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

4 Confidence regions

Let

$$\mathbf{Y} \sim N_n(\mathbf{f}(\boldsymbol{\beta}), \boldsymbol{\Sigma}) \quad \text{and} \quad \mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}. \tag{5}$$

Lemma 4.1 *In the model (5) the* $(1-\alpha)$*-confidence region is*

$$\left\{\boldsymbol{\beta} : \mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}, [\mathbf{Y} - \mathbf{f}(\boldsymbol{\beta})]'\mathbf{U}[\mathbf{Y} - \mathbf{f}(\boldsymbol{\beta})] \leq \chi^2_{k-q}(1-\alpha)\right\}, \tag{6}$$

where

$$\begin{aligned}
\mathbf{U} &= \boldsymbol{\Sigma}^{-1}\mathbf{F}(\boldsymbol{\beta})\,\mathrm{Var}(\hat{\hat{\boldsymbol{\beta}}})\mathbf{F}'(\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1},\\
\mathbf{F}(\boldsymbol{\beta}) &= \partial\mathbf{f}(\boldsymbol{\beta})/\partial\boldsymbol{\beta}',\\
\mathbf{C}(\boldsymbol{\beta}) &= \mathbf{F}'(\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{F}(\boldsymbol{\beta}),\\
\mathrm{Var}(\hat{\hat{\boldsymbol{\beta}}}) &= \mathbf{C}^{-1}(\boldsymbol{\beta}) - \mathbf{C}^{-1}(\boldsymbol{\beta})\mathbf{G}'(\boldsymbol{\beta})[\mathbf{G}(\boldsymbol{\beta})\mathbf{C}^{-1}(\boldsymbol{\beta})\mathbf{G}'(\boldsymbol{\beta})]^{-1}\mathbf{G}(\boldsymbol{\beta})\mathbf{C}^{-1}(\boldsymbol{\beta}),\\
\mathbf{G}(\boldsymbol{\beta}) &= \partial\mathbf{g}(\boldsymbol{\beta})/\partial\boldsymbol{\beta}'.
\end{aligned}$$

Proof cf. [5].

It is to be remarked that in the case of linearity of the model (and the constraints), the confidence region from Lemma 4.1 can be expressed as the confidence ellipsoid from Lemma 2.3.

In the following text we shall assume that the model (5) can be approximated by the model (1), where

$$\begin{aligned}
\mathbf{f}_0 &= \mathbf{f}(\boldsymbol{\beta}_0), \quad \mathbf{F} = \partial\mathbf{f}(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0',\\
\mathbf{F}_i &= \partial^2\mathbf{f}(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0\partial\boldsymbol{\beta}_0', \quad i = 1,\dots,n,\\
\mathbf{g}(\boldsymbol{\beta}_0) &= \mathbf{0}, \quad \mathbf{G} = \partial\mathbf{g}(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0,\\
\mathbf{G}_i &= \partial^2\mathbf{g}(\boldsymbol{\beta}_0)/\partial\boldsymbol{\beta}_0\partial\boldsymbol{\beta}_0', \quad i = 1,\dots,q.
\end{aligned}$$

The following problem arises, under which conditions the confidence region (6) can be approximated by the ellipsoid (3).

Theorem 4.2 *Let the model (1) be under consideration. Let* δ_{max} *be the solution of the equation*

$$P\left\{\chi^2_{t(\delta)} = \frac{k-q+\delta}{k-q+2\delta}\left(\sqrt{\chi^2_{k-q}(1-\alpha)} - \sqrt{\delta}\right)^2\right\} = 1 - \alpha - \varepsilon,$$

where $t(\delta) = (k-q+\delta)^2/(k-q+2\delta)$. *Then the implication*

$$\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\sqrt{\delta_{max}}}{C^{(par)}_{I,\delta\beta}} \Rightarrow P\{(\boldsymbol{\beta} - \hat{\hat{\boldsymbol{\beta}}})'\mathbf{C}(\boldsymbol{\beta} - \hat{\hat{\boldsymbol{\beta}}}) \leq \chi^2_{k-q}(1-\alpha)\} \geq 1 - \alpha - \varepsilon$$

is valid.

Proof Let (1) be the considered model; then with respect to Lemma 4.1 the $(1-\alpha)$-confidence region is

$$\Bigg[\boldsymbol{\beta} = \boldsymbol{\beta}_0 + \delta\boldsymbol{\beta} : P\Bigg(\Bigg\{\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\left[\mathbf{Y} - \mathbf{f}_0 - \mathbf{F}\delta\boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right]\Bigg\}'\boldsymbol{\Sigma}^{-1}$$

$$\times\, \mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\left[\mathbf{Y} - \mathbf{f}_0 - \mathbf{F}\delta\boldsymbol{\beta} - \frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right] \le \chi^2_{k-q}(1-\alpha)\Bigg) \ \&\ \mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0}\Bigg].$$

Further

$$\left[\mathbf{F}(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}}) + \mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right]'\boldsymbol{\Sigma}^{-1}\left[\mathbf{F}(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}}) + \mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right] =$$

$$= (\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{C}(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})$$

$$+ 2(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) + \frac{1}{4}\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$$

$$\le \left(\sqrt{(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{C}(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})} + \frac{1}{2}\sqrt{\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})}\right)^2.$$

(The last inequality is a consequence of the Schwarz inequality;

$$(\mathbf{x}+\mathbf{y})'\mathbf{W}(\mathbf{x}+\mathbf{y}) \le \left(\sqrt{\mathbf{x}'\mathbf{W}\mathbf{x}} + \sqrt{\mathbf{y}'\mathbf{W}\mathbf{y}}\right)^2,$$

where $\mathbf{x}$ and $\mathbf{y}$ are n-dimensional vectors and $\mathbf{W}$ an $n \times n$ p.d. matrix.) Further

$$\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) =$$

$$= \boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{M}_{G'}(\mathbf{M}_{G'}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{M}_{G'})^{+}\mathbf{M}_{G'}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$$

$$= \boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{F}[\mathbf{C}^{-1} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}\mathbf{C}^{-1}]\mathbf{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$$

and $(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})\mathbf{C}(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}}) \sim \chi^2_{k-q}(\delta)$, where (cf. Lemma 3.1) $\delta = \mathbf{b}'(\delta\boldsymbol{\beta})\mathbf{C}\mathbf{b}(\delta\boldsymbol{\beta})$,

$$\mathbf{b}(\delta\boldsymbol{\beta}) = [\mathbf{I} - \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\mathbf{G}]\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\frac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})$$

$$+ \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}).$$

In the following text the approximation (cf. [2])

$$\chi^2_f(\delta) \sim \frac{f+2\delta}{f+\delta}\chi^2_{t(\delta)}(0), \qquad t(\delta) = \frac{(f+\delta)^2}{f+2\delta}$$

will be used. We have

$$P\left\{\left(\sqrt{(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{C}(\delta\boldsymbol{\beta} - \widehat{\widehat{\delta\boldsymbol{\beta}}})} + \frac{1}{2}\sqrt{\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})}\right)^2 \le \chi^2_{k-q}(1-\alpha)\right\}$$

$$= P\left\{\left(\sqrt{\frac{k-q+2\delta}{k-q+\delta}\chi^2_{t(\delta)}(0)} + \frac{1}{2}\sqrt{\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta}}\right)^2 \le \chi^2_{k-q}(1-\alpha)\right\}.$$

Since

$$\begin{aligned} &\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta(\boldsymbol{\beta}) \leq \\ &\leq \boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta(\boldsymbol{\beta}) + \boldsymbol{\gamma}'(\delta\boldsymbol{\beta})(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) \\ &= 4\mathbf{b}'(\delta\boldsymbol{\beta})\mathbf{C}\mathbf{b}(\delta\boldsymbol{\beta}) = \delta, \end{aligned}$$

we have

$$\begin{aligned} &P\left\{\left(\sqrt{(\delta\boldsymbol{\beta}-\widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{C}(\delta\boldsymbol{\beta}-\widehat{\widehat{\delta\boldsymbol{\beta}}})}+\frac{1}{2}\sqrt{\boldsymbol{\kappa}'(\delta\boldsymbol{\beta})\boldsymbol{\Sigma}^{-1}\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})}\right)^2 \leq \chi^2_{k-q}(1-\alpha)\right\} \\ &\geq P\left\{\left(\sqrt{(\delta\boldsymbol{\beta}-\widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{C}(\delta\boldsymbol{\beta}-\widehat{\widehat{\delta\boldsymbol{\beta}}})}+\sqrt{\mathbf{b}'(\delta\boldsymbol{\beta})\mathbf{C}\mathbf{b}(\delta\boldsymbol{\beta})}\right)^2 \leq \chi^2_{k-q}(1-\alpha)\right\} \\ &= P\left\{\sqrt{\chi^2_{k-q}(\delta)}+\sqrt{\delta} \leq \sqrt{\chi^2_{k-q}(1-\alpha)}\right\} \\ &= P\left\{\chi^2_{t(\delta)}(0) \leq \frac{k-q+\delta}{k-q+2\delta}\left(\sqrt{\chi^2_{k-q}(1-\alpha)}-\sqrt{\delta}\right)^2\right\}. \end{aligned}$$

Thus if

$$P\left\{\chi^2_{t(\delta_{max})}(0) \leq \frac{k-q+\delta_{max}}{k-q+2\delta_{max}}\left(\sqrt{\chi^2_{k-q}(1-\alpha)}-\sqrt{\delta_{max}}\right)^2\right\} = 1-\alpha-\varepsilon,$$

then

$$\begin{aligned} &P\Big\{\Big(\Big\{\mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\left[\mathbf{Y}-\mathbf{f}_0-\mathbf{F}\delta\boldsymbol{\beta}-\tfrac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right]\Big\}'\boldsymbol{\Sigma}^{-1} \\ &\times \mathbf{P}^{\Sigma^{-1}}_{FM_{G'}}\left[\mathbf{Y}-\mathbf{f}_0-\mathbf{F}\delta\boldsymbol{\beta}-\tfrac{1}{2}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right] \leq \chi^2_{k-q}(1-\alpha)\Big)\Big\} \\ &\geq P\left\{(\delta\boldsymbol{\beta}-\widehat{\widehat{\delta\boldsymbol{\beta}}})'\mathbf{C}(\delta\boldsymbol{\beta}-\widehat{\widehat{\delta\boldsymbol{\beta}}}) \leq \chi^2_{k-q}(1-\alpha)\right\} \geq 1-\alpha-\varepsilon. \end{aligned}$$

Since $\delta = \mathbf{b}'(\delta\boldsymbol{\beta})\mathbf{C}\mathbf{b}(\delta\boldsymbol{\beta})$ and

$$\frac{2\sqrt{\mathbf{b}'(\delta\boldsymbol{\beta})\mathbf{C}\mathbf{b}(\delta\boldsymbol{\beta})}}{\delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s}} \leq C^{(par)}_{I,\beta} \Rightarrow 2\sqrt{\mathbf{b}'(\delta\boldsymbol{\beta})\mathbf{C}\mathbf{b}(\delta\boldsymbol{\beta})} \leq \delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s}C^{(par)}_{I,\beta},$$

we obtain

$$\delta\mathbf{s}'\mathbf{K}'_G\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\sqrt{\delta_{max}}}{C^{(par)}_{I,\beta}} \Rightarrow \delta \leq \delta_{max} \text{ and so (7) is valid}$$

and thus the statement is proved. □

Corollary 4.3 *If the model (1) is linear, i.e.* $\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) = \mathbf{0}$, *then*

$$\mathbf{b}(\delta\boldsymbol{\beta}) = \mathbf{C}^{-1}\mathbf{G}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\frac{1}{2}\boldsymbol{\gamma}(\delta\boldsymbol{\beta})$$

and Theorem 4.2 can be reformulated as follows.

Let δ_{max} *be solution of the equation*

$$P\Big\{\chi^2_{t(\delta_{max})}(0) \leq \frac{k-q+\delta_{max}}{k-q+2\delta_{max}}\chi^2_{k-q}(1-\alpha)\Big\} = 1-\alpha-\varepsilon. \tag{7}$$

Then

$$\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\sqrt{\delta_{max}}}{C^{(constr)}} \Rightarrow \delta \leq \delta_{max}$$

(cf. Definition 3.4).

Corollary 4.4 *If the constraints in the model (1) are linear, i.e.* $\boldsymbol{\gamma}(\delta\boldsymbol{\beta}) = \mathbf{0}$, *then the reformulation of Theorem 4.2 is as follows.*

Let δ_{max} *be the solution of the equation*

$$P\left\{\chi^2_{t(\delta)} = \frac{k-q+\delta}{k-q+2\delta}\left(\sqrt{\chi^2_{k-q}(1-\alpha)}-\sqrt{\delta}\right)^2\right\} = 1-\alpha-\varepsilon, \tag{8}$$

where $t(\delta) = (k-q+\delta)^2/(k-q+2\delta)$. *Then*

$$\delta\mathbf{s}'\mathbf{K}_G'\mathbf{C}\mathbf{K}_G\delta\mathbf{s} \leq \frac{2\sqrt{\delta_{max}}}{K^{(par)}_{\delta s}} \Rightarrow \delta \leq \delta_{max}$$

(cf. Definition 3.8).

The solution of the equation (7) for several values of the number $k-q$ is given in Table 4.1

$k-q$	1	2	3	4	5
δ_{max}	0.46	0.64	0.78	0.92	1.05
χ^2_{k-q}	3.84	5.99	7.81	9.49	11.1
$C^{(constr)}$	0.353	0.267	0.226	0.202	0.185

Table 4.1
$1-\alpha = 0.95,\ \varepsilon = 0.05$

When we use this table in practice, it is necessary to attain the value of $C^{(constr)}$ smaller than $2\sqrt{\delta_{max}}/\chi^2_{n-q}(1-\alpha)$ in order to linearize the constraints. Maximal admissible values of $C^{(constr)}$ are given also in Table 4.1

Analogously the solution of the equation (8) for several values of the number $k-q$ is given in Table 4.2

$k-q$	1	2	3	4	5
δ_{max}	0.07	0.07	0.065	0.065	0.065
χ^2_{k-q}	3.84	5.99	7.81	9.49	11.1
$C^{(par)}_{I,\delta\beta}(K^{(par)})$	0.138	0.088	0.020	0.051	0.046

Table 4.2
$1-\alpha = 0.95$, $\varepsilon = 0.05$

Table 4.2 can be used also in the case that both the model and the constraints are nonlinear. In that case it is necessary to design the experiment in such a way that

$$2\sqrt{\delta_{max}/\chi^2_{n-q}(1-\omega)} \gg C^{(par)}_{I,\delta\beta}(K^{(par)})$$

in order to linearize the model and the constraints. Maximal admissible values of $C^{(par)}_{I,\delta\beta}$ $(K^{(par)})$ are given also in Table 4.2.

In all cases the inequality for $C^{(constr)}$, $K^{(par)}$, $C^{(par)}_{I,\delta\beta}$ must be attained for a sufficiently small ω in order to be practically sure that the value $\boldsymbol{\beta}_0$ is in a sufficiently small neigbourhood of the actual value of the parameter $\boldsymbol{\beta}$.

5 Numerical example

Let (cf. also Example 4.3 in [5])

$$\mathbf{Y} \sim N_n(\mathbf{f}(\boldsymbol{\beta}), \sigma^2\mathbf{I}), \qquad \mathbf{g}(\boldsymbol{\beta}) = \mathbf{0}$$

be under consideration. Here

$$f_i(\boldsymbol{\beta}) = \begin{cases} l_1(x_i,\beta_1) &= \beta_1 x_i, \quad x_i \le 5, \\ l_2(x_i,\beta_2,\beta_3) &= \beta_2\exp(\beta_3 x_i), \; x_i \ge 5, \end{cases}$$

$$g(\beta_1,\beta_2,\beta_3) = l_1(5,\beta_1) - l_2(5,\beta_2,\beta_3) = 5\beta_1 - \beta_2\exp(5\beta_3).$$

Further

$$\begin{aligned} \beta_1 &= 1.473, & \beta_2 &= 33, & \beta_3 &= -0.299954, \\ \beta_1^{(0)} &= 1.473, & \beta_2^{(0)} &= 33, & \beta_3^{(0)} &= -0.299954, \end{aligned}$$

$$\begin{aligned} \partial l_1(x_i,\beta_1)/\partial(\beta_1,\beta_2,\beta_3) &= (x_i,0,0), \\ \partial l_2(x_i,\beta_2,\beta_3))/\partial(\beta_1,\beta_2,\beta_3) &= (0,\exp(x_i\beta_3), x_i\beta_2\exp(x_i\beta_3)), \\ \partial g(\beta_1,\beta_2,\beta_3))/\partial(\beta_1,\beta_2,\beta_3) &= (5,-\exp(5\beta_3), -5\beta_2\exp(5\beta_3)). \end{aligned}$$

x	1	2	3	6	7	8
y	1.2	3.2	4.9	5.1	3.8	2.5
$l_1(x,\beta_1)$	1.473	2.945	4.418			
$l_2(x,\beta_2,\beta_3)$				5.455	4.041	2.994

Table 5.1
$\sigma^2 = (0.5)^2$, $\alpha = 0.05$

In this case we obtain $C^{(par)} = 5.5672$ (cf. [8]) and we cannot assume that the confidence region from Lemma 4.1 can be approximated by the confidence ellipsoid from Lemma 1.3. Thus let us assume the situation given in Table 5.2.

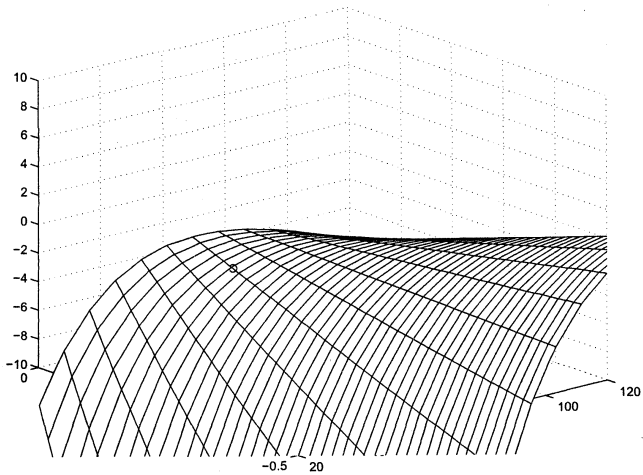

Fig. 5.1
Graph of function $5 \times 1.473 - \beta_2 e^{\beta_3}$.

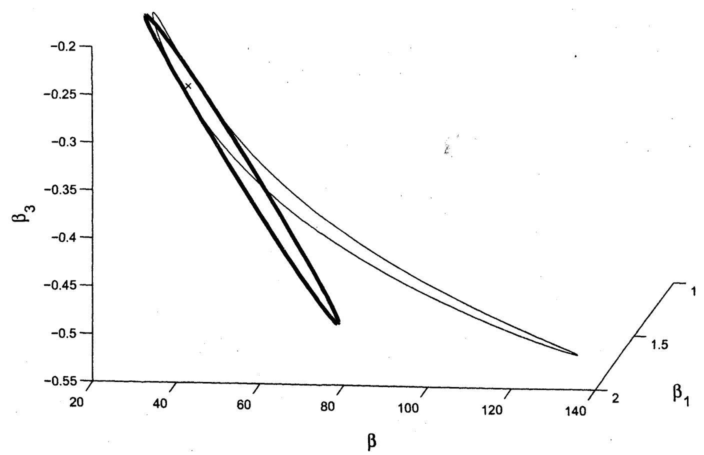

Fig. 5.2
The confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on 3D space for data from Table 5.1

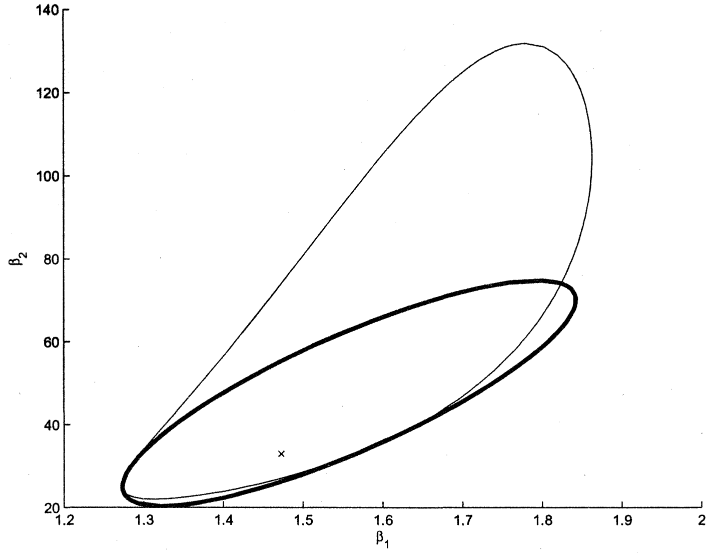

Fig. 5.3
Projection of the confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on the coordinate axes β_1, β_2 for data from Table 5.1

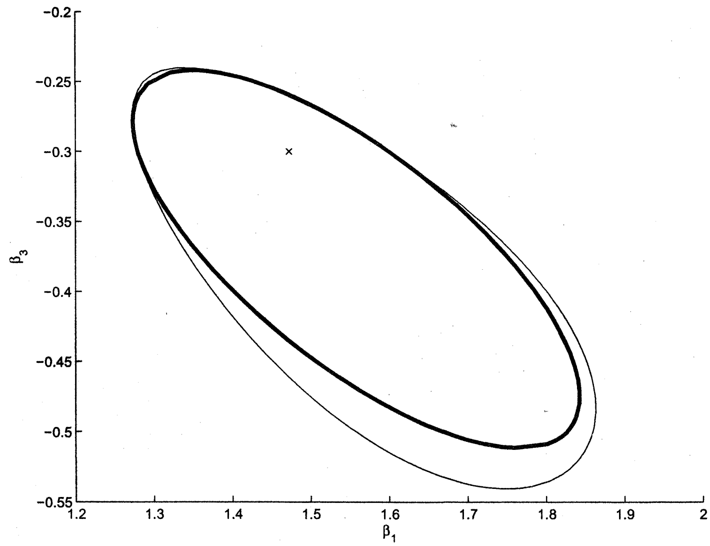

Fig. 5.4
Projection of the confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on the coordinate axes β_1, β_3 for data from Table 5.1

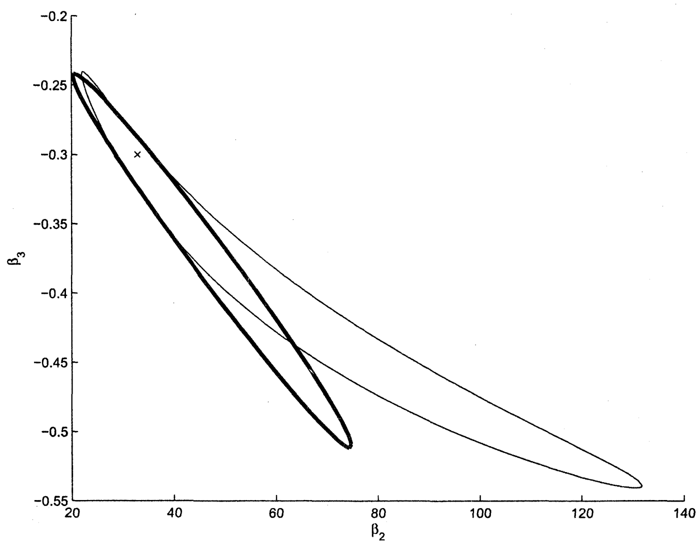

Fig. 5.5
Projection of the confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on the coordinate axes β_2, β_3 for data from Table 5.1

x	1	2	3	6	7	8
y	1.48	2.94	4.42	5.46	4.03	2.98
$l_1(x, \beta_1)$	1.473	2.945	4.418			
$l_2(x, \beta_2, \beta_3)$				5.455	4.041	2.994

Table 5.2
$\sigma^2 = (0.01)^2$, $\alpha = 0.05$

In this case $C^{(par)} = 0.111\,344$ (cf. [8]) and the agreement between confidence region from Lemma 4.1 and Lemma 1.3 should be satisfactory. The following figures ([9]) show this fact.

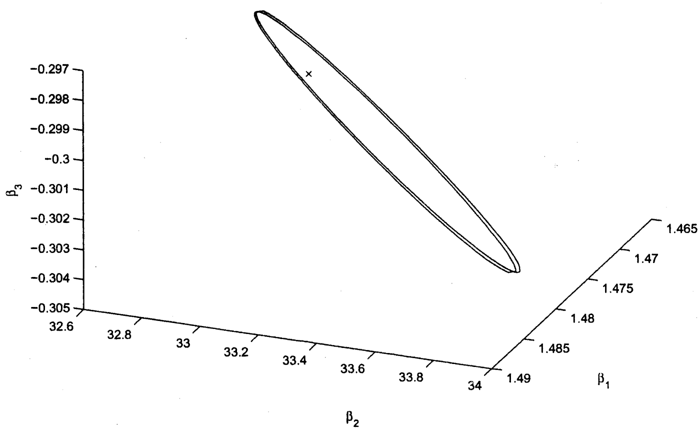

Fig. 5.6
The confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on 3D space for data from Table 5.2

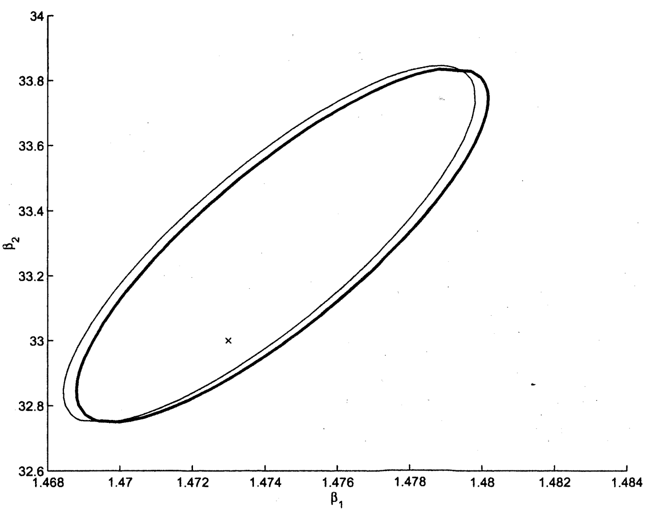

Fig. 5.7
Projection of the confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on the coordinate axes β_1, β_2 for data from Table 5.2

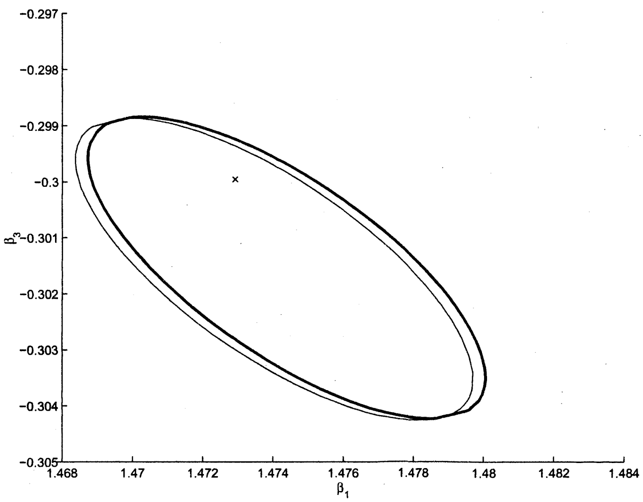

Fig. 5.8
Projection of the confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on the coordinate axes β_1, β_3 for data from Table 5.2

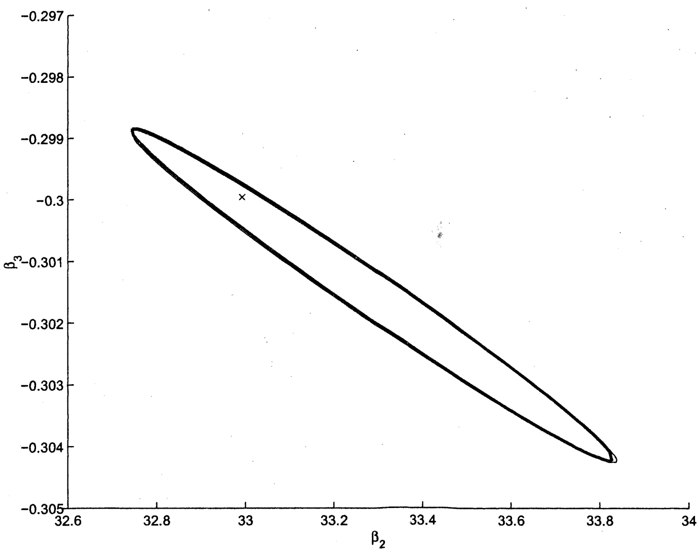

Fig. 5.9
Projection of the confidence region (Lemma 4.1) and confidence ellipse (Lemma 1.3) on the coordinate axes β_2, β_3 for data from Table 5.2

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