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Linearization Regions for a Determination of a Calibration Curve *

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Abstract

A calibration problem can be described by a regression model with constraints on parameters. These constraints are nonlinear and thus the linearization procedures has been used. The problem is to find the conditions under which the linearization does not affect the unbiasedness of the estimation significantly.

Key words: Regression model with constraints, linearization, bias, measures of nonlinearity.

1991 Mathematics Subject Classification: 62J05, 62F99

Introduction

One of the calibration problems is to determine the values of the parameters $\beta_1$ and $\beta_2$ from the measured values $\mu_1, \ldots, \mu_n$ and $\nu_1, \ldots, \nu_n$, when simultaneously the relation $\nu_i = \beta_1 + \beta_2 \mu_i$, $i = 1, \ldots, n$, is assumed.

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Under stochastically independent measurements of the values \( \mu \) and \( \nu \), the model of measurement is

\[
E \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} I, 0 \\ 0, I \end{pmatrix} \begin{pmatrix} \mu \\ \nu \end{pmatrix}, \quad \text{Var} \begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \sigma_1^2 I, 0 \\ 0, \sigma_2^2 I \end{pmatrix}.
\]

Here \( E(\frac{X}{Y}) \) is the mean value of the observation vector \( (\frac{X}{Y}) \), \( \text{Var} (\frac{X}{Y}) \) is the covariance matrix of this vector, \( \sigma_1^2 \) and \( \sigma_2^2 \) are dispersions in the measurement of the values \( \mu \) and \( \nu \), respectively, \( I \) is the \( n \times n \) identity matrix. The unknown parameters occur in the constraints

\[
1 \beta_1 + \mu \beta_2 - \nu = 0,
\]

only (here \( I = (1, \ldots, 1)' \in R^n \)). The constraints (2) are nonlinear; their linearization in approximate values \( \mu_0, \nu_0, \beta_{1,0} \) and \( \beta_{2,0} \) can be written in the form

\[
1 \beta_{1,0} + \mu_0 \beta_{2,0} - \nu_0 + (\beta_{2,0} I, -I) \begin{pmatrix} \delta \mu \\ \delta \nu \end{pmatrix} + (1, \mu_0) \begin{pmatrix} \delta \beta_1 \\ \delta \beta_2 \end{pmatrix} = 0.
\]

The neglected quadratic term is \( \delta \mu \delta \beta_2 \); here \( \delta \mu = \mu - \mu_0, \delta \nu = \nu - \nu_0, \delta \beta_1 = \beta_1 - \beta_{1,0} \) and \( \delta \beta_2 = \beta_2 - \beta_{2,0} \).

The problem is to determine boundaries of the region where the changes of \( \delta \beta_2 \) and \( \delta \mu \) cannot cause a significant bias in estimators of the parameters \( \beta_1 \) and \( \beta_2 \). It will be shown that the relation between \( \sigma_1 \) and \( \sigma_2 \) is decisive.

\section{Notation and auxiliary statements}

The notation

\[
H_1 = (\beta_{2,0} I, -I), \quad H_2 = (1, \mu_0), \quad \frac{1}{2} \omega (\delta \mu, \delta \beta_2) = \delta \mu \delta \beta_2
\]

will be used in the following.

\textbf{Lemma 1.1} In the model (1) with the linearized constraints (3) the best linear unbiased estimators (BLUE) of the parameters \( \delta \mu, \delta \nu, \delta \beta_1 \) and \( \delta \beta_2 \) are given by the relations

\[
\delta \mu = X - \mu_0 + \frac{\sigma_1^2 \beta_{2,0}}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_{1, \mu_0} [Y - \beta_{2,0} (X - \mu_0)],
\]

\[
\delta \nu = Y - \nu_0 - \frac{\sigma_2^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_{1, \mu_0} [Y - \beta_{2,0} (X - \mu_0)],
\]

\[
\begin{pmatrix} \delta \beta_1 \\ \delta \beta_2 \end{pmatrix} = - \begin{pmatrix} \beta_{1,0} \\ \beta_{2,0} \end{pmatrix} + \begin{pmatrix} n, 1' \mu_0 \\ \mu_0 1, \mu_0 \mu_0 \end{pmatrix}^{-1} \begin{pmatrix} 1' \\ \mu_0 \end{pmatrix} [Y - \beta_{2,0} (X - \mu_0)].
\]

Here

\[
M_{1, \mu_0} = I - (1, \mu_0) \begin{pmatrix} n, 1' \mu_0 \\ \mu_0 1, \mu_0 \mu_0 \end{pmatrix}^{-1} \begin{pmatrix} 1' \\ \mu_0 \end{pmatrix}.
\]
The variances and cross-covariance matrices of the estimators are

\[
\text{Var}(\hat{\mu}) = \sigma_1^2 \left( I - \frac{\sigma_1^2 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_{1,\mu_0} \right),
\]

\[
\text{cov}(\hat{\mu}, \hat{\nu}) = \frac{\sigma_1^2 \sigma_2^2 \beta_{2,0}}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_{1,\mu_0},
\]

\[
\text{cov}(\hat{\mu}, (\hat{\beta}_1)) = -\sigma_1^2 \beta_{2,0} (1, \mu_0) \left( \begin{array}{c} n, 1' \mu_0 \\ \mu_0' 1, \mu_0 \mu_0 \end{array} \right)^{-1},
\]

\[
\text{Var}(\hat{\nu}) = \sigma_2^2 \left( I - \frac{\sigma_2^2 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_{1,\mu_0} \right),
\]

\[
\text{cov}(\hat{\nu}, (\hat{\beta}_1)) = -\sigma_2^2 (1, \mu_0) \left( \begin{array}{c} n, 1' \mu_0 \\ \mu_0' 1, \mu_0 \mu_0 \end{array} \right)^{-1},
\]

\[
\text{Var}(\hat{\beta}_1) = (\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2) \left( \begin{array}{c} n, 1' \mu_0 \\ \mu_0' 1, \mu_0 \mu_0 \end{array} \right)^{-1}.
\]

**Proof** see in [1].

**Remark 1.2** The coefficients \( \frac{\sigma_1^2 \beta_{2,0}}{\sigma_1^2 \beta_{2,0} + \sigma_2^2} \) and \( -\frac{\sigma_2^2 \beta_{2,0}}{\sigma_1^2 \beta_{2,0} + \sigma_2^2} \), which occur in the estimators \( \hat{\mu} \) and \( \hat{\nu} \), show that the task of the estimation of the parameters \( \beta_1 \) and \( \beta_2 \) can be formulated as follows. To determine \( \beta_1 \) and \( \beta_2 \) in such a way that the sum of squared distances of the points \( (X_i, Y_i), i = 1, \ldots, n \), from the resulting position of the line \( y = \beta_1 + \beta_2 x \) be minimized; the distances are given in the Mahalanobis norm \( \| (x, y) \| = \sqrt{x^2 + \frac{y^2}{\sigma_1^2}} \). It means that the function

\[
\Phi(\beta_1, \beta_2) = \sum_{i=1}^{n} \frac{(Y_i - \beta_1 - \beta_2 X_i)^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}
\]

must be minimized.

**Lemma 1.3** Let \( \xi_i = X_i - \bar{X}, \eta_i = Y_i - \bar{Y}, i = 1, \ldots, n \), where \( \bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i \), \( \bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i \). Let

\[
\Phi(\beta_1, \beta_2) = \sum_{i=1}^{n} \frac{(Y_i - \beta_1 - \beta_2 X_i)^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}
\]

and \( \hat{\beta}_1 \) and \( \hat{\beta}_2 \) minimize the function \( \Phi(\cdot, \cdot) \). Then \( \hat{\beta}_1 = \bar{Y} - \hat{\beta}_2 \bar{X} \) and

\[
\hat{\beta}_2 = \frac{1}{2 \sigma_1^2 \sum_{i=1}^{n} \xi_i \eta_i} \left\{ -\sum_{i=1}^{n} (\sigma_2^2 \xi_i^2 - \sigma_1^2 \eta_i^2) + \\
+ \sqrt{\left[ \sum_{i=1}^{n} (\sigma_2^2 \xi_i^2 - \sigma_1^2 \eta_i^2) \right]^2 + 4 \sigma_1^2 \sigma_2^2 \left( \sum_{i=1}^{n} \xi_i \eta_i \right)^2} \right\}.
\]


Proof It holds

\[
\frac{\partial \Phi(\beta_1, \beta_2)}{\partial \beta_1} \bigg|_{\beta=\hat{\beta}} = -\sum_{i=1}^{n} \frac{2(Y_i - \hat{\beta}_1 - \hat{\beta}_2 X_i)}{\sigma^2_{\hat{\beta}_2} + \sigma^2_2} = 0
\]

\[\Rightarrow \hat{\beta}_1 = \bar{Y} - \hat{\beta}_2 \bar{X}\]

\[\Rightarrow \phi(\hat{\beta}_2) = \sum_{i=1}^{n} \frac{[Y_i - \hat{\beta}_1 - \hat{\beta}_2 X_i - (\bar{Y} - \hat{\beta}_1 - \hat{\beta}_2 \bar{X})]^2}{\sigma^2_{\hat{\beta}_2} + \sigma^2_2} = \sum_{i=1}^{n} \frac{(\eta_i - \hat{\beta}_2 \xi_i)^2}{\sigma^2_{\hat{\beta}_2} + \sigma^2_2}.
\]

To finish the proof it is sufficient to solve the equation \(d\phi(\hat{\beta}_2)/d\hat{\beta}_2 = 0\). \(\Box\)

Remark 1.4 If the procedure for the estimators \(\hat{\beta}_1\) and \(\hat{\beta}_2\) from Lemma 1.1 (with some iterations) is used, we obtain the values from Lemma 1.3. Even Lemma 1.3 is suitable from the numerical viewpoint, it is not suitable for an investigation of statistical properties because of the nonlinearity. Therefore in the following we will start from Lemma 1.1. In addition it is to be said that Lemma 1.3 cannot be used in the case of a nonlinear calibration curve, however Lemma 1.1 is a good basis for any form of a calibration curve. It is sufficient to change properly the linearized constraints.

2 Nonlinearity of the model and linearization regions

Lemma 2.1 The bias of the estimator \(\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix}\) from Lemma 1.1 is

\[
E \left( \begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} \right) - \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} n, \\ \mu'_0, \mu_0' \mu_0 \end{pmatrix}^{-1} \begin{pmatrix} 1' \\ \mu'_0 \end{pmatrix} \delta \mu \delta \beta_2.
\]

Proof is obvious. \(\Box\)

In the following the symbol \(K_A\) means the matrix with the properties \(A_{m,n} K_A = 0\), \(K_A\) is of the type \(n \times [n - r(A)]\) and \(r(K_A)\) (the rank of the matrix \(K_A\)) = \(n - r(A)\). Obviously \(\text{Ker}(A) = \{u : Au = 0\} = M(K_A)\) (here \(M(\cdot)\) denotes the column space of the proper matrix).

Lemma 2.2 Let \(H = (H_1, H_2)\); then

\[
K_H = \begin{pmatrix} K_1 \\ \cdots \\ K_2 \end{pmatrix} = \begin{pmatrix} I, & 1, & -\mu_0 \\ \beta_{2,0} I, & \mu_0, & 1 \\ \cdots & \cdots & \cdots \\ 0', & -\beta_{2,0}, & 1 \\ 0', & 1, & \beta_{2,0} \end{pmatrix}.
\]
Proof Obviously $HK_H = 0$. With respect to our assumption $r(H_1, H_2) = n$, $r(H_2) = 2$. Since $K_H$ is the matrix of type $(2n + 2) \times (n + 2)$ and its rank is $r(K_H) = n + 2$, the assertion is proved.

Lemma 2.3 Model (1) with the constraints (2) is, with the exception of the terms of the higher order than two, equivalent to the model

$$E\left(\begin{array}{c} X \\ Y \end{array}\right) = K_1 \kappa - T \frac{1}{2} \omega(K_H \kappa), \quad (4)$$

where

$$\begin{pmatrix} T \\ U \end{pmatrix} = (H_1, H_2)^{-1} = \begin{pmatrix} \beta_{2,0} I \\ -I \\ \cdots \\ n, 1' \mu_0 \\ \mu_0' 1, \mu_0 \mu_0 \end{pmatrix} \left[ (1 + \beta_{2,0}^2) I + P_{1, \mu_0} \right]^{-1},$$

$$-T \frac{1}{2} \omega(K_H \kappa) = -\begin{pmatrix} \beta_{2,0} I \\ -I \end{pmatrix} \left[ (1 + \beta_{2,0}^2) I + P_{1, \mu_0} \right]^{-1} (I, L^T, -\mu_0) \kappa (0', 1, \beta_{2,0}) \kappa.$$

Proof The constraint

$$H_1 \begin{pmatrix} \delta \mu \\ \delta \nu \end{pmatrix} + H_2 \begin{pmatrix} \delta \beta_1 \\ \delta \beta_2 \end{pmatrix} + \frac{1}{2} \omega(\delta \mu, \delta \beta_1, \delta \beta_2) = 0$$

enables us to determine the parameters $\delta \mu, \delta \nu, \delta \beta_1$ and $\delta \beta_2$ in the form

$$\begin{pmatrix} \delta \mu \\ \delta \nu \\ \delta \beta_1 \\ \delta \beta_2 \end{pmatrix} = \begin{pmatrix} K_1 \\ K_2 \end{pmatrix} \kappa + \frac{1}{2} \tau(\kappa),$$

where $\tau$ is a vector of the quadratic forms of the vector $\kappa$. Since

$$(H_1, H_2) \tau + \omega = 0,$$

we obtain

$$\tau = -\begin{pmatrix} T \\ U \end{pmatrix} \omega$$

and simultaneously the vectors $\delta \mu, \delta \nu, \delta \beta_1, \delta \beta_2$ in $\omega$ can be substituted by the vector $K_H \kappa$. In our case

$$\frac{1}{2} \omega(\delta \mu, \delta \nu, \delta \beta_1, \delta \beta_2) = \delta \mu \delta \beta_2$$

and thus

$$\delta \mu = (I, 1, -\mu_0) \kappa, \quad \delta \beta_2 = (0', 1, \beta_{2,0}) \kappa.$$

The form of the matrices $T$ and $U$ can be verified directly from the relation

$$(H_1, H_2) \begin{pmatrix} T \\ U \end{pmatrix} = I.$$
Remark 2.4 Nonlinear models of the form (4) are investigated in [2]. Further investigation is restricted to the determination of the linearization region with respect to the bias of the estimators $\beta_1$ and $\beta_2$.

Remark 2.5 Let $n \times n$ matrix $A$ be symmetric and positive definite and $B$ be an arbitrary $n \times k$ matrix. Obviously

$$\{x : x'Ax \leq c^2\} \cap M(B) = \{By : y'B'ABy \leq c^2\}.$$ 

If it is necessary to determine the boundaries of the set on the right hand side and simultaneously the boundaries of the set $\{x : x'Ax \leq c^2\}$ can be determined in an easier way, then the easier way will be chosen. If some condition is satisfied on the set $\{x : x'Ax \leq c^2\}$, then it is obviously satisfied on the set $\{By : y'B'ABy \leq c^2\}$ as well. This simple fact will be utilized in the following.

Lemma 2.6 Let $a \in \mathbb{R}^n$ and the quadratic form be given by the relation

$$a'xy = (x', y)\left(\begin{array}{cc} 0, & \frac{1}{2}a' \\ \frac{1}{2}a', & 0 \end{array}\right)\left(\begin{array}{c} x \\ y \end{array}\right) = c^2, \quad x \in \mathbb{R}^n, \ y \in \mathbb{R}^1.$$ 

Then the matrix

$$A = \left(\begin{array}{cc} 0, & \frac{1}{2}a' \\ \frac{1}{2}a', & 0 \end{array}\right)$$

has nonzero eigenvalues equal to

$$\sqrt{a'a}/2, -\sqrt{a'a}/2$$

and the corresponding eigenvectors are

$$f_1 = \frac{1}{\sqrt{2}} \left(\begin{array}{c} a/\sqrt{a'a} \\ 1 \end{array}\right), \quad f_2 = \frac{1}{\sqrt{2}} \left(\begin{array}{c} a/\sqrt{a'a} \\ -1 \end{array}\right).$$

Proof

$$\det\left[\left(\begin{array}{cc} 0, & \frac{1}{2}a' \\ \frac{1}{2}a', & 0 \end{array}\right) - \lambda \left(\begin{array}{cc} 1, & 0' \\ 0', & 1 \end{array}\right)\right] = (-1)^n\lambda^{n-1} \left(-\lambda^2 + \frac{a'a}{4}\right).$$

By the solution of the equation

$$(-1)^n\lambda^{n-1} \left(-\lambda^2 + \frac{a'a}{4}\right) = 0$$

and by the verification of the equalities

$$Af_i = \lambda_if_i, \quad i = 1, 2,$$

the assertion is proved. $\square$
Theorem 2.7 If

\[ \delta \mu' \delta \mu + \delta \beta_2^2 \leq 2 \varepsilon_1 \sqrt{1'M_{\mu_0}1} \left( \frac{2 \varepsilon_1 \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}}{\text{Var}(\hat{\beta}_1)} \right), \]

then \( |E(\hat{\beta}_1) - \beta_1| \leq \varepsilon_1 \).

Proof With respect to Lemma 2.1 we have

\[
\begin{align*}
\mu_1 &= \left\{ \left( \begin{array}{c} n, \\
\mu_0' \mu_0 \end{array} \right)^{-1} \right\} \left( \begin{array}{c} 1' \\
\mu_0' \end{array} \right) \delta \mu \delta \beta_2 \\
&= ([n - 1'\mu_0(\mu_0'\mu_0)^{-1} \mu_0']^{-1}, -[n - 1'\mu_0(\mu_0'\mu_0)^{-1} \mu_0']^{-1} 1'\mu_0(\mu_0'\mu_0)^{-1}) \\
&\quad \times \left( \begin{array}{c} 1' \\
\mu_0' \end{array} \right) \delta \mu \delta \beta_2 = (1'M_{\mu_0}1)^{-1} 1'M_{\mu_0} \delta \mu \delta \beta_2.
\end{align*}
\]

Regarding Lemma 2.6

\[
(1'M_{\mu_0}1)^{-1} 1'M_{\mu_0} \delta \mu \delta \beta_2 = \\
= (\delta \mu', \delta \beta_2) \begin{pmatrix}
\frac{1}{2} (1'M_{\mu_0}1)^{-1} 1'M_{\mu_0} & 0 \\
0 & \frac{1}{2} (1'M_{\mu_0}1)^{-1} 1'M_{\mu_0}
\end{pmatrix} \begin{pmatrix}
\delta \mu \\
\delta \beta_2
\end{pmatrix}
\]

and the nonzero eigenvalues of this quadratic form are

\[
\lambda_{1,2} = \left\{ \begin{array}{cl}
\frac{1}{2} \sqrt{(1'M_{\mu_0}1)^{-1} 1'M_{\mu_0}M_{\mu_0} 1(1'M_{\mu_0}1)^{-1}} = \frac{1}{2} \sqrt{(1'M_{\mu_0}1)^{-1}}, \\
-\frac{1}{2} \sqrt{(1'M_{\mu_0}1)^{-1} 1'M_{\mu_0}M_{\mu_0} 1(1'M_{\mu_0}1)^{-1}} = -\frac{1}{2} \sqrt{(1'M_{\mu_0}1)^{-1}}.
\end{array} \right.
\]

The set of those vectors \( \left( \delta \mu', \delta \beta_2 \right) \) for which \( |b_1| \leq \varepsilon_1 \), is hyperbolic cylinder

\[
|\langle \delta \mu', \delta \beta_2 \rangle \lambda_1 (f_1 f_1' - f_2 f_2') \left( \begin{array}{c} \delta \mu \\
\delta \beta_2
\end{array} \right)| \leq \varepsilon_1, \quad (5)
\]

where \( \lambda_1 = 1/(2 \sqrt{1'M_{\mu_0}1}) \) and \( f_1 \) and \( f_2 \) are eigenvectors corresponding with \( \lambda_1 \) and \( \lambda_2 = -\lambda_1 \), respectively.

Thus if

\[
(\delta \mu', \delta \beta_2) \left( \begin{array}{c} \delta \mu \\
\delta \beta_2
\end{array} \right) \leq 2 \varepsilon_1 \sqrt{1'M_{\mu_0}1},
\]

then (5) is valid and \( |b_1| \leq \varepsilon_1 \).

\[ \square \]

Remark 2.8 Since \( 1'M_{\mu_0}1 = n \sin^2 \phi \), where \( \phi \) is an angle between the vectors \( 1 \) and \( \mu_0 \), it is desirable to have the vector \( \mu_0 \) as orthogonal to the vector \( 1 \) as possible, i.e. \( 1'\mu_0 \) should be as near to zero as possible.
Theorem 2.9 If

\[ \delta \mu' \delta \mu + \delta \beta_2^2 \leq 2 \varepsilon_2 \sqrt{\mu_0' M_n \mu_0} \left( \frac{2 \varepsilon_2 \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}}{\sqrt{\text{Var}(\hat{\beta}_2)}} \right), \]

where \( M_n = I_{n,n} - \frac{1}{n} 1'1 \), then

\[ |b_2| = |E(\hat{\beta}_2) - \beta_2| \leq \varepsilon_2. \]

Proof  Analogously as in Theorem 2.7

\[ b_2 = \left\{ \left( \begin{array}{c} \mu_0' \mu_0 \\ \mu_0' 1, \mu_0' \mu_0 \end{array} \right)^{-1} \right\} \cdot \left( \begin{array}{c} 1' \\ \mu_0' \mu_0 \end{array} \right) \delta \mu \delta \beta_2 = (\mu_0' M_n \mu_0)^{-1} \mu_0' M_n \delta \mu \delta \beta_2. \]

Now Lemma 2.6 is used and the proof is finished in the same way as in Theorem 2.7.

Remark 2.10 Since

\[ \mu_0' M_n \mu_0 = \sum_{i=1}^{n} (\mu_{0,i} - \overline{\mu}_0)^2, \]

where \( \overline{\mu}_0 = \frac{1}{n} \sum_{i=1}^{n} \mu_{0,i} \), it is desirable to spread the values \( \mu_{0,1}, \ldots, \mu_{0,n} \) on the as large interval as possible.

Example 2.11 Let the values \( \mu_i \in \{1, 2, 3, 4, 5, 6, 7\} \) be measured with the accuracy characterized by the standard deviation \( \sigma_1 = 0.1 \) and the corresponding values \( \nu \) with the same accuracy, i.e. \( \sigma_2 = \sigma_1 = 0.1 \). The approximate value of \( \beta_2 \) is \( \beta_{2,0} = 1 \).

The linearization region for \( \beta_1 \) (Theorem 2.7) is

\[ \left\{ \left( \begin{array}{c} \delta \mu \\ \delta \beta_2 \end{array} \right) : \delta \mu' \delta \mu + \delta \beta_2^2 \leq 2.366 \varepsilon_1 \right\} \]

and for \( \beta_2 \) (Theorem 2.9)

\[ \left\{ \left( \begin{array}{c} \delta \mu \\ \delta \beta_2 \end{array} \right) : \delta \mu' \delta \mu + \delta \beta_2^2 \leq 10.583 \varepsilon_2 \right\}. \]

If \( \varepsilon_1 = \frac{1}{4} \sqrt{\text{Var}(\hat{\beta}_1)} \) and \( \varepsilon_2 = \frac{1}{4} \sqrt{\text{Var}(\hat{\beta}_2)} \), then \( 2.366 \varepsilon_1 = 10.582 \varepsilon_2 = 0.071 \);

\( \sqrt{\text{Var}(\hat{\beta}_1)} = 0.120, \sqrt{\text{Var}(\hat{\beta}_2)} = 0.026. \) The uncertainty in \( \delta \mu \) is thus decisive. The a priori confidence region for \( \mu \) is

\[ \{ \mu : (\mu - \mathbf{X})'(\mu - \mathbf{X}) \leq \sigma_1^2 \chi^2_{\alpha}(0,1 - \alpha) \}; \]

if \( \sigma_1 = 0.1 \) and \( 1 - \alpha = 0.95 \), then \( \sigma_1^2 \chi^2_{\alpha}(0,0.95) = 0.1407 \). Thus the linearization is not admissible, since 0.1407 > 0.071.
If \( \sigma_1 = 0.01 \), then \( \sigma_1^2 \chi^2_1(0;0.95) = 0.00147 \) and the requirements on the linearization are satisfied very well; \( 2.366 \sqrt{\text{Var}(\hat{\beta}_1)/4} = 10.583 \sqrt{\text{Var}(\hat{\beta}_2)/4} = 0.0071 > 0.00147 \). For \( \sigma_1 = \sigma_2 = 0.048 \) the equality

\[
\sigma_1^2 \chi^2_1(0;0.95) = 2.366 \sqrt{\text{Var}(\hat{\beta}_1)/4} = 10.583 \sqrt{\text{Var}(\hat{\beta}_2)/4}
\]

holds. (Cf. further Theorem 2.15 and Example 2.16).

**Remark 2.12** The bias in estimators of parameters is expressed usually in the \( \varepsilon \)-multiple of the standard deviation. Since

\[
\sqrt{\text{Var}(\hat{\beta}_1)} = \sqrt{\frac{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}{n - 1} \mu_0 (\mu_0^\prime \mu_0)^{-1} \mu_0^\prime \mathbf{1}} = \sqrt{\frac{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}{1' \mathbf{M}_{\mu_0} \mathbf{1}}},
\]

the linearization region (in our case it is a ball) must have the radius

\[
R = \sqrt{2 \varepsilon \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}}
\]

in order to be valid

\[
\delta \mu' \delta \mu + \delta \beta_2^2 \leq 2 \varepsilon \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} \Rightarrow |b_1| \leq \varepsilon \sqrt{\text{Var}(\hat{\beta}_1)}.
\]

Analogously for the parameter \( \beta_2 \)

\[
\delta \mu' \delta \mu + \delta \beta_2^2 \leq 2 \varepsilon \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} \Rightarrow |b_2| \leq \varepsilon \sqrt{\text{Var}(\hat{\beta}_2)}.
\]

The linearization region for both parameters is the same; it is a certain advantage.

In general the linearization region must cover the confidence region for the parameters \( \delta \mu \) and \( \delta \beta_2 \) significantly. In the case that the inequalities \( |b_i| \leq \varepsilon \sqrt{\text{Var}(\hat{\beta}_i)}, i = 1, 2 \), are required, it must hold

\[
\left\{ \begin{pmatrix} \delta \mu \\ \delta \beta_2 \end{pmatrix} : \left( \delta \mu - \delta \hat{\mu} \right)' \left[ \text{Var} \left( \begin{pmatrix} \delta \hat{\mu} \\ \delta \hat{\beta}_2 \end{pmatrix} \right) \right]^{-1} \left( \delta \mu - \delta \hat{\mu} \right) \leq \chi^2_{1 + 1}(0;1 - \alpha) \right\}
\]

\[
\subset \left\{ \begin{pmatrix} \delta \mu \\ \delta \beta_2 \end{pmatrix} : \delta \mu' \delta \mu + \delta \beta_2^2 \leq 2 \varepsilon \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} \right\}
\]

for a sufficiently small \( \alpha \).

**Lemma 2.13** It holds

\[
\left[ \text{Var} \left( \begin{pmatrix} \delta \hat{\mu} \\ \delta \hat{\beta}_2 \end{pmatrix} \right) \right]^{-1} = \begin{pmatrix} \frac{1}{\sigma_1^2} \mathbf{I} + \frac{\beta_{2,0}^2}{\sigma_2^2} \mathbf{M}_n, & \frac{\beta_{2,0}^2}{\sigma_2^2} \mu_0 \mathbf{M}_n, \\ \frac{\beta_{2,0}^2}{\sigma_2^2} \mathbf{M}_n \mu_0, & \frac{1}{\sigma_2^2} \mu_0' \mathbf{M}_n \mu_0 \end{pmatrix}.
\]
Proof With respect to Lemma 1.1

\[
\text{Var} \left( \frac{\delta \mu}{\delta \beta_2} \right) = \left( \begin{array}{ccc}
\sigma_1^2 - \frac{\sigma_1^4 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} & M_{1,\mu_0} & -\sigma_1^2 \beta_{2,0} M_{1,\mu_0} (\mu_0 M_n \mu_0)^{-1} \\
-\left( \mu_0 M_n \mu_0 \right)^{-1} \mu_0 M_{1,\beta_2,0} \sigma_1^2 & \sigma_1^2 \beta_{2,0} + \frac{\sigma_2^2}{\sigma_1^2} & \left( \sigma_1^2 \beta_{2,0}^2 + \sigma_2^2 \right) (\mu_0' M_n \mu_0)^{-1}
\end{array} \right).
\]

Now the Rohde formula in the form

\[
(A, B, C) = \left( \begin{array}{ccc}
(A - BC^{-1} B')^{-1} & -(A - BC^{-1} B')^{-1} BC^{-1} \\
-C^{-1} B'(A - BC^{-1} B')^{-1} & (C - B' A^{-1} B')^{-1}
\end{array} \right)
\]

will be used; here

\[
A - BC^{-1} B' =
\]

\[
= \sigma_1^2 I - \frac{\sigma_1^4 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_{1,\mu_0} - \frac{\sigma_1^4 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_n \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' M_n.
\]

In the next step the equality

\[
M_{1,\mu_0} + M_n \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' M_n = M_n
\]

must be proved.

With respect to definition

\[
M_{1,\mu_0} = I - 1, \mu_0 \end{array} \right) \end{array} \right)
\]

\[
= I - (1, \mu_0) \left( \begin{array}{ccc}
\frac{1}{n} + \frac{1}{n} \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' 1 \frac{1}{n}, & -\frac{1}{n} \mu_0 (\mu_0' M_n \mu_0)^{-1} 1 \frac{1}{n}
\end{array} \right)
\]

Further

\[
M_{1,\mu_0} + M_n \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' M_n =
\]

\[
= I - \frac{1}{n} 11' - \frac{1}{n} 11' \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' 1 \frac{1}{n} + \frac{1}{n} 11' \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0
\]

\[
= M_n - M_n \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' M_n + M_n \mu_0 (\mu_0' M_n \mu_0)^{-1} \mu_0' M_n = M_n.
\]

Thus we obtain

\[
A - BC^{-1} B' = \sigma_1^2 I - \frac{\sigma_1^4 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} M_n = \frac{\sigma_1^2 \sigma_2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} I + \frac{\sigma_1^4 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} \frac{1}{n} 11'
\]

and

\[
(A - BC^{-1} B')^{-1} =
\]

\[
= \frac{\sigma_1^2 \beta_{2,0} + \sigma_2^2}{\sigma_1^2 \beta_{2,0}^2} I - \frac{\sigma_1^4 \beta_{2,0}^2 + \sigma_2^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} \frac{1}{\sqrt{n}} \frac{\sigma_1^2 \beta_{2,0} + \sigma_2^2}{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2} \frac{1}{\sqrt{n}}
\]

\[
= \frac{\sigma_1^2 \beta_{2,0} + \sigma_2^2}{\sigma_1^2 \beta_{2,0}^2} I - \frac{\sigma_1^4 \beta_{2,0}^2}{\sigma_1^2 \beta_{2,0}^2} \frac{1}{n} = \frac{1}{\sigma_1^2} I + \frac{\beta_{2,0}^2}{\sigma_2^2} M_n.
\]
The further steps of the proof are simple and therefore they are omitted. □

**Lemma 2.14** The eigenvalues of the matrix

\[
\left[ \text{Var} \left( \frac{\delta \mu}{\delta \beta_2} \right) \right]^{-1} = \begin{pmatrix}
\frac{1}{\sigma^2_1} I + \frac{\beta^2_{2,0}}{\sigma_2^2} M_n, & \frac{\beta_{2,0}}{\sigma_2^2} \mu_0' M_n, \\
\frac{\beta_{2,0}}{\sigma_2^2} \mu_0' M_n, & \frac{1}{\sigma_2^2} \mu_0' M_n \mu_0
\end{pmatrix}
\] *(6)*

are

\[
\frac{1}{\sigma^2_1}, \quad \frac{1}{\sigma^2_2} + \frac{\beta^2_{2,0}}{\sigma_2^2}
\]

and

\[
\lambda_{1,2} = \left\{ \begin{array}{l}
\frac{1}{2} \left\{ \left[ \frac{1}{\sigma^2_1} \mu_0' M_n \mu_0 - \left( \frac{1}{\sigma^2_1} + \frac{\beta^2_{2,0}}{\sigma_2^2} \right) \right] + \\
+ \sqrt{\left[ \frac{1}{\sigma^2_1} \mu_0' M_n \mu_0 - \left( \frac{1}{\sigma^2_1} + \frac{\beta^2_{2,0}}{\sigma_2^2} \right) \right]^2 + 4 \frac{\beta^2_{2,0}}{\sigma_2^2} \mu_0' M_n \mu_0} \right\}, \\
\frac{1}{2} \left\{ \left[ \frac{1}{\sigma^2_1} \mu_0' M_n \mu_0 + \left( \frac{1}{\sigma^2_1} + \frac{\beta^2_{2,0}}{\sigma_2^2} \right) \right] - \\
- \sqrt{\left[ \frac{1}{\sigma^2_1} \mu_0' M_n \mu_0 - \left( \frac{1}{\sigma^2_1} + \frac{\beta^2_{2,0}}{\sigma_2^2} \right) \right]^2 + 4 \frac{\beta^2_{2,0}}{\sigma_2^2} \mu_0' M_n \mu_0} \right\}
\right\}
\]

Let \( \frac{1}{\sigma^2_1} < \frac{\mu_0' M_n \mu_0}{\sigma_2^2} \). Then the smallest eigenvalue is greater than \( \frac{1}{2 \sigma^2_1} \).

**Proof** Let

\[
b_0 = M_n \mu_0 / \sqrt{\mu_0' M_n \mu_0},
\]

and \( B_0 \) be a matrix of the type \( n \times (n - 2) \) such that \( M(b_0, B_0) = M(M_n) \), \( b_0' B_0 = 0 \), \( B_0 B_0 = I_{n-2,n-2} \). Then obviously \( M_n = b_0 b_0' + B_0 B_0 \) and the matrix \( (b_0, B_0, 1/\sqrt{n}) \) is orthogonal.

The vector \( \begin{pmatrix} 1/\sqrt{n} \\ 0 \end{pmatrix} \) is an eigenvector of the matrix (6) with the eigenvalue equal to \( \frac{1}{\sigma^2_1} \).

The columns of the matrix \( \begin{pmatrix} B_0' \\ 0' \end{pmatrix} \) are also eigenvectors of the matrix (6) with the common eigenvalue equal to \( \frac{1}{\sigma^2_1} + \frac{\beta^2_{2,0}}{\sigma_2^2} \).

The matrix

\[
\begin{pmatrix}
\frac{1}{\sigma^2_1} I + \frac{\beta^2_{2,0}}{\sigma_2^2} M_n, & \frac{\beta_{2,0}}{\sigma_2^2} \mu_0' M_n, \\
\frac{\beta_{2,0}}{\sigma_2^2} \mu_0' M_n, & \frac{1}{\sigma_2^2} \mu_0' M_n \mu_0
\end{pmatrix}
- \begin{pmatrix}
\frac{1}{\sigma^2_1} 11' / \sqrt{n} + \left( \frac{1}{\sigma^2_1} + \frac{\beta^2_{2,0}}{\sigma_2^2} \right) B_0 B_0', 0 \\
0', \\
\frac{\beta^2_{2,0}}{\sigma_2^2} \mu_0' M_n \mu_0 b_0, \\
\frac{1}{\sigma_2^2} \mu_0' M_n \mu_0
\end{pmatrix}
\]

is
can be expressed as
\[ \lambda_1 f_1 f_1' + \lambda_2 f_2 f_2', \]
where \( \lambda_1 \) and \( \lambda_2 \) are the last two not yet determined eigenvalues.

Obviously the vectors \( f_i, i = 1, 2 \) must be of the form \( \frac{1}{\sqrt{1+y^2}} (b_0, y) \) and the equality
\[
\left( \begin{pmatrix} \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} & \frac{\beta_{2,0}}{\sigma_2^2} \sqrt{\mu_0'M_n\mu_0} b_0 \\ \frac{\beta_{2,0}}{\sigma_2^2} \sqrt{\mu_0'M_n\mu_0} b_0 & \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 \end{pmatrix} \right) \begin{pmatrix} b_0 \\ y \end{pmatrix} = \lambda \begin{pmatrix} b_0 \\ y \end{pmatrix},
\]
must be satisfied.

The last equality contains two unknowns, i.e. \( \lambda \) and \( y \). The quadratic equation for \( \lambda \) has two solutions, given in the assertion of the lemma. Here the solution is omitted, since it is elementary.

As far as the \( \lambda_1 \) is concerned it is valid
\[
\lambda_1 = \frac{1}{2} \left\{ \left[ \frac{1}{\sigma_1^2} \mu_0'M_n\mu_0 + \left( \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \right] \right. \\
+ \sqrt{ \left[ \frac{1}{\sigma_1^2} \mu_0'M_n\mu_0 - \left( \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \right]^2 + 4 \frac{\beta_{2,0}^2}{\sigma_2^4} \mu_0'M_n\mu_0 } \\
\left. > \frac{1}{2} \left\{ \left[ \frac{1}{\sigma_1^2} \mu_0'M_n\mu_0 + \left( \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \right] \right. \\
\left. + \sqrt{ \left[ \frac{1}{\sigma_1^2} \mu_0'M_n\mu_0 - \left( \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \right]^2 } \right\} \\
= \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0. \\
\]

As far as the \( \lambda_2 \) is concerned, we have for the expression under the square root
\[
\left[ \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 - \left( \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \right]^2 + 4 \frac{\beta_{2,0}^2}{\sigma_2^4} \mu_0'M_n\mu_0 = \\
= \left( \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 - \frac{\beta_{2,0}^2}{\sigma_2^2} \right)^2 - 2 \left( \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 - \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \frac{1}{\sigma_1^2} + \frac{1}{\sigma_1^4} + 4 \frac{\beta_{2,0}^2}{\sigma_2^4} \mu_0'M_n\mu_0 \\
= \left( \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 + \frac{\beta_{2,0}^2}{\sigma_2^2} \right)^2 + \frac{1}{\sigma_1^2} - 2 \left( \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 - \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \frac{1}{\sigma_1^2} \\
< \left( \frac{1}{\sigma_2^2} \mu_0'M_n\mu_0 + \frac{\beta_{2,0}^2}{\sigma_2^2} \right)^2;
thus
\[
\lambda_2 > \frac{1}{2} \left\{ \left[ \frac{1}{\sigma_1^2} \mu_0 M_n \mu_0 + \left( \frac{1}{\sigma_1^2} + \frac{\beta_{2,0}^2}{\sigma_2^2} \right) \right] - \sqrt{\left\{ \frac{1}{\sigma_2^2} \mu_0' M_n \mu_0 + \frac{\beta_{2,0}^2}{\sigma_2^2} \right\}} \right\} = \frac{1}{2\sigma_1^2}.
\]

**Theorem 2.15** Let \( \frac{1}{\sigma_1^2} < \frac{\mu_0' M_n \mu_0}{\sigma_2^2} \). If
\[
\sigma_1 << \sqrt{\varepsilon^2 \beta_{2,0}^2 + \varepsilon \sqrt{\varepsilon^2 \beta_{2,0}^4 + 4\sigma_2^2 \chi_{n+1}^2(0; 1 - \alpha)}} / \left( \sqrt{\chi_{n+1}^2(0; 1 - \alpha)} \right) \quad (7)
\]
and \( \alpha \) is sufficiently small, then
\[
|b_1| < \varepsilon \sqrt{\text{Var}(\beta_1)} \quad \& \quad |b_2| < \varepsilon \sqrt{\text{Var}(\beta_2)}.
\]

**Proof** With respect to Remark 2.12 the radius \( R \) of the linearization region is
\[
R = 2\varepsilon \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}. \]
The largest semiaxis of the confidence ellipsoid for the vector \( (\delta \mu, \delta \beta_2) \) is smaller than
\[
\sqrt{2\sigma_1 \sqrt{\chi_{n+1}^2(0; 1 - \alpha)}}.
\]
If
\[
\sqrt{2\sigma_1 \sqrt{\chi_{n+1}^2(0; 1 - \alpha)}} << \sqrt{2\varepsilon \sqrt{\sigma_1^2 \beta_{2,0}^2 + \sigma_2^2}}, \quad (8)
\]
then with respect to Remark 2.12 \( |b_1| \leq \varepsilon \sqrt{\text{Var}(\beta_1)} \) and \( |b_2| \leq \varepsilon \sqrt{\text{Var}(\beta_2)} \).

However (7) and (8) are equivalent, what can be proved easily.

**Example 2.16** (continuation of Example 2.11) The values of \( \lambda_1 \) and \( \lambda_2 \) for data from Example 2.11 are \( \lambda_1 = 2903.567 \) and \( \lambda_2 = 96.433 > \frac{1}{2\sigma_1^2} = 50 \).

The following two tables enables us to imagine the proper relations between \( \sigma_1 \) and \( \sigma_2 \) in order to make the linearization possible.

**Table 2.1**
\[
\chi^2(0; 0.95) = 15.5, \quad \varepsilon = 0.25, \quad \beta_{2,0} = 1
\]

<table>
<thead>
<tr>
<th>( \sigma_2 )</th>
<th>0.01</th>
<th>0.02</th>
<th>0.03</th>
<th>0.04</th>
<th>0.05</th>
<th>0.1</th>
<th>0.2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_1 ) ( \ll )</td>
<td>0.018</td>
<td>0.022</td>
<td>0.025</td>
<td>0.028</td>
<td>0.031</td>
<td>0.042</td>
<td>0.058</td>
<td>0.128</td>
</tr>
</tbody>
</table>

**Table 2.2**
\[
\chi^2(0; 0.95) = 15.5, \quad \varepsilon = 0.25, \quad \beta_{2,0} = 2
\]

<table>
<thead>
<tr>
<th>( \sigma_2 )</th>
<th>0.01</th>
<th>0.02</th>
<th>0.03</th>
<th>0.04</th>
<th>0.05</th>
<th>0.1</th>
<th>0.2</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \sigma_1 ) ( \ll )</td>
<td>0.031</td>
<td>0.034</td>
<td>0.035</td>
<td>0.037</td>
<td>0.038</td>
<td>0.047</td>
<td>0.062</td>
<td>0.129</td>
</tr>
</tbody>
</table>
References
