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ISOBESTIC POINTS: SENSITIVENESS AND LINEARIZATION

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ABSTRACT. Problems of a nonlinearity occur in a determination of isobestic points even in the case when linear regression functions are crossed. Further problem is created by a priori unknown variance components. More complicated problems occur when nonlinear regression functions must be taken into account. Some criteria for a decision whether empirical variances and a linearization of a model can be used, are given in the paper.

1. Introduction

Let regression functions $f_i(x, \boldsymbol{\beta}_i)$, $i = 1, \dots, s$, be under consideration. Let at points $x_{i,1}, \dots, x_{i,n_i}$ values $y_{i,j} = f_i(x_{i,j}, \boldsymbol{\beta}_i)$, $j = 1, \dots, n_i$, be measured. A symbol $\boldsymbol{\beta}_i$ denotes a k_i-dimensional unknown parameter of the ith regression function $f_i(x, \boldsymbol{\beta}_i)$. There exists a point T (isobestic point) on a real line, where all functions $f_i(x, \boldsymbol{\beta}_i)$ have the same value, i.e.,

$$f_1(T, \boldsymbol{\beta}_1) = \dots = f_s(T, \boldsymbol{\beta}_s) = \eta .$$

The problem is to determine this point T on the basis of the measurement results $y_{i,j}$, $j = 1, \dots, n_i$, $i = 1, \dots, s$. Sometimes not only the value T but also the vector $(T, \eta)'$ must be estimated.

The problem occurs in chemistry (cf. [3]), nevertheless, it is interesting by itself. Some consideration is given in [5], [6], but no numerical study is presented there.

The aim of the paper is to continue the study mainly from the numerical viewpoint. A theory is given in [7].

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2. Notations and auxiliary statements

The following model
$$\boldsymbol{Y} \sim N_n(\boldsymbol{f}(\boldsymbol{\beta}), \boldsymbol{\Sigma}), \tag{1}$$
is considered, where
$$\boldsymbol{Y} = (\boldsymbol{Y}_1', \dots, \boldsymbol{Y}_s')', \ \boldsymbol{f}(\boldsymbol{\beta}) = (\boldsymbol{f}_1'(\boldsymbol{\beta}_1), \dots, \boldsymbol{f}_s'(\boldsymbol{\beta}_s))',$$
$$\boldsymbol{\beta} = (\boldsymbol{\beta}_1', \dots, \boldsymbol{\beta}_s')', \ \boldsymbol{\Sigma} = \mathrm{diag}\{\sigma_1^2 \boldsymbol{V}_1, \dots, \sigma_s^2 \boldsymbol{V}_s\},$$
$$\boldsymbol{f}_j(\boldsymbol{\beta}_j) = (f_j(x_{j,1}, \boldsymbol{\beta}_j), \dots, f_j(x_{j,n_j}, \boldsymbol{\beta}_j))', \qquad j = 1, \dots, s, \quad n = \sum_{i=1}^{s} n_i,$$
either with constraints
$$f_1(T, \boldsymbol{\beta}_1) = \dots = f_s(T, \boldsymbol{\beta}_s) \tag{2}$$
or with constraints
$$f_1(T, \boldsymbol{\beta}_1) = \dots = f_s(T, \boldsymbol{\beta}_s) = \eta. \tag{3}$$
Here $\boldsymbol{Y}_i$, $i = 1, \dots, s$, is an n_i-dimensional random vector (observation vector) with the mean value $E(\boldsymbol{Y}_i) = \boldsymbol{f}_i(\boldsymbol{\beta}_i)$ and with the covariance matrix $\sigma_i^2 \boldsymbol{V}_i$, where σ_i^2 is an unknown parameter and $\boldsymbol{V}_i$ is a given $n_i \times n_i$ symmetric and positive definite matrix. The symbol diag means a diagonal matrix.

Both given models, (1), (2) and (1), (3), respectively, will be considered in the linear and the quadratic version. The linear version of (1) is written in the form
$$\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\beta}^{(0)}) \sim N_n(\boldsymbol{F}\delta\boldsymbol{\beta}, \boldsymbol{\Sigma}), \quad \delta\boldsymbol{\beta} = \boldsymbol{\beta} - \boldsymbol{\beta}^{(0)}, \tag{4}$$
where $\boldsymbol{F} = \partial \boldsymbol{f}(\boldsymbol{u})/\partial \boldsymbol{u}'\big|_{u=\beta^{(0)}}$ and $\boldsymbol{\beta}^{(0)}$ is an approximate value of the vector $\boldsymbol{\beta}$. Linear forms of constraints (2) and (3) are given by
$$\boldsymbol{H}\delta\boldsymbol{\beta} + \boldsymbol{b}\delta T = \boldsymbol{0}, \quad \delta T = T - T^{(0)} \tag{5}$$
and
$$\boldsymbol{G}\delta\boldsymbol{\beta} + (\boldsymbol{a}, -\boldsymbol{1})\begin{pmatrix}\delta T \\ \delta\eta\end{pmatrix} = \boldsymbol{0}, \quad \delta T = T - T^{(0)}, \quad \delta\eta = \eta - \eta^{(0)}, \tag{6}$$
respectively. Here $T^{(0)}$ and $\eta^{(0)}$ are approximate values of the x-coordinate and the y-coordinate of the isobestic point, respectively. Further
$$\boldsymbol{H} = \mathrm{diag}\{\boldsymbol{g}_1' - \boldsymbol{g}_2', \ \boldsymbol{g}_2' - \boldsymbol{g}_3', \dots, \boldsymbol{g}_{s-1}' - \boldsymbol{g}_s'\}, \quad \boldsymbol{G} = \mathrm{diag}\{\boldsymbol{g}_1', \ \boldsymbol{g}_2', \dots, \boldsymbol{g}_s'\},$$
$$\boldsymbol{b} = (a_1 - a_2, \dots, a_{s-1} - a_s)', \quad \boldsymbol{a} = (a_1, \dots, a_s)', \quad \boldsymbol{1} = (1, \dots, 1)',$$
$$\boldsymbol{g}_i' = \partial f_i(T^{(0)}, \boldsymbol{u})/\partial \boldsymbol{u}'\big|_{u=\beta_i^{(0)}}, \quad a_i = \partial f_i(x, \boldsymbol{\beta}_i^{(0)})/\partial x\big|_{x=T^{(0)}}, \quad i = 1, \dots, s.$$
The quadratic version is treated in Section 4.

It is to be emphasized that approximate values $\boldsymbol{\beta}^{(0)}$, $T^{(0)}$ and $\eta^{(0)}$ must be chosen in such a way that (2) and (3) are satisfied (in more detail cf. [4]). Obviously, approximate values must be sufficiently close to actual values.

The estimator of δT from the model (4), (5) is the same as the estimator from (4), (6) (cf. [5]). Consequently, although in the following only the problem of the x-coordinate of the isobestic point will be studied, the model (4), (6) will be also under consideration, since expressions in this model have simpler structure. The model (4), (6) will be supposed to be regular, i.e., the rank of the matrix $\boldsymbol{F}_{n\times k}$, $k = k_1 + \dots + k_s$, is $r(\boldsymbol{F}) = k < n$, $\boldsymbol{\Sigma}$ is positive definite, $r(\boldsymbol{G}, \boldsymbol{a}, \mathbf{1}) = s < k+2$ and $r(\boldsymbol{a}, \mathbf{1}) = 2 < s$.

All the following assertions are proved in [7].

Lemma 2.1. *The best linear unbiased estimators* (BLUE) *of the parameter* δT *and* $\delta\eta$ *in the model* (4) *and* (6) *are*

$$\widehat{\delta T} = -\left[\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{a}\right]^{-1}\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{G}\widetilde{\delta\boldsymbol{\beta}}\,,$$

$$\widehat{\delta\eta} = \left[\mathbf{1}'(\boldsymbol{M}_a \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_a)^+\mathbf{1}\right]^{-1}\mathbf{1}'(\boldsymbol{M}_a \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_a)^+\boldsymbol{G}\widetilde{\delta\boldsymbol{\beta}}\,,$$

$$\operatorname{Var}(\widehat{\delta T}) = \left[\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{a}\right]^{-1},$$

$$\operatorname{Var}(\widehat{\delta\eta}) = \left[\mathbf{1}'(\boldsymbol{M}_a \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_a)^+\mathbf{1}\right]^{-1},$$

where

$$\begin{aligned}(\boldsymbol{M}_1 \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+ &= (\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1} \\ &\quad - (\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1}\mathbf{1}\left[\mathbf{1}'(\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1}\mathbf{1}\right]^{-1}\mathbf{1}'(\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1},\end{aligned}$$

$$\begin{aligned}(\boldsymbol{M}_a \boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_a)^+ &= (\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1} \\ &\quad - (\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1}\boldsymbol{a}\left[\boldsymbol{a}'(\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1}\boldsymbol{a}\right]^{-1}\boldsymbol{a}'(\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}')^{-1},\end{aligned}$$

$$\widetilde{\delta\boldsymbol{\beta}} = \boldsymbol{C}^{-1}\boldsymbol{F}'\boldsymbol{\Sigma}^{-1}\big(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\beta}^{(0)})\big), \quad \boldsymbol{C} = \boldsymbol{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{F}\,.$$

Here the symbol $\boldsymbol{A}^+$ means Moore-Penrose g-inverse of the matrix $\boldsymbol{A}$ (cf. [10]), symbols $\widehat{\ }$ and $\widetilde{\ }$ denote estimators in the model (4), (6) (the model with constraints) and in the model (4) (the model without constraints), respectively.

3. Insensitivity regions

The notation

$$\boldsymbol{\vartheta} = (\sigma_1^2, \dots, \sigma_s^2)' \in \underline{\boldsymbol{\vartheta}}, \quad \underline{\boldsymbol{\vartheta}} = \{\boldsymbol{\vartheta} :\ \boldsymbol{\vartheta} \in \mathbb{R}^s,\ \vartheta_1 > 0, \dots, \vartheta_s > 0\}$$

will be used in the following. Let $\boldsymbol{\Sigma} = \sum_{i=1}^{s} \vartheta_i \overline{\boldsymbol{V}}_i$, i.e., $\overline{\boldsymbol{V}}_i$, $i = 1, \dots, s$, be the $n \times n$ symmetric and positive semidefinite matrix with the matrix $\boldsymbol{V}_i$ at the ith diagonal position and with zero blocks otherwise.

Let $\boldsymbol{\vartheta}_0$ be true value of the parameter $\boldsymbol{\vartheta}$. Evidently, a change $\boldsymbol{\vartheta}_0 + \delta\boldsymbol{\vartheta}$, $\delta\boldsymbol{\vartheta} \in \mathbb{R}^s$, $\delta\vartheta_i > -\vartheta_{0,i}$, $i = 1, \dots, s$, can destroy the optimum quality of the $\boldsymbol{\vartheta}_0$-LBLUE $\widehat{\delta T}$ ($\boldsymbol{\vartheta}_0$-locally BLUE), the confidence ellipsoid, the power function of the test, etc. This problem can be analyzed by using an insensitivity region. It is a region defined in the parameter space $\underline{\boldsymbol{\vartheta}}$ such that shifts $\delta\boldsymbol{\vartheta}$ of $\boldsymbol{\vartheta}_0$ inside this region do not cause any essential damage of chosen statistical characteristic.

Since $\widehat{\delta T}$ is unbiased $\forall \boldsymbol{\vartheta}$, the shift $\delta\boldsymbol{\vartheta}$ influences its variance only. For the sake of simplicity, only the insensitivity region for the variance of $\widehat{\delta T}$ is considered. A consideration of other statistical characteristics cf. [4], [8] and [9].

DEFINITION 3.1. Let $\varepsilon > 0$ be a number chosen by a user. The insensitivity region for the variance of the estimator $\widehat{\delta T}$ is the set

$$\mathcal{N}_{\delta T,\varepsilon} = \left\{ \delta\boldsymbol{\vartheta} : \delta\boldsymbol{\vartheta} \in \mathbb{R}^s, \operatorname{Var}\left[\partial \widehat{\delta T}(\boldsymbol{Y}, \boldsymbol{u}) / \partial \boldsymbol{u}' \big|_{u=\vartheta_0} \delta\boldsymbol{\vartheta}\right] \leq \varepsilon^2 \operatorname{Var}\left[\widehat{\delta T}(\boldsymbol{Y}, \boldsymbol{\vartheta}_0)\right] \right\}.$$

THEOREM 3.2. *The explicite expression of the region* $\mathcal{N}_{\delta T,\varepsilon}$ *is*

$$\mathcal{N}_{\delta T,\varepsilon} = \left\{ \delta\boldsymbol{\vartheta} :\ \delta\boldsymbol{\vartheta} \in \mathbb{R}^s,\ \delta\boldsymbol{\vartheta}' \boldsymbol{W}_{\delta T} \delta\boldsymbol{\vartheta} \leq \varepsilon^2 \left[\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ \boldsymbol{a}\right]^{-1} \right\},$$

where

$$\begin{aligned} \boldsymbol{W}_{\delta T} = \boldsymbol{K}' \boldsymbol{F} \boldsymbol{C}^{-1} \boldsymbol{G}' \Big\{ &(\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ - (\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ \\ &\times \boldsymbol{a} \left[\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ \Big\} \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{F}' \boldsymbol{K}, \end{aligned}$$

$$\boldsymbol{K} = (\boldsymbol{k}_1, , \dots, \boldsymbol{k}_s),$$

$$\begin{aligned} \boldsymbol{k}_i' = \left[\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ \boldsymbol{a}\right]^{-1} &\boldsymbol{a}'(\boldsymbol{M}_1 \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{G}' \boldsymbol{M}_1)^+ \boldsymbol{G} \boldsymbol{C}^{-1} \boldsymbol{F}' \\ &\times \boldsymbol{\Sigma}^{-1} \overline{\boldsymbol{V}}_i \boldsymbol{\Sigma}^{-1}, \quad i = 1, \dots, s. \end{aligned}$$

4. Linearization region for the bias

In the first step the bias of the estimator $\widehat{\delta T}$ in the quadratic version

$$\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\beta}^{(0)}) \sim N_n\left(\boldsymbol{F} \delta\boldsymbol{\beta} + \frac{1}{2} \boldsymbol{\kappa}(\delta\boldsymbol{\beta}), \boldsymbol{\Sigma} \right), \tag{7}$$

$$\boldsymbol{G} \delta\boldsymbol{\beta} + (\boldsymbol{a}, -\boldsymbol{1}) \begin{pmatrix} c\delta T \\ \delta\eta \end{pmatrix} + \frac{1}{2} \boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta) = \boldsymbol{0} \tag{8}$$

of the model (1) and (3) is considered. Here

$$\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) = \big(\boldsymbol{\kappa}_1'(\delta\boldsymbol{\beta}_1), \dots, \boldsymbol{\kappa}_s'(\delta\boldsymbol{\beta}_s)\big)',$$

$$\boldsymbol{\kappa}_{i,j} = \delta\boldsymbol{\beta}_i' \, \partial^2 f_i(x_{i,j}, \boldsymbol{u})/\partial\boldsymbol{u}\,\partial\boldsymbol{u}'\big|_{u=\beta_i^{(0)}} \delta\boldsymbol{\beta}_i, \qquad i = 1, \dots, s, \ j = 1, \dots, n_i\,,$$

$$\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta) = \big(\boldsymbol{\omega}_1(\delta\boldsymbol{\beta}_1, \delta T, \delta\eta), \dots, \boldsymbol{\omega}_s(\delta\boldsymbol{\beta}_s, \delta T, \delta\eta)\big)',$$

$$\boldsymbol{\omega}_i(\delta\boldsymbol{\beta}_i, \delta T, \delta\eta) = (\delta\boldsymbol{\beta}_i', \delta T, \delta\eta)\boldsymbol{U}_i \begin{pmatrix} \delta\boldsymbol{\beta}_i \\ \delta T \\ \delta\eta \end{pmatrix}, \qquad i = 1, \dots, s\,,$$

$$\boldsymbol{U}_i = \begin{pmatrix} \partial^2 f_i(T^{(0)}, \boldsymbol{u})/\partial\boldsymbol{u}\,\partial\boldsymbol{u}'\big|_{u=\beta_i^{(0)}}\,, & \partial^2 f_i(t, \boldsymbol{u})/\partial\boldsymbol{u}\,\partial t\big|_{u=\beta_i^{(0)}, t=T^{(0)}}\,, & \mathbf{0} \\ \partial^2 f_i(t, \boldsymbol{u})/\partial\boldsymbol{u}'\,\partial t\big|_{u=\beta_i^{(0)}, t=T^{(0)}}, & \partial^2 f_i(t, \boldsymbol{\beta}^{(0)})/\partial t^2\big|_{t=T^{(0)}}\,, & 0 \\ \mathbf{0}\,, & 0\,, & 0 \end{pmatrix}.$$

Lemma 4.1. *The bias of the estimator* $\widehat{\delta T}$ *in the quadratic model* (7), (8) *is*

$$b_T = E(\widehat{\delta T}) - \delta T = -\big[\boldsymbol{a}'(\boldsymbol{M}_1\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\boldsymbol{M}_1\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+ \times \left[-\frac{1}{2}\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta) + \frac{1}{2}\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{F}'\boldsymbol{\Sigma}^{-1}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right].$$

Quantities δT and $\delta\eta$ are functions of $\delta\boldsymbol{\beta}$, which follows from assumptions, the vector $\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta)$ can be expressed as the function of $\delta\boldsymbol{\beta}$ as well. Instead of δT, $\delta\eta$ in $\boldsymbol{\omega}$ it is sufficient to use the linear approximation (cf. Lemma 2.1)

$$\delta T = -\big[\boldsymbol{a}'(\boldsymbol{M}_1\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\boldsymbol{M}_1\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{G}\delta\boldsymbol{\beta}\,,$$

$$\delta\eta = \big[\mathbf{1}'(\boldsymbol{M}_a\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_a)^+\mathbf{1}\big]^{-1}\mathbf{1}'(\boldsymbol{M}_a\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_a)^+\boldsymbol{G}\delta\boldsymbol{\beta}\,.$$

In order to find a set of such shifts of $\delta\boldsymbol{\beta}$ which don't create any essential bias in $\widehat{\delta T}$, the following measure of the nonlinearity for δT will be utilized.

Definition 4.2. The *measure of the nonlinearity* of the quadratic model (7) and (8) with respect to the bias of the estimator $\widehat{\delta T}$ is

$$C_{\delta T} = \sup\left\{\frac{2\sqrt{b_T\big[\boldsymbol{a}'(\boldsymbol{M}_1\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{a}\big]b_T}}{\delta\boldsymbol{\beta}'\boldsymbol{C}\delta\boldsymbol{\beta}} : \delta\boldsymbol{\beta} \in \mathbb{R}^k\right\}.$$

Here $k = k_1 + \dots + k_s$, where k_i is a dimension of the parameter $\boldsymbol{\beta}_i$ in the ith regression function, $\big[\boldsymbol{a}'(\boldsymbol{M}_1\boldsymbol{G}\boldsymbol{C}^{-1}\boldsymbol{G}'\boldsymbol{M}_1)^+\boldsymbol{a}\big]^{-1} = \mathrm{Var}(\widehat{\delta T})$, $\boldsymbol{C}^{-1} = \mathrm{Var}(\widehat{\delta\boldsymbol{\beta}})$.

Definition 4.3. Let tol > 0 be a tolerance chosen by user. The *linearization region* for the bias of the estimator $\widehat{\delta T}$ is

$$\mathcal{L}_{\delta T, \mathrm{tol}} = \left\{\delta\boldsymbol{\beta} : \ \delta\boldsymbol{\beta} \in \mathbb{R}^k, \ \delta\boldsymbol{\beta}'\boldsymbol{C}\delta\boldsymbol{\beta} \le \frac{2\,\mathrm{tol}}{C_{\delta T}}\right\}.$$

Theorem 4.4. *It holds*

$$\delta\boldsymbol{\beta}'\boldsymbol{C}\delta\boldsymbol{\beta} \le \frac{2\,\mathrm{tol}}{C_{\delta T}} \implies |b_T| \le \mathrm{tol}\sqrt{\mathrm{Var}(\widehat{\delta T})}\,.$$

Remark 4.5. The linearization region $\mathcal{L}_{\delta T,\mathrm{tol}}$ can be used in practice under some condition. We have to be practically sure that the actual value $\boldsymbol{\beta}^*$ of the parameter $\boldsymbol{\beta}$ satisfies the condition $\boldsymbol{\beta}^* - \boldsymbol{\beta}^{(0)} \in \mathcal{L}_{\delta T,\mathrm{tol}}$. This can be attained if the $(1-\alpha)$-confidence region for $\delta\boldsymbol{\beta}$, for a sufficiently high level of confidence, is included into $\mathcal{L}_{\delta T,\mathrm{tol}}$. Thus it must hold $\chi_k^2(1-\alpha) \ll 2\,\mathrm{tol}/C_{\delta T}$ (weak nonlinearity with respect to the bias of $\widehat{\delta T}$). Here $\chi_k^2(1-\alpha)$ is the $(1-\alpha)$-quantile of chi-square distribution with k degrees of freedom.

5. Numerical example

Let three linear regression functions $f_i(x,\boldsymbol{\beta}_i) = \beta_{i,1} + \beta_{i,2}x$, $i = 1,2,3$, be under consideration. Let each straight line be measured one time at points $x = 2,4,6,8$ with different accuracy, i.e.,

$$\boldsymbol{Y}_i \sim N_4\left[\begin{pmatrix} 1, & 2\\ 1, & 4\\ 1, & 6\\ 1, & 8\end{pmatrix}\begin{pmatrix}\beta_{i,1}\\ \beta_{i,2}\end{pmatrix};\ \sigma_i^2\boldsymbol{I}\right], \qquad i = 1,2,3\,.$$

Let the x-coordinate of the intersection point of $f_i(x,\boldsymbol{\beta}_i)$, $i = 1,2,3$, be T. The condition for the determination of the isobestic point T is given by equalities

$$\beta_{1,1} + \beta_{1,2}T = \beta_{2,1} + \beta_{2,2}T = \beta_{3,1} + \beta_{3,2}T\,. \tag{9}$$

The main goal of this example is to study the relationship between the configuration of straight lines (their gradients $\beta_{1,2}$, $\beta_{2,2}$, $\beta_{3,2}$), the accuracy of the measurement (σ_1, σ_2, σ_3), the possibility of the linearization of the condition (9) subject to the bias of $\widehat{\delta T}$, and the possibility of using approximate values of σ_1, σ_2, σ_3 instead of their true values subject to the variance of $\widehat{\delta T}$.

For the sake of the simplicity let the following straight lines

$$f_1\colon y = x\,, \quad f_2\colon y = 5\,, \quad f_3\colon y = -x + 10$$

be under consideration (cf. Fig. 1). Let the tolerance for the insensitivity region $\mathcal{N}_{\delta T,\varepsilon}$ be $\varepsilon = 0.1$. It means that tolerated shifts $\delta\boldsymbol{\vartheta}$ ($\delta\boldsymbol{\sigma}$) can make only 1 % (10 %) increase of the variance (the standard error) of the estimator $\widehat{\delta T}$. Let the tolerance for the linearization region $\mathcal{L}_{\delta T,\mathrm{tol}}$ be $\mathrm{tol} = 0.5$. It means that $\sqrt{\mathrm{MSE}(\widehat{\delta T})}$ (mean square error) can increase of 12.5 % only, since it holds

$$\sqrt{\mathrm{MSE}(\widehat{\delta T})} \le \sqrt{\mathrm{Var}(\widehat{\delta T}) + \mathrm{tol}^2\,\mathrm{Var}(\widehat{\delta T})} \doteq \sqrt{\mathrm{Var}(\widehat{\delta T})}\left(1 + \frac{\mathrm{tol}^2}{2}\right).$$

Numerical results are presented in dependence on approximate values of σ_1, σ_2 and σ_3 in Table 1. Symbols $\boldsymbol{v}_i$, $i = 1,2,3$, and λ denote eigenvectors and their corresponding eigenvalues from the spectral decomposition of the matrix $\boldsymbol{W}_{\delta T}$ ($\boldsymbol{W}_{\delta T} = \sum_{i=1}^{3} \lambda_i \boldsymbol{v}_i \boldsymbol{v}_i'$). The symbol γ_i, $i = 1,2,3$, means the length of the ith semiaxis of the region $\mathcal{N}_{\delta T,0.1}(\delta\boldsymbol{\vartheta})$ in the direction $\boldsymbol{v}_i$ ($\gamma_i = \sqrt{0.1^2\,\mathrm{Var}(\widehat{\delta T})/\lambda_i}$). Symbols $\delta\vartheta_{i,\max}$ and $\delta\sigma_{i,\max}$, $i = 1,2,3$, mean maximum tolerable shifts $\delta\vartheta_i$ of $\vartheta_i = \sigma_i^2$ if $\delta\vartheta_j = 0$ $\forall j \ne i$ and shifts $\delta\sigma_i$ ($\delta\sigma_i = \sqrt{\vartheta_i + \delta\vartheta_i} - \sigma_i$) of σ_i if $\delta\sigma_j = 0$ $\forall j \ne i$, respectively. Finally, $r = 2\,\mathrm{tol}/C_{\delta T}$.

Firstly, the problem of the linearization will be discussed. The 0.95-confidence ellipsoid for $\delta\boldsymbol{\beta}$ and the linearization region for the bias of $\widehat{\delta T}$ are

$$\mathcal{E}_{0.95}(\delta\boldsymbol{\beta}) = \{\delta\boldsymbol{\beta} :\ \delta\boldsymbol{\beta} \in \mathbb{R}^6,\ (\delta\boldsymbol{\beta} - \widetilde{\delta\boldsymbol{\beta}})'\boldsymbol{C}(\delta\boldsymbol{\beta} - \widetilde{\delta\boldsymbol{\beta}}) \le 12.592\},$$
$$\mathcal{L}_{\delta T,0.5}(\delta\boldsymbol{\beta}) = \{\delta\boldsymbol{\beta} :\ \delta\boldsymbol{\beta} \in \mathbb{R}^6,\ \delta\boldsymbol{\beta}'\boldsymbol{C}\delta\boldsymbol{\beta} \le r\}.$$

From Table 1 it holds: $r = 63,2455$ in cases I, II and $r = 34,2995$ in the case III. It implies $12.592 \ll r$. Hence the condition (9) can be linearized, i.e., shifts of the vector $\delta\boldsymbol{\beta}$ don't make the bias in $\widehat{\delta T}$ larger than tolerable one.

Now, the problem of the accuracy of the measurement will be discussed. Firstly, let all straight lines be measured with the same accuracy $\sigma_i = 0.1$, $i = 1,2,3$, (cf. Table 1, case I). From the spectral decomposition of $\boldsymbol{W}_{\delta T}$ it follows, that the shift $\delta\vartheta_2$ can be arbitrarily large and it doesn't influence shifts $\delta\vartheta_1$ and $\delta\vartheta_3$. By contrast, shifts $\delta\vartheta_1$ and $\delta\vartheta_3$ are closely connected. The projection of $\mathcal{N}_{\delta T,0.1}$ on the subspace of $\delta\vartheta_1 \times \delta\vartheta_3$ is the band in the direction of the vector $(1,1)'$ with the width equal to $2 \times 0.0025 = 0.005$ (cf. Fig 2). The whole region $\mathcal{N}_{\delta T,0.1}$ is the layer given by the shifting of this band along the orthogonal vector $(0,\delta\vartheta_2,0)'$, $\delta\vartheta_2 > -0.01$. Hence, in this case, the determination of T is indifferent to the measurement of f_2. On the other hand, there are high demands on the accuracy of the measurement of f_1 and f_3. If the inaccuracy in σ_1, σ_3 can make the standard deviation of $\widehat{\delta T}$ larger of 10 % ($\varepsilon = 0.1$), then, e.g., $\sigma_1 = 0.1$ can change maximally of 16 % ($\delta\sigma_{1,\max} = 0.016$) provided that $\sigma_3 = 0.1$ is known precisely and vice versa.

The above mentioned conclusion, that the determination of T is independent of the measurement of f_2, is verified by the case $\sigma_1 = \sigma_3 = 0.1$ and $\sigma_2 = 0.5$

TABLE 1. Numerical results of $\widehat{\delta T}$, $\mathcal{L}_{\delta T,0.5}$ and $\mathcal{N}_{\delta T,0.1}$ in dependence on $\boldsymbol{\sigma}$.

I.	$\sigma_1 = 0.1$, $\sigma_2 = 0.1$, $\sigma_3 = 0.1$						
	$C_{\delta T} = 0.0158$		$r = 63.2455$	$\mathrm{Var}(\widehat{\delta T}) = 0.0013$		$\sqrt{\mathrm{Var}(\widehat{\delta T})} = 0.0361$	
i	$\boldsymbol{v}_1$	$\boldsymbol{v}_2$	$\boldsymbol{v}_3$	λ	γ	$\delta\vartheta_{\max}$	$\delta\sigma_{\max}$
1	0	-0.7071	-0.7071	0	∞	0.0035	0.0160
2	1	0	0	0	∞	∞	∞
3	0	-0.7071	0.7071	2.0833	0.0025	0.0035	0.0160

II.	$\sigma_1 = 0.1$, $\sigma_2 = 0.5$, $\sigma_3 = 0.1$						
	$C_{\delta T} = 0.0158$		$r = 63.2455$	$\mathrm{Var}(\widehat{\delta T}) = 0.0013$		$\sqrt{\mathrm{Var}(\widehat{\delta T})} = 0.0361$	
i	$\boldsymbol{v}_1$	$\boldsymbol{v}_2$	$\boldsymbol{v}_3$	λ	γ	$\delta\vartheta_{\max}$	$\delta\sigma_{\max}$
1	0	-0.7071	-0.7071	0	∞	0.0143	0.0558
2	1	0	0	0	∞	∞	∞
3	0	-0.7071	0.7071	0.0125	0.0103	0.0143	0.0558

III.	$\sigma_1 = 0.5$, $\sigma_2 = 0.1$, $\sigma_3 = 0.1$						
	$C_{\delta T} = 0.0292$		$r = 34.2995$	$\mathrm{Var}(\widehat{\delta T}) = 0.0043$		$\sqrt{\mathrm{Var}(\widehat{\delta T})} = 0.0656$	
i	$\boldsymbol{v}_1$	$\boldsymbol{v}_2$	$\boldsymbol{v}_3$	λ	γ	$\delta\vartheta_{\max}$	$\delta\sigma_{\max}$
1	-0.0544	0.9927	0.1301	2.8167	0.0039	0.0714	0.0669
2	0.8703	0.0998	-0.4799	0	∞	0.0045	0.0203
3	0.4895	-0.0671	0.8676	0	∞	0.0079	0.0339

(cf. Table 1, case II). Although the standard deviation σ_2 is 5 times larger, i.e., the dispersion is 25 times larger, the standard deviation of $\widehat{\delta T}$ is 0.0361, i.e., it is the same as in the case $\sigma_2 = 0.1$. For the completeness' sake, the projection of $\mathcal{N}_{\delta T,0.1}$ on $\delta\vartheta_1 \times \delta\vartheta_3$ is the band in the direction $(1,1)'$ with the width 0.0206. The whole region $\mathcal{N}_{\delta T,0.1}$ is also the layer given by the shifting of the obtained band along the orthogonal vector $(0, \delta\vartheta_2, 0)'$, $\delta\vartheta_2 > -0.25$.

Obviously, straight lines f_1 and f_3 have the same weight in the measurement if they have the same accuracy of the measurement. Let us consider $\sigma_1 = 0.5$ and $\sigma_2 = \sigma_3 = 0.1$ (Table 1, case III). Obviously, the measurement of f_2 influences the accuracy of the variance of $\widehat{\delta T}$. The insensitivity region is also the layer in $\mathbb{R}^3$ given by appropriate eigenvectors $\boldsymbol{v}_i$ and semiaxes γ_i, $i = 1,2,3$.

From the example it follows, that the linearization of the condition for the determination of the isobestic point T can be made without any essential change. But the accuracy of the determination of T depends on the configuration of linear functions, on the accuracy of the measurement, etc.

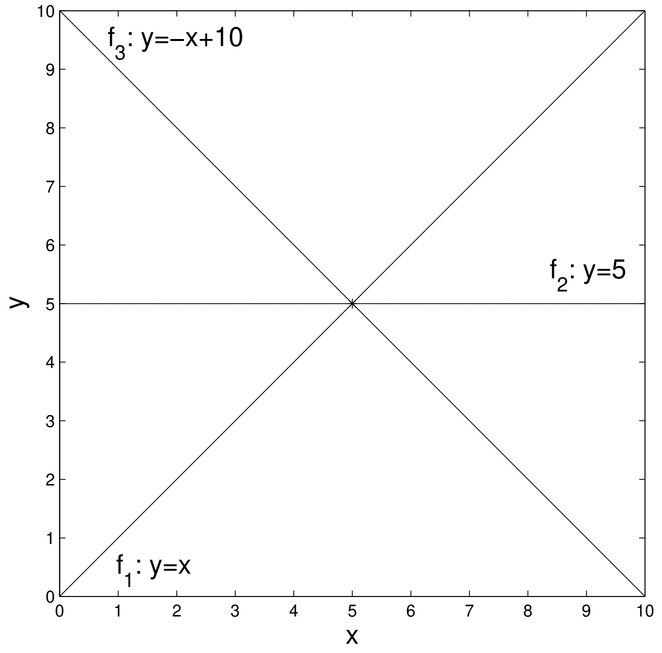

FIGURE 1. Regression functions.

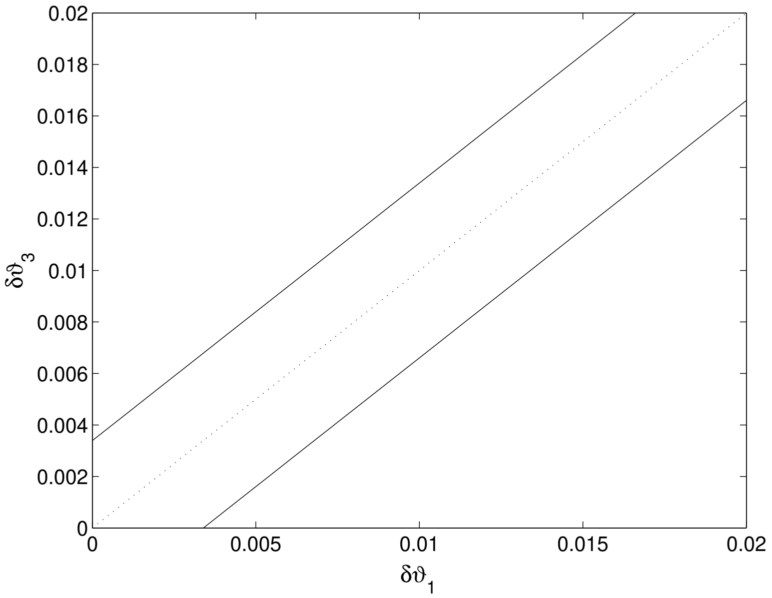

FIGURE 2. Projection of $\mathcal{N}_{\delta T,0.1}$ on $\delta\vartheta_1 \times \delta\vartheta_3$ from the case I.

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