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PROBLEMS OF SENSITIVENESS AND LINEARIZATION IN A DETERMINATION OF ISOBESTIC POINTS

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ABSTRACT. A determination of isobestic points (i.e., points where several regression functions are crossed) is a typical problem of chemistry. From the statistical viewpoint the problem is nonlinear even in the case when linear regression functions are dealt with and further problems occur when variance components are unknown. Some criteria for a decision whether empirical variances and a linearization of a model can be used are given in the paper.

1. Introduction

A determination of isobestic points is a typical problem of chemistry however it is interesting by itself. It is usually employed with reference to a set of absorption spectra, plotted on the same chart for a set of solutions in which the sum of the concentrations of two principal absorbing components is constant. The curves of absorbance against wavelength (or frequency) for such a set of mixtures often all intersect at one or more points, called isobestic points (cf. [3]).

Let at known points $x_{i,1},\dots,x_{i,n_i}$, $i = 1,\dots,s$, on the real line values $y_{i,j} = f_i(x_{i,j},\beta_i)$, $j = 1,\dots,n_i$, $i = 1,\dots,s$, be measured. An analytical form of the function $f_i(x,\beta_i)$ is assumed to be known however a k_i-dimensional parameter β_i, $i = 1,\dots,s$, is unknown. From the theory, there exists a point T (an isobestic point) on the real line, where all functions $f_i(\cdot,\beta_i)$ have the same

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value, i.e.,

$$f_1(T,\beta_1) = \cdots = f_s(T,\beta_s) = \eta\,.$$

The problem is to determine this point T on the basis of 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.

Some consideration is given in [5] and [6], however, no numerical study is presented there. Some survey of results, obtained in the process of developing and utilizing algorithms which solve the above mentioned problems, is given in [7].

2. Notations and auxiliary statements

The following model

$$\boldsymbol{Y} \sim N_n\big(\boldsymbol{f}(\boldsymbol{\beta}),\boldsymbol{\Sigma}\big) \tag{1}$$

is considered, where

$$\boldsymbol{Y} = \begin{pmatrix} \boldsymbol{Y}_1 \\ \vdots \\ \boldsymbol{Y}_s \end{pmatrix}, \qquad \boldsymbol{f}(\boldsymbol{\beta}) = \begin{pmatrix} \boldsymbol{f}_1(\boldsymbol{\beta}_1) \\ \vdots \\ \boldsymbol{f}_s(\boldsymbol{\beta}_s) \end{pmatrix}, \qquad \boldsymbol{f}_j(\boldsymbol{\beta}_j) = \begin{pmatrix} f_j(x_{j,1},\boldsymbol{\beta}_j) \\ \vdots \\ f_j(x_{j,n_j},\boldsymbol{\beta}_j) \end{pmatrix},$$

$$\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{1,1}, & \mathbf{0}, & \dots, & \mathbf{0} \\ \mathbf{0}, & \boldsymbol{\Sigma}_{2,2}, & \dots, & \mathbf{0} \\ \dots & \dots & \dots & \dots \\ \mathbf{0}, & \mathbf{0}, & \dots, & \boldsymbol{\Sigma}_{s,s} \end{pmatrix}, \qquad n = \sum_{i=1}^{s} n_i\,,$$

either with constraints

$$f_1(T,\boldsymbol{\beta}_1) = \cdots = f_s(T,\boldsymbol{\beta}_s)\,, \tag{2}$$

or with constraints

$$\eta = f_1(T,\boldsymbol{\beta}_1) = \cdots = f_s(T,\boldsymbol{\beta}_s)\,. \tag{3}$$

Here $\boldsymbol{Y}_i$, $i = 1,\dots,s$, is an n_i-dimensional random vector (observation vector) with the mean value $E(\boldsymbol{Y}_i) = \boldsymbol{f}_i(\boldsymbol{\beta}_i)$, $\boldsymbol{\beta}_i \in \mathbb{R}^{k_i}$, is an unknown vector, and with the covariance matrix $\boldsymbol{\Sigma}_{i,i}$. The covariance matrix will be considered in two forms, i.e., either $\boldsymbol{\Sigma}_{i,i}$ is known in advance, or $\boldsymbol{\Sigma}_{i,i} = \sigma_i^2\mathbf{V}_i$, where σ_i^2 is unknown parameter and $\mathbf{V}_i$ is given $n_i \times n_i$ symmetric and p.d. (positive definite) matrix.

Both given models, i.e., (1), (2) and (1), (3), respectively, will be considered in the linear and in the quadratic version. The quadratic version is treated in Section 4. The linear version of the model (1), (2) is written in the form

$$\boldsymbol{Y} - \boldsymbol{f}\big(\boldsymbol{\beta}^{(0)}\big) \sim N_n\,(\mathbf{F}\delta\boldsymbol{\beta},\boldsymbol{\Sigma})\,, \qquad \delta\boldsymbol{\beta} = \boldsymbol{\beta} - \boldsymbol{\beta}^{(0)}, \tag{4}$$

$$\mathbf{H}\delta\boldsymbol{\beta} + \boldsymbol{b}\delta T = \boldsymbol{0}, \qquad \delta T = T - T^{(0)}, \tag{5}$$

where $\boldsymbol{\beta}^{(0)}$ is an approximate value of the vector $\boldsymbol{\beta} = \left(\boldsymbol{\beta}_1', \dots, \boldsymbol{\beta}_s'\right)'$, $T^{(0)}$ is an approximate value of the x-coordinate of the isobestic point and

$$\boldsymbol{g}_i' = \frac{\partial f_i(T^{(0)}, \boldsymbol{u})}{\partial \boldsymbol{u}'}\Big|_{\boldsymbol{u}=\boldsymbol{\beta}_i^{(0)}}, \quad a_i = \frac{\partial f_i(t, \boldsymbol{\beta}_i^{(0)})}{\partial t}\Big|_{t=T^{(0)}}, \qquad i = 1, \dots, s,$$

$$\mathbf{H} = \begin{pmatrix} \boldsymbol{g}_1' - \boldsymbol{g}_2', & \boldsymbol{0}, & \dots, & \boldsymbol{0} \\ \boldsymbol{0}, & \boldsymbol{g}_2' - \boldsymbol{g}_3', & \dots, & \boldsymbol{0} \\ \dots & \dots & \dots & \dots \\ \boldsymbol{0}, & \boldsymbol{0}, & \dots, & \boldsymbol{g}_{s-1}' - \boldsymbol{g}_s' \end{pmatrix}, \qquad \boldsymbol{b} = \begin{pmatrix} a_1 - a_2 \\ \vdots \\ a_{s-1} - a_s \end{pmatrix},$$

$$\mathbf{F} = \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial \boldsymbol{u}'}\Big|_{\boldsymbol{u}=\boldsymbol{\beta}^{(0)}}.$$

It is to be mentioned that the vector $\boldsymbol{\beta}^{(0)}$ and the value $T^{(0)}$ can be given with sufficient accuracy in chemical experiments.

Linear version of the model (1), (3) is (4) and

$$\mathbf{G}\delta\boldsymbol{\beta} + (\boldsymbol{a}, -\boldsymbol{1})\begin{pmatrix} \delta T \\ \delta\eta \end{pmatrix} = \boldsymbol{0}, \qquad \delta T = T - T^{(0)}, \ \ \delta\eta = \eta - \eta^{(0)}, \tag{6}$$

where

$$\mathbf{G} = \begin{pmatrix} \boldsymbol{g}_1', & \boldsymbol{0}, & \dots, & \boldsymbol{0} \\ \boldsymbol{0}, & \boldsymbol{g}_2', & \dots, & \boldsymbol{0} \\ \dots & \dots & \dots & \dots \\ \boldsymbol{0}, & \boldsymbol{0}, & \dots, & \boldsymbol{g}_s' \end{pmatrix}, \qquad \boldsymbol{a} = \begin{pmatrix} a_1 \\ \vdots \\ a_s \end{pmatrix}, \qquad \boldsymbol{1} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

and $\eta^{(0)}$ is an approximate value of the y-coordinate of the isobestic point.

Both models will be supposed to be regular, i.e., the rank of the matrix $\mathbf{F}_{n\times k}$, $k = k_1 + \dots + k_s$, is $r(\mathbf{F}) = k < n$, the covariance matrix $\boldsymbol{\Sigma}$ is positive definite, $r(\mathbf{H}, \boldsymbol{b}) = s - 1 < k + 1$, $r(\mathbf{G}, \boldsymbol{a}, \boldsymbol{1}) = s < k + 2$ and $r(\boldsymbol{a}, \boldsymbol{1}) = 2 < s$.

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]). In practice, it is suitable to choose the value $T^{(0)}$ and $\eta^{(0)}$ in the first step and then to calculate $\boldsymbol{\beta}^{(0)}$ in such a way that $f_1\left(T^{(0)}, \boldsymbol{\beta}_1^{(0)}\right) = \dots = f_s\left(T^{(0)}, \boldsymbol{\beta}_s^{(0)}\right)$. The graphical record of measurement results enables us to do it easily.

Let $\mathbf{X}$ be any $n \times k$ matrix. The symbol $\mathcal{M}(\mathbf{X}) = \{\mathbf{X}\boldsymbol{u} : \boldsymbol{u} \in \mathbb{R}^k\}$ denotes a column space of the matrix $\mathbf{X}$. We will denote $\mathbf{P}_{\mathbf{X}}$ an orthogonal projector in the Euclidean norm on $\mathcal{M}(\mathbf{X})$ and $\mathbf{M}_{\mathbf{X}} = \mathbf{I} - \mathbf{P}_{\mathbf{X}}$. Let $\mathbf{W}$ be a positive semidefinite matrix and $\mathbf{A}$ be a matrix with the same number of columns as the dimension of the matrix $\mathbf{W}$. Then the symbol $\mathbf{A}^-_{m(\mathbf{W})}$ means the minimum $\mathbf{W}$-seminorm g-inverse of the matrix $\mathbf{A}$, i.e., the matrix with properties

$$\mathbf{A}\mathbf{A}^-_{m(\mathbf{W})}\mathbf{A} = \mathbf{A} \qquad \text{and} \qquad \mathbf{W}\mathbf{A}^-_{m(\mathbf{W})}\mathbf{A} = \left(\mathbf{W}\mathbf{A}^-_{m(\mathbf{W})}\mathbf{A}\right)'$$

and $\mathbf{A}^+$ means the Moore-Penrose g-inverse of the matrix $\mathbf{A}$, i.e.,

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

In more detail, cf. [10].

In the following text, the symbol $\widehat{\ }$ denotes an estimator in a model with constraints and $\widetilde{\ }$ denotes an estimator in a model without constraints.

The following two lemmas are given under condition that the covariance matrix $\boldsymbol{\Sigma}$ (cf. (1)) is given. If $\boldsymbol{\Sigma}_{i,i} = \sigma_i^2\mathbf{V}_i$, where σ_i^2 is unknown, $i = 1,\dots,s$, but ratios $\sigma_1^2 : \sigma_2^2 : \dots : \sigma_s^2$ are known, i.e.,

$$\boldsymbol{\Sigma} = \sigma_1^2\left(\mathbf{V}_1 + \frac{\sigma_2^2}{\sigma_1^2}\mathbf{V}_2 + \dots + \frac{\sigma_s^2}{\sigma_1^2}\mathbf{V}_s\right) = \sigma_1^2\mathbf{V}\,,$$

estimators of the parameter $\delta\boldsymbol{\beta}$, δT and $\delta\eta$ are invariant to σ_1^2 and thus these lemmas can be used after a simple modification. If ratios $\sigma_1^2 : \sigma_2^2 : \dots : \sigma_s^2$ are unknown, then $(\sigma_{10}^2,\dots,\sigma_{s0}^2)$-locally best linear unbiased estimators of $\delta\boldsymbol{\beta}$, δT and $\delta\eta$ can be determined only; the vector $(\sigma_{10}^2,\dots,\sigma_{s0}^2)$ is an approximate value of the true value of the vector $(\sigma_1^2,\dots,\sigma_s^2)$.

LEMMA 2.1. *The best linear unbiased estimator* (*BLUE*) *of the parameter* δT *and* $\delta\eta$ *in the model* (4) *and* (6) *is*

$$\begin{pmatrix}\widehat{\delta T}\\ \widehat{\delta\eta}\end{pmatrix} = -\left[\begin{pmatrix}\boldsymbol{a}'\\ -\boldsymbol{1}'\end{pmatrix}^-_{m(GC^{-1}G')}\right]'\mathbf{G}\widetilde{\delta\boldsymbol{\beta}}$$
$$= \begin{pmatrix}-\left[\boldsymbol{a}'(\mathbf{M}_{\boldsymbol{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{1}})^+\boldsymbol{a}\right]^{-1}\boldsymbol{a}'(\mathbf{M}_{\boldsymbol{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{1}})^+\\ \left[\boldsymbol{1}'(\mathbf{M}_{\boldsymbol{a}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{a}})^+\boldsymbol{1}\right]^{-1}\boldsymbol{1}'(\mathbf{M}_{\boldsymbol{a}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{a}})^+\end{pmatrix}\mathbf{G}\widetilde{\delta\boldsymbol{\beta}}\,,$$

where

$$\mathbf{M}_{\boldsymbol{1}} = \mathbf{I} - [1/\boldsymbol{1}'\boldsymbol{1}]\boldsymbol{1}\boldsymbol{1}'\,, \qquad \mathbf{M}_{\boldsymbol{a}} = \mathbf{I} - [1/\boldsymbol{a}'\boldsymbol{a}]\boldsymbol{a}\boldsymbol{a}'\,,$$
$$(\mathbf{M}_{\boldsymbol{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{1}})^+$$
$$= (\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1} - (\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\boldsymbol{1}\left[\boldsymbol{1}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\boldsymbol{1}\right]^{-1}\boldsymbol{1}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\,,$$
$$(\mathbf{M}_{\boldsymbol{a}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{a}})^+$$
$$= (\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1} - (\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\boldsymbol{a}\left[\boldsymbol{a}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\boldsymbol{a}\right]^{-1}\boldsymbol{a}'(\mathbf{G}\mathbf{C}^{-1}\mathbf{G}')^{-1}\,,$$
$$\widetilde{\delta\boldsymbol{\beta}} = \mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\left(\boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\beta}^{(0)})\right)\,, \qquad \mathbf{C} = \mathbf{F}'\boldsymbol{\Sigma}^{-1}\mathbf{F}\,.$$

Further

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

P r o o f . In the model (4) and (6) the BLUE of the parameter $(\delta\boldsymbol{\beta}', \delta T, \delta\eta)'$ is given by the relation

$$\begin{pmatrix} \widehat{\delta\beta} \\ \widehat{\delta T} \\ \widehat{\delta\eta} \end{pmatrix} = \left[\begin{pmatrix} \mathbf{F}', & \mathbf{G}' \\ \mathbf{0}, & \begin{pmatrix} \boldsymbol{a}' \\ -\boldsymbol{1}' \end{pmatrix} \end{pmatrix}^{-}_{m\begin{pmatrix} \boldsymbol{\Sigma}, \mathbf{0} \\ \mathbf{0}, \mathbf{0} \end{pmatrix}} \right]' \begin{pmatrix} \boldsymbol{Y} - \boldsymbol{f}(\boldsymbol{\beta}^{(0)}) \\ \boldsymbol{0} \end{pmatrix}.$$

Now it is sufficient to use relationships (cf. [10])

$$\left[(\mathbf{X}')^{-}_{m(\mathbf{W})} \right]' = [\mathbf{X}'(\mathbf{W} + \mathbf{X}\mathbf{X}')^{-}\mathbf{X}]^{-}\mathbf{X}'(\mathbf{W} + \mathbf{X}\mathbf{X}')^{-},$$

which is valid for any positive semidefinite matrix $\mathbf{W}$, and

$$\begin{pmatrix} \mathbf{A}, & \mathbf{B} \\ \mathbf{B}', & \mathbf{C} \end{pmatrix}^{-} = \begin{pmatrix} (\mathbf{A} - \mathbf{B}\mathbf{C}^{-}\mathbf{B}')^{+}, & -(\mathbf{A} - \mathbf{B}\mathbf{C}^{-}\mathbf{B}')^{+}\mathbf{B}\mathbf{C}^{-} \\ -(\mathbf{C} - \mathbf{B}'\mathbf{A}^{-}\mathbf{B})^{+}\mathbf{B}'\mathbf{A}^{-}, & (\mathbf{C} - \mathbf{B}'\mathbf{A}^{-}\mathbf{B})^{+} \end{pmatrix},$$

which is valid for any positive semidefinite matrix $\begin{pmatrix} \mathbf{A}, & \mathbf{B} \\ \mathbf{B}', & \mathbf{C} \end{pmatrix}$. After a simple, however, tedious calculation we can obtain the statement. □

Lemma 2.2. *The estimator* $\widehat{\delta T}$ *of* δT *from the model* (4), (6) *is the same as the estimator from the model* (4), (5).

P r o o f . Cf. [5; Theorem 4.1]. □

3. Insensitivity regions

The notation

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

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

$$\overline{\mathbf{V}}_i = \begin{pmatrix} \mathbf{0}, & \mathbf{0}, & \mathbf{0}, & \dots, & \mathbf{0} \\ \dots & \dots & \dots & \dots & \dots \\ \mathbf{0}, & \dots, & \mathbf{V}_i, & \dots, & \mathbf{0} \\ \dots & \dots & \dots & \dots & \dots \\ \mathbf{0}, & ,\mathbf{0} & \dots, & \mathbf{0}, & \mathbf{0} \end{pmatrix}, \qquad i = 1, \dots, s.$$

Let $\boldsymbol{\vartheta}^*$ be the true value of the parameter $\boldsymbol{\vartheta}$. Evidently, a change $\boldsymbol{\vartheta}^* + \delta\boldsymbol{\vartheta}$, $\delta\boldsymbol{\vartheta} \in \mathbb{R}^s$, $\delta\vartheta_i > -\vartheta_i^*$, $i = 1, \dots, s$, can destroy the optimum quality of the

$\boldsymbol{\vartheta}^*$-LBLUE $\widehat{\delta T}$ ($\boldsymbol{\vartheta}^*$-locally best linear unbiased estimator), 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 the parameter $\boldsymbol{\vartheta}$ around $\boldsymbol{\vartheta}^*$ inside this region do not cause any essential damage of the chosen statistical characteristic.

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

With respect to Lemma 2.1, we have

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

LEMMA 3.1. *It holds that*

$$\frac{\partial(\widehat{\delta T})}{\partial\vartheta_i} = \left[\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}\right]^{-1}\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{G}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\times$$
$$\times\overline{\mathbf{V}}_i\boldsymbol{\Sigma}^{-1}\mathbf{F}\mathbf{C}^{-1}\mathbf{G}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\left[\mathbf{G}\widetilde{\delta\boldsymbol{\beta}} + \mathbf{a}\widehat{\delta T}\right].$$

Proof. Let any $n \times k$ matrix $\mathbf{A}$ depend on a parameter t and

$$\mathcal{M}\left[\frac{\partial\mathbf{A}(t)}{\partial t}\right] \subset \mathcal{M}\left[\mathbf{A}(t)\right].$$

Then

$$\frac{\partial\mathbf{A}^+(t)}{\partial t} = -\mathbf{A}^+(t)\frac{\partial\mathbf{A}(t)}{\partial t}\mathbf{A}^+(t).$$

It is a consequence of the definition of the Moore-Penrose g-inverse and of the following relationships

$$\mathcal{M}(\mathbf{A}) = \mathcal{M}(\mathbf{A}^+),$$
$$\frac{\partial}{\partial t}\left[\mathbf{A}(t)\mathbf{A}^+(t)\mathbf{A}(t)\right] = \frac{\partial}{\partial t}\mathbf{A}(t),$$
$$\frac{\partial}{\partial t}\left[\mathbf{A}(t)\mathbf{A}^+(t)\mathbf{A}(t)\right] = \left[\frac{\partial}{\partial t}\mathbf{A}(t)\right]\mathbf{A}^+(t)\mathbf{A}(t) + \mathbf{A}(t)\left[\frac{\partial}{\partial t}\mathbf{A}^+(t)\right]\mathbf{A}(t)$$
$$+ \mathbf{A}(t)\mathbf{A}^+(t)\left[\frac{\partial}{\partial t}\mathbf{A}(t)\right],$$

$$\mathbf{A}^+(t)\left[\frac{\partial}{\partial t}\mathbf{A}(t)\right]\mathbf{A}^+(t)$$
$$= \mathbf{A}^+(t)\left[\frac{\partial}{\partial t}\mathbf{A}(t)\right]\mathbf{A}^+(t)\mathbf{A}(t)\mathbf{A}^+(t) + \mathbf{A}^+(t)\mathbf{A}(t)\left[\frac{\partial}{\partial t}\mathbf{A}^+(t)\right]\mathbf{A}(t)\mathbf{A}^+(t)$$
$$+ \mathbf{A}^+(t)\mathbf{A}(t)\mathbf{A}^+(t)\left[\frac{\partial}{\partial t}\mathbf{A}(t)\right]\mathbf{A}^+(t).$$

Now it is sufficient to use the assumption $\mathcal{M}[\partial \mathbf{A}(t)/\partial t] \subset \mathcal{M}[\mathbf{A}(t)]$.

When the matrix $\mathbf{A}(t)$ is regular, then obviously

$$\frac{\partial \mathbf{A}^{-1}(t)}{\partial t} = -\mathbf{A}^{-1}(t)\left[\frac{\partial \mathbf{A}(t)}{\partial t}\right]\mathbf{A}^{-1}(t).$$

Regarding our assumption and just proved relationships, we obtain

$$\begin{aligned}\frac{\partial \widehat{\delta T}}{\partial \vartheta_i} = & -\frac{\partial\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\right]^{-1}}{\partial \vartheta_i}\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\mathbf{G}\widetilde{\delta\boldsymbol{\beta}} \\ & - \left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\right]^{-1}\boldsymbol{a}'\frac{\partial[(\mathbf{M_1 G C^{-1} G' M_1})^+]}{\partial \vartheta_i}\mathbf{G}\widetilde{\delta\boldsymbol{\beta}} \\ & - \left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\right]^{-1}\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\mathbf{G}\frac{\partial \widetilde{\delta\boldsymbol{\beta}}}{\partial \vartheta_i},\end{aligned}$$

where

$$\begin{aligned}&\frac{\partial\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\right]^{-1}}{\partial \vartheta_i} \\ &\quad = \left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\right]^{-1}\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\mathbf{G C^{-1} F'}\Sigma^{-1}\overline{\mathbf{V}}_i \times \\ &\qquad \times \Sigma^{-1}\mathbf{F C^{-1} G'}(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+\boldsymbol{a}\right]^{-1},\end{aligned}$$

$$\begin{aligned}&\frac{\partial[(\mathbf{M_1 G C^{-1} G' M_1})^+]}{\partial \vartheta_i} \\ &\quad = -(\mathbf{M_1 G C^{-1} G' M_1})^+\mathbf{G C^{-1} F'}\Sigma^{-1}\overline{\mathbf{V}}_i\Sigma^{-1}\mathbf{F C^{-1} G'}(\mathbf{M_1 G C^{-1} G' M_1})^+,\end{aligned}$$

and finally

$$\frac{\partial \widetilde{\delta\boldsymbol{\beta}}}{\partial \vartheta_i} = \boldsymbol{0}$$

since

$$\begin{aligned}\widetilde{\delta\boldsymbol{\beta}}_i &= (\mathbf{F}_i'\Sigma_{i,i}^{-1}\mathbf{F}_i)^{-1}\mathbf{F}_i'\Sigma_{i,i}^{-1}\left(\boldsymbol{Y}_i - \boldsymbol{f}_i(\boldsymbol{\beta}_i^{(0)})\right) \\ &= (\mathbf{F}_i'\mathbf{V}_{i,i}^{-1}\mathbf{F}_i)^{-1}\mathbf{F}_i'\mathbf{V}_{i,i}^{-1}\left(\boldsymbol{Y}_i - \boldsymbol{f}_i(\boldsymbol{\beta}_i^{(0)})\right), \qquad i = 1,\dots,s.\end{aligned}$$

Now it is obvious how to finish the proof. □

Lemma 3.2. *The random vectors*

$$\widehat{\delta T} \qquad \text{and} \qquad \frac{\partial[(\mathbf{M_1 G C^{-1} G' M_1})^+]}{\partial \vartheta_i}(\mathbf{G}\widetilde{\delta\boldsymbol{\beta}} + \boldsymbol{a}\widehat{\delta T})$$

are not correlated.

Proof. According to Lemma 2.1, the term

$$\frac{\partial[(\mathbf{M_1 G C^{-1} G' M_1})^+]}{\partial \vartheta_i}(\mathbf{G}\widetilde{\delta\boldsymbol{\beta}} + \boldsymbol{a}\widehat{\delta T})$$

can be written in the form

$$\frac{\partial[(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+]}{\partial\vartheta_i}\Big[\mathbf{I}-\boldsymbol{a}\big[\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\Big]\mathbf{G}\widetilde{\delta\beta}.$$

Now it is sufficient to prove that the term

$$(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\Big\{\mathbf{I}-\boldsymbol{a}\big[\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\Big\}\mathbf{G}\widetilde{\delta\beta}$$

is not correlated with the term

$$\big[\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\mathbf{G}\widetilde{\delta\beta}.$$

□

LEMMA 3.3. *When the second and higher derivatives are neglected, then*

$$\mathrm{Var}\big[\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{\vartheta}^*+\delta\boldsymbol{\vartheta})\big] = \mathrm{Var}\big[\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{\vartheta}^*)\big] + \mathrm{Var}\left[\delta\boldsymbol{\vartheta}'\frac{\partial\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{u})}{\partial\boldsymbol{u}}\Big|_{\boldsymbol{u}=\boldsymbol{\vartheta}^*}\right].$$

P r o o f . It is a consequence of Lemma 3.2. □

Let the shift $\delta\boldsymbol{\vartheta}$ be tolerated if

$$\mathrm{Var}\Big\{\big[\partial\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{u})/\partial\boldsymbol{u}'|_{\boldsymbol{u}=\boldsymbol{\vartheta}^*}\big]\delta\boldsymbol{\vartheta}\Big\} \le \varepsilon^2\,\mathrm{Var}\big[\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{\vartheta}^*)\big],$$

where $\varepsilon > 0$ is chosen by a user. Now the definition of the insensitivity region can be given.

DEFINITION 3.4. Let $\varepsilon > 0$ be a chosen number. The *insensitivity region for the dispersion* of the estimator $\widehat{\delta T}$ is the set

$$\mathcal{N}_{\delta T,\varepsilon} = \Big\{\delta\boldsymbol{\vartheta}:\ \delta\boldsymbol{\vartheta}\in\mathbb{R}^s,\ \delta\vartheta_i > -\vartheta_i^*,\ i=1,\dots,s,$$
$$\mathrm{Var}\left[\delta\boldsymbol{\vartheta}'\frac{\partial\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{u})}{\partial\boldsymbol{u}}\Big|_{\boldsymbol{u}=\boldsymbol{\vartheta}^*}\right] \le \varepsilon^2\,\mathrm{Var}\big[\widehat{\delta T}(\boldsymbol{Y},\boldsymbol{\vartheta}^*)\big]\Big\}.$$

THEOREM 3.5. *The explicit expression of the insensitivity region* $\mathcal{N}_{\delta T,\varepsilon}$ *is*

$$\mathcal{N}_{\delta T,\varepsilon} = \Big\{\delta\boldsymbol{\vartheta}:\ \delta\boldsymbol{\vartheta}\in\mathbb{R}^s,\ \delta\vartheta_i > -\vartheta_i^*,\ i=1,\dots,s,$$
$$\delta\boldsymbol{\vartheta}'\mathbf{W}_{\delta T}\delta\boldsymbol{\vartheta} \le \varepsilon^2\big[\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\boldsymbol{a}\big]^{-1}\Big\},$$

where

$$\mathbf{W}_{\delta T} = \mathbf{K}'\mathbf{F}\mathbf{C}^{-1}\mathbf{G}'\Big\{(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+ - (\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\times$$
$$\times\,\boldsymbol{a}\big[\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\Big\}\mathbf{G}\mathbf{C}^{-1}\mathbf{F}'\mathbf{K},$$

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

$$\boldsymbol{k}_i' = \big[\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\boldsymbol{a}\big]^{-1}\boldsymbol{a}'(\mathbf{M}_1\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_1)^+\mathbf{G}\mathbf{C}^{-1}\mathbf{F}'\boldsymbol{\Sigma}^{-1}\overline{\mathbf{V}}_i\boldsymbol{\Sigma}^{-1}$$
$$i=1,\dots,s.$$

P r o o f . According to Lemma 3.1 it holds that

$$\frac{\partial(\widehat{\delta T})}{\partial \vartheta_i} = \mathbf{k}_i'\mathbf{F}\mathbf{C}^{-1}\mathbf{G}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+[\mathbf{G}\widetilde{\delta\beta} + \mathbf{a}\widehat{\delta T}],$$

where

$$\mathbf{k}_i' = [\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}]^{-1}\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{G}\mathbf{C}^{-1}\mathbf{F}'\Sigma^{-1}\overline{\mathbf{V}}_i\Sigma^{-1}.$$

Let $\mathbf{K} = (\mathbf{k}_1, \dots, \mathbf{k}_s)$. Then

$$\begin{aligned}\mathrm{Var}\left(\delta\boldsymbol{\vartheta}'\frac{\partial(\widehat{\delta T})}{\partial\boldsymbol{\vartheta}}\right) &= \mathrm{Var}\left[\delta\boldsymbol{\vartheta}'\mathbf{K}'\mathbf{F}\mathbf{C}^{-1}\mathbf{G}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+(\mathbf{G}\widetilde{\delta\beta} + \mathbf{a}\widehat{\delta T})\right] \\ &= \delta\boldsymbol{\vartheta}'\mathbf{K}'\,\mathrm{Var}\Big(\mathbf{F}\mathbf{C}^{-1}\mathbf{G}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+(\mathbf{G}\widetilde{\delta\beta} + \mathbf{a}\widehat{\delta T})\Big)\mathbf{K}\delta\boldsymbol{\vartheta}.\end{aligned}$$

Further, with respect to Lemma 2.1,

$$\mathbf{G}\widetilde{\delta\beta} + \mathbf{a}\widehat{\delta T} = \{\mathbf{I} - \mathbf{a}[\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}]^{-1}\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\}\mathbf{G}\widetilde{\delta\beta};$$

thus

$$\begin{aligned}&\mathrm{Var}[(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+(\mathbf{G}\widetilde{\delta\beta} + \mathbf{a}\widehat{\delta T})] \\ &= \{(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+ - (\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}[\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}]^{-1}\times \\ &\qquad \times \mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\{(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+ \\ &\qquad - (\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}[\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}]^{-1}\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\} \\ &= (\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+ - (\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}[\mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{a}]^{-1}\times \\ &\qquad \times \mathbf{a}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+,\end{aligned}$$

since

$$(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'(\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+ = (\mathbf{M}_{\mathbf{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{1}})^+.$$

Now it is obvious how to finish the proof. □

Remark 3.6. The insensitivity region is to be calculated for the true value $\boldsymbol{\vartheta}^*$ of the vector $\boldsymbol{\vartheta}$. Since it is unknown, we calculated it for some near value $\boldsymbol{\vartheta}^{(0)}$. In practice, the approximate value $\vartheta_i^{(0)}$ of the parameter ϑ_i can be determined e.g. from measurement results of the ith regression function, $i = 1, \dots, s$, i.e.,

$$\vartheta_i^{(0)} = \frac{1}{n_i - k_i}[\mathbf{Y}_i - \mathbf{f}_i(\beta_i^{(0)})]'(\mathbf{M}_{\mathbf{F}_i}\mathbf{V}_i\mathbf{M}_{\mathbf{F}_i})^+[\mathbf{Y}_i - \mathbf{f}_i(\beta_i^{(0)})],$$

where $\mathbf{M}_{\mathbf{F}_i} = \mathbf{I} - \mathbf{F}_i(\mathbf{F}_i'\mathbf{F}_i)^-\mathbf{F}_i'$.

If values $\vartheta_i^{(0)}$ are used instead of ϑ_i^*, $i = 1,\dots,s$, the investigation of the sensitivity is valid for the point $\boldsymbol{\vartheta}^{(0)} = \big(\vartheta_1^{(0)},\dots,\vartheta_s^{(0)}\big)'$ only. It can be assumed that an investigation at a point $\boldsymbol{\vartheta}^{(0)}$ near to $\boldsymbol{\vartheta}^*$ gives similar insensitivity region. To be sure about it, it would be useful to do it for several points $\boldsymbol{\vartheta}^{(0)}$ in the neighbourhood of $\boldsymbol{\vartheta}^*$. In the paper it is not done since emphasis on the methodology is given only.

It is to be remarked also that the estimator $\widehat{\boldsymbol{\vartheta}}$ of the parameter $\boldsymbol{\vartheta}$ in an experiment should be calculated in the whole model and not in the partial ones. It is useful to use the MINQUE procedure (in more detail cf. [11]).

4. Linearization

The quadratic version of the model (1) and (3) is given by

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

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

where

$$\begin{aligned}
\boldsymbol{\kappa}(\delta\boldsymbol{\beta}) &= \big[\boldsymbol{\kappa}_1'(\delta\boldsymbol{\beta}_1),\dots,\boldsymbol{\kappa}_s'(\delta\boldsymbol{\beta}_s)\big]',\\
\boldsymbol{\kappa}_i'(\delta\boldsymbol{\beta}_i) &= \big[\kappa_{i,1}(\delta\boldsymbol{\beta}_i),\dots,\kappa_{i,n_i}(\delta\boldsymbol{\beta}_i)\big], && i = 1,\dots,s,\\
\kappa_{i,j} &= \delta\boldsymbol{\beta}_i'\partial^2 f_i(x_{i,j},\boldsymbol{u})/\partial\boldsymbol{u}\partial\boldsymbol{u}'\big|_{\boldsymbol{u}=\boldsymbol{\beta}_i^{(0)}}\delta\boldsymbol{\beta}_i, && i = 1,\dots,s,\ \ j = 1,\dots,n_i,
\end{aligned}$$

$$\begin{aligned}
\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta) &= \big[\omega_1(\delta\boldsymbol{\beta}_1, \delta T, \delta\eta),\dots,\omega_s(\delta\boldsymbol{\beta}_s, \delta T, \delta\eta)\big]',\\
\omega_i(\delta\boldsymbol{\beta}_i, \delta T, \delta\eta) &= (\delta\boldsymbol{\beta}_i', \delta T, \delta\eta)\mathbf{U}_i\begin{pmatrix}\delta\boldsymbol{\beta}_i\\ \delta T\\ \delta\eta\end{pmatrix}, \qquad i = 1,\dots,s,
\end{aligned}$$

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

In this section it is assumed the validity of the quadratic model (7), (8) and the full information on the covariance matrix $\boldsymbol{\Sigma}$. The estimator $\widehat{\delta T}$ from Lemma 2.1 is investigated here. It is to be remarked that $\widehat{\delta T}$ is the BLUE of δT in the models (4), (5) and (4), (6).

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

$$\begin{aligned} b_T &= E(\widehat{\delta T}) - \delta T \\ &= -\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \times \\ &\qquad \times \left[-\frac{1}{2}\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta) + \frac{1}{2}\mathbf{G C^{-1} F' \Sigma^{-1}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right]. \end{aligned}$$

Proof. With respect to Lemma 2.1 we obtain

$$\begin{aligned} E(\widehat{\delta T}) &= -\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \mathbf{G} E(\widetilde{\delta\boldsymbol{\beta}}) \\ &= -\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \times \\ &\qquad \times \mathbf{G}\left(\mathbf{C^{-1} F' \Sigma^{-1} F}\delta\boldsymbol{\beta} + \frac{1}{2}\mathbf{C^{-1} F' \Sigma^{-1}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right) \\ &= -\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \times \\ &\qquad \times \left(\mathbf{G}\delta\boldsymbol{\beta} + \frac{1}{2}\mathbf{G C^{-1} F' \Sigma^{-1}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right) \\ &= \delta T - \left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \times \\ &\qquad \times \left[-\frac{1}{2}\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta) + \frac{1}{2}\mathbf{G C^{-1} F' \Sigma^{-1}}\boldsymbol{\kappa}(\delta\boldsymbol{\beta})\right]. \end{aligned}$$

□

Quantities δT and $\delta\eta$ are functions of $\delta\boldsymbol{\beta}$, which is implied by assumptions, thus the vector $\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta)$ can be expressed as the function of $\delta\boldsymbol{\beta}$ as well. In $\boldsymbol{\omega}$, instead of δT and $\delta\eta$, it is sufficient to use the linear approximation given as a solution of the equation

$$\mathbf{G}\delta\boldsymbol{\beta} + (\boldsymbol{a}, -\boldsymbol{1})\begin{pmatrix}\delta T \\ \delta\eta\end{pmatrix} = \boldsymbol{0}.$$

A suitable solution is

$$\begin{aligned} \delta T &= -\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right]^{-1} \boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \mathbf{G}\delta\boldsymbol{\beta}, \\ \delta\eta &= \quad \left[\boldsymbol{1}'(\mathbf{M_a G C^{-1} G' M_a})^+ \boldsymbol{1}\right]^{-1} \boldsymbol{1}'(\mathbf{M_a G C^{-1} G' M_a})^+ \mathbf{G}\delta\boldsymbol{\beta}. \end{aligned}$$

Therefore, instead of $\boldsymbol{\omega}(\delta\boldsymbol{\beta}, \delta T, \delta\eta)$, the function $\overline{\boldsymbol{\omega}}(\delta\boldsymbol{\beta})$ can be used.

In order to find a set of such shifts of the vector $\delta\boldsymbol{\beta}$ which do not create any essential bias in $\widehat{\delta T}$, the following measure of the nonlinearity for δT will be utilized. (It was motivated by [2].)

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

$$C_{\delta T} = \sup\left\{ \frac{2\sqrt{b_T\left[\boldsymbol{a}'(\mathbf{M_1 G C^{-1} G' M_1})^+ \boldsymbol{a}\right] b_T}}{\delta\boldsymbol{\beta}'\mathbf{C}\,\delta\boldsymbol{\beta}} : \ \delta\boldsymbol{\beta} \in \mathbb{R}^k \right\}.$$

Here $k = k_1 + \cdots + k_s$, where k_i is a dimension of the parameter $\boldsymbol{\beta}_i$ in the ith regression function and

$$\left[\boldsymbol{a}'(\mathbf{M}_{\boldsymbol{1}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\boldsymbol{1}})^{+}\boldsymbol{a}\right]^{-1} = \mathrm{Var}(\widehat{\delta T}), \qquad \mathbf{C}^{-1} = \mathrm{Var}(\widetilde{\delta\boldsymbol{\beta}}).$$

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

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

THEOREM 4.4. *It holds that*

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

P r o o f . The following implications follow from Definition 4.2

$$\delta\boldsymbol{\beta}'\mathbf{C}\delta\boldsymbol{\beta} \le \frac{2\,\mathrm{tol}}{C_{\delta T}} \implies 2\sqrt{b_T\left[\mathrm{Var}(\widehat{\delta T})\right]^{-1}b_T} \le \delta\boldsymbol{\beta}'\mathbf{C}\delta\boldsymbol{\beta}C_{\delta T} \le \frac{2\,\mathrm{tol}}{C_{\delta T}}C_{\delta T} = 2\,\mathrm{tol}.$$

Further $\sqrt{b_T\left[\mathrm{Var}(\widehat{\delta T})\right]^{-1}b_T} \le \mathrm{tol}$ is equivalent to $|b_T| \le \mathrm{tol}\sqrt{\mathrm{Var}(\widehat{\delta T})}$. □

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 that

$$\chi^2_k(1-\alpha) \ll \frac{2\,\mathrm{tol}}{C_{\delta T}}$$

(weak nonlinearity with respect to the bias of $\widehat{\delta T}$). Here $\chi^2_k(1-\alpha)$ is the $(1-\alpha)$-quantile of chi-square distribution with k degrees of freedom.

It is a consequence of the following consideration. Let in the model (4), (6) the matrix $(\boldsymbol{a}, -\boldsymbol{1})$ be denoted as $\mathbf{R}$. Then

$$\mathrm{Var}(\widehat{\delta\boldsymbol{\beta}}) = \mathbf{C}^{-1} - \mathbf{C}^{-1}\mathbf{G}'\left(\mathbf{M}_{\mathbf{R}}\mathbf{G}\mathbf{C}^{-1}\mathbf{G}'\mathbf{M}_{\mathbf{R}}\right)^{+}\mathbf{G}\mathbf{C}^{-1}$$

is the covariance matrix of the estimator $\widehat{\delta\boldsymbol{\beta}}$ (the BLUE of $\delta\boldsymbol{\beta}$ in the model (4), (6)). Since $\mathrm{Var}(\widetilde{\delta\boldsymbol{\beta}}) = \mathbf{C}^{-1}$ ($\widetilde{\delta\boldsymbol{\beta}}$ is the BLUE of $\delta\boldsymbol{\beta}$ in the model (4)), the matrix $\mathrm{Var}(\widetilde{\delta\boldsymbol{\beta}}) - \mathrm{Var}(\widehat{\delta\boldsymbol{\beta}})$ is positive semidefinite and thus the $(1-\alpha)$-confidence ellipsoid based on the estimator $\widehat{\delta\boldsymbol{\beta}}$ is included in the $(1-\alpha)$-confidence ellipsoid based on the estimator $\widetilde{\delta\boldsymbol{\beta}}$ (if for the realization of $\widehat{\delta\boldsymbol{\beta}}$ and $\widetilde{\delta\boldsymbol{\beta}}$, respectively, $\widehat{\delta\boldsymbol{\beta}} = \widetilde{\delta\boldsymbol{\beta}}$ is valid). The $(1-\alpha)$-confidence ellipsoid based on $\widetilde{\delta\boldsymbol{\beta}}$ is

$$\mathcal{E}_{1-\alpha}(\delta\boldsymbol{\beta}) = \left\{\boldsymbol{u}:\ \boldsymbol{u} \in \mathbb{R}^k\,,\ \left(\boldsymbol{u} - \widetilde{\delta\boldsymbol{\beta}}\right)'\mathbf{C}\left(\boldsymbol{u} - \widetilde{\delta\boldsymbol{\beta}}\right) \le \chi_k^2(1-\alpha)\right\}.$$

If for sufficiently large $(1-\alpha)$ it is true that $\mathcal{E}_{1-\alpha}(\delta\boldsymbol{\beta}) \subset \mathcal{L}_{\delta T,\mathrm{tol}}$, we can be practically sure that $\boldsymbol{\beta}^*$ satisfies the condition $\boldsymbol{\beta}^* - \boldsymbol{\beta}^{(0)} \in \mathcal{L}_{\delta T,\mathrm{tol}}$. In practice we substitute the condition $\mathcal{E}_{1-\alpha}(\delta\boldsymbol{\beta}) \subset \mathcal{L}_{\delta T,\mathrm{tol}}$ by the condition $\chi_k^2(1-\alpha) \ll 2\,\mathrm{tol}\,/C_{\delta T}$.

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.,

$$\boldsymbol{Y}_i \sim N_4\left[\begin{pmatrix} 1, & 2\\ 1, & 4\\ 1, & 6\\ 1, & 8 \end{pmatrix}\begin{pmatrix}\beta_{i,1}\\ \beta_{i,2}\end{pmatrix};\sigma_i^2\mathbf{I}\right], \qquad i = 1,2,3. \tag{9}$$

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

$$\beta_{1,1} + \beta_{1,2}T = \beta_{2,1} + \beta_{2,2}T = \beta_{3,1} + \beta_{3,2}T. \tag{10}$$

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 (standard errors σ_1, σ_2, σ_3), the possibility of the linearization of the condition (10) 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 $\widehat{\delta T}$.

Although models (9) are linear, the condition (10) is nonlinear. Hence the linear form of each model and of the condition is given as (using expressions (4), (6))

$$\begin{pmatrix} Y_{i,1}-\beta_{i,1}^{(0)}-2\beta_{i,2}^{(0)} \\ Y_{i,2}-\beta_{i,1}^{(0)}-4\beta_{i,2}^{(0)} \\ Y_{i,3}-\beta_{i,1}^{(0)}-6\beta_{i,2}^{(0)} \\ Y_{i,4}-\beta_{i,1}^{(0)}-8\beta_{i,2}^{(0)} \end{pmatrix} \sim N_4\left[\begin{pmatrix} 1, & 2 \\ 1, & 4 \\ 1, & 6 \\ 1, & 8 \end{pmatrix}\begin{pmatrix} \delta\beta_{i,1} \\ \delta\beta_{i,2} \end{pmatrix}; \sigma_i^2 \mathbf{I}\right], \tag{11}$$

$$\begin{pmatrix} 1, & T^{(0)}, & 0, & 0, & 0, & 0 \\ 0, & 0, & 1, & T^{(0)}, & 0, & 0 \\ 0, & 0, & 0, & 0, & 1, & T^{(0)} \end{pmatrix}\delta\boldsymbol{\beta} + \begin{pmatrix} \beta_{1,2}^{(0)} \\ \beta_{2,2}^{(0)} \\ \beta_{3,2}^{(0)} \end{pmatrix}\delta T - \mathbf{1}\delta\eta = \mathbf{0}, \tag{12}$$

$$\delta\boldsymbol{\beta} = \boldsymbol{\beta} - \boldsymbol{\beta}^{(0)}, \qquad \delta T = T - T^{(0)}, \qquad \delta\eta = \eta - \eta^{(0)},$$

$$\delta\boldsymbol{\beta} = \left(\delta\beta_{1,1}, \delta\beta_{1,2}, \delta\beta_{2,1}, \delta\beta_{2,2}, \delta\beta_{3,1}, \delta\beta_{3,2}\right)'.$$

For the sake of simplicity let the following straight lines

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

be under consideration (cf. Fig. 1).

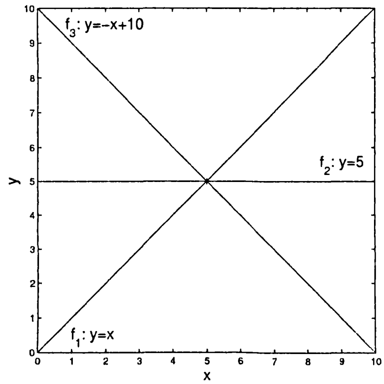

FIGURE 1. Regression functions.

Simulated data are given in dependence on approximate values of standard errors σ_1, σ_2 and σ_3 in Table 1. In this case, approximate values of parameters $\boldsymbol{\beta}$, T and η can be chosen as

$$\boldsymbol{\beta}^{(0)} = (0,1,5,0,10,-1)', \qquad T^{(0)} = 5, \qquad \eta^{(0)} = 5,$$

i.e., $\boldsymbol{\beta}^{(0)}$, $T^{(0)}$ and $\eta^{(0)}$ are true values of $\boldsymbol{\beta}$, T and η, respectively. Hence parameters $\delta\boldsymbol{\beta}$, δT and $\delta\eta$ denote differences of parameters $\boldsymbol{\beta}$, T and η from their corresponding true values. $(\sigma_1^2,\sigma_2^2,\sigma_3^2)$-LBLUEs of the parameter $\delta\boldsymbol{\beta}$ in the model (11) (the model without constraints) are

$$\begin{aligned}
\widetilde{\delta\beta}'_I &= 10^{-6}(0.5341, -0.1155, -1.5004, 0.2718, 0.8373, 0.0069)\,,\\
\widetilde{\delta\beta}'_{II} &= 10^{-6}(0.6680, -0.1430, 26183.6430, -3558.7150, -0.0798, -0.3299)\,,\\
\widetilde{\delta\beta}'_{III} &= 10^{-6}(-6381.4139, -585.0412, 0.5870, 0.0142, 0.5067, -0.0498)\,,\\
\widetilde{\delta\beta}'_{IV} &= 10^{-6}(0.7020, -0.2054, 0.9725, -0.1231, 14787.0050, -3286.3492)\,,
\end{aligned}$$

i.e., estimated values of straight lines coefficients are

$$\begin{aligned}
\widetilde{\beta}'_I &= (\ \ 0.0000,\ 1.0000,\ 5.0000,\ \ 0.0000,\ 10.0000,\ -1.0000)\,,\\
\widetilde{\beta}'_{II} &= (\ \ 0.0000,\ 1.0000,\ 5.0262,\ -0.0036,\ 10.0000,\ -1.0000)\,,\\
\widetilde{\beta}'_{III} &= (-0.0064,\ 0.9994,\ 5.0000,\ \ 0.0000,\ 10.0000,\ -1.0000)\,,\\
\widetilde{\beta}'_{IV} &= (\ \ 0.0000,\ 1.0000,\ 5.0000,\ \ 0.0000,\ 10.0148,\ -1.0033)\,.
\end{aligned}$$

For each case I–IV estimators $\left(\widetilde{\delta\beta}_{i,1}, \widetilde{\delta\beta}_{i,2}\right)'$ are stochastically independent for different regression functions f_i, $i = 1, 2, 3$, and their covariance matrices are

$$\begin{aligned}
\operatorname{Var}\left[\begin{pmatrix}\widetilde{\delta\beta}_{i,1}\\ \widetilde{\delta\beta}_{i,2}\end{pmatrix}\right] &= \begin{pmatrix}0.0150, & -0.0025\\ -0.0025, & 0.0005\end{pmatrix} \qquad \text{if } \sigma_i = 0.1\,,\\
\operatorname{Var}\left[\begin{pmatrix}\widetilde{\delta\beta}_{i,1}\\ \widetilde{\delta\beta}_{i,2}\end{pmatrix}\right] &= \begin{pmatrix}0.3750, & -0.0625\\ -0.0625, & 0.0125\end{pmatrix} \qquad \text{if } \sigma_i = 0.5\,.
\end{aligned}$$

$(\sigma_1^2, \sigma_2^2, \sigma_3^2)$-LBLUEs of parameters δT, T, $\delta\eta$ and η in the model (11), (12) (the model with constraints) are given in the Table 2.

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 tol $= 0.5$. It means that $\sqrt{\mathrm{MSE}(\widehat{\delta T})}$ (mean square error) can increase of 12.5% only, since there holds

$$\begin{aligned}
\sqrt{\mathrm{MSE}(\widehat{\delta T})} &= \sqrt{\operatorname{Var}(\widehat{\delta T}) + b_T^2} \le \sqrt{\operatorname{Var}(\widehat{\delta T}) + \mathrm{tol}^2 \operatorname{Var}(\widehat{\delta T})}\\
&\doteq \sqrt{\operatorname{Var}(\widehat{\delta T})}\left(1 + \frac{\mathrm{tol}^2}{2}\right).
\end{aligned}$$

TABLE 1. SIMULATED DATA.

	I. $\sigma_1=\sigma_2=\sigma_3=0.1$			II. $\sigma_1=\sigma_3=0.1,\ \sigma_2=0.5$		
	f_1	f_2	f_3	f_1	f_2	f_3
$y_{i,1}$	1.9931	4.9856	8.0082	2.0119	5.1269	7.9919
$y_{i,2}$	4.0086	5.0057	6.0071	3.9880	5.4231	6.0053
$y_{i,3}$	6.0125	4.9960	4.0129	5.9998	5.1478	4.0022
$y_{i,4}$	7.9841	5.0069	2.0067	7.9984	4.8391	1.9974

	III. $\sigma_2=\sigma_3=0.1,\ \sigma_1=0.5$			IV. $\sigma_1=\sigma_2=0.1,\ \sigma_3=0.5$		
	f_1	f_2	f_3	f_1	f_2	f_3
$y_{i,1}$	1.9056	5.0043	8.0004	2.0021	5.0108	8.0818
$y_{i,2}$	3.9260	5.0090	6.0068	4.0024	4.9987	6.0585
$y_{i,3}$	5.6312	5.0073	4.0057	5.9899	5.0039	4.0054
$y_{i,4}$	7.9415	5.0058	1.9974	7.9926	5.0009	1.7490

TABLE 2. ESTIMATED VALUES OF δT, T, $\delta\eta$ AND η IN THE MODEL (11), (12).

case	$\widehat{\delta T}$	$\widehat{T}$	$\mathrm{Var}(\widehat{\delta T})$	$\widehat{\delta\eta}$	$\widehat{\eta}$	$\mathrm{Var}(\widehat{\delta\eta})$
I.	$0.4575\cdot10^{-6}$	5.0000	0.0013	$0.2278\cdot10^{-6}$	5.0000	0.0008
II.	$-0.0989\cdot10^{-6}$	5.0000	0.0013	$164.3682\cdot10^{-6}$	5.0002	0.0012
III.	$930.3673\cdot10^{-6}$	5.0009	0.0043	$-619.8537\cdot10^{-6}$	4.9994	0.0022
IV.	$-163.8959\cdot10^{-6}$	4.9998	0.0043	$-109.3615\cdot10^{-6}$	4.9999	0.0022

Numerical results important for the determination of the linearization and the insensitivity region are presented in dependence on approximate values of σ_1, σ_2 and σ_3 in Table 3. Symbols $\mathbf{v}_i$ and λ_i, $i=1,2,3$, denote eigenvectors and their corresponding eigenvalues from the spectral decomposition of the matrix $\mathbf{W}_{\delta T}$, i.e, $\mathbf{W}_{\delta T}=\sum_{i=1}^{3}\lambda_i\mathbf{v}_i\mathbf{v}_i'$. 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 $\mathbf{v}_i$, i.e., $\gamma_i=\sqrt{0.1^2\,\mathrm{Var}(\widehat{\delta T})/\lambda_i}$. 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 $\delta\vartheta_j=0$ for all $j\neq i$ and maximum tolerable shifts $\delta\sigma_i$ of σ_i if $\delta\sigma_j=0$ for all $j\neq i$, respectively. Evidently, $\delta\sigma_i=\sqrt{\vartheta_i+\delta\vartheta_i}-\sigma_i$. Finally, $r=2\,\mathrm{tol}/C_{\delta T}$.

TABLE 3. NUMERICAL RESULTS FOR THE DETERMINATION OF $\mathcal{L}_{\delta T,0.5}$ AND $\mathcal{N}_{\delta T,0.1}$.

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

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

Firstly, the problem of the linearization will be discussed. The 0.95-confidence ellipsoid for $\delta\boldsymbol{\beta}$ is

$$\mathcal{E}_{0.95}(\delta\boldsymbol{\beta}) = \left\{\delta\boldsymbol{\beta}:\ \delta\boldsymbol{\beta} \in \mathbb{R}^6\ ,\ \ (\delta\boldsymbol{\beta} - \widetilde{\delta\boldsymbol{\beta}})'\mathbf{C}(\delta\boldsymbol{\beta} - \widetilde{\delta\boldsymbol{\beta}}) \leq 12.592\right\}$$

$(\chi_6^2(0.95) = 12.592)$ and the linearization region for the bias of $\widehat{\delta T}$ is

$$\mathcal{L}_{\delta T,0.5}(\delta\boldsymbol{\beta}) = \left\{\delta\boldsymbol{\beta}:\ \delta\boldsymbol{\beta} \in \mathbb{R}^6\ ,\ \ \delta\boldsymbol{\beta}'\mathbf{C}\delta\boldsymbol{\beta} \leq r\right\}.$$

From Table 3 it follows that: $r = 63,2455$ in cases I, II and $r = 34,2995$ in cases III and IV. It implies $12.592 \ll r$. Hence the condition (10) can be linearized, i.e., shifts of the vector $\delta\boldsymbol{\beta}$ do not cause the bias in $\widehat{\delta T}$ larger than tolerable one.

Now, there will be discussed the problem of the accuracy of the measurement. Firstly, let all straight lines be measured with the same accuracy $\sigma_i = 0.1$, $i = 1,2,3$ (cf. Table 3, case I). From the spectral decomposition of the matrix $\mathbf{W}_{\delta T}$ it follows that the shift $\delta\vartheta_2$ can be arbitrarily large and it doesn't influence shifts $\delta\vartheta_1$ and $\delta\vartheta_3$. On the contrary, shifts $\delta\vartheta_1$ and $\delta\vartheta_3$ are closely connected. The insensitivity region $\mathcal{N}_{\delta T,0.1}$ is the layer in $\mathbb{R}^3$ with the width equal to $2\cdot\gamma = 2\cdot 0.0025 = 0.005$. Its boundary is given by planes with the normal vector $\boldsymbol{v}_3 = (-0.7071, 0, 0.7071)'$. The orthogonal projection of $\mathcal{N}_{\delta T,0.1}$ on the subspace $\delta\vartheta_1 \times \delta\vartheta_3$ is the band in the direction of the vector $(1,1)'$ (see Fig. 2). It is to be reminded that tolerated shifts $\delta\vartheta_i$ must satisfy $\delta\vartheta_i > -0.01$, $i = 1,2,3$. Hence, in this case, the determination of T is indifferent to the measurement of the straight line $y = 5$. On the other hand, there are high demands on the accuracy of the measurement of $y = x$ and $y = -x + 10$. If the inaccuracy in σ_1 and 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.

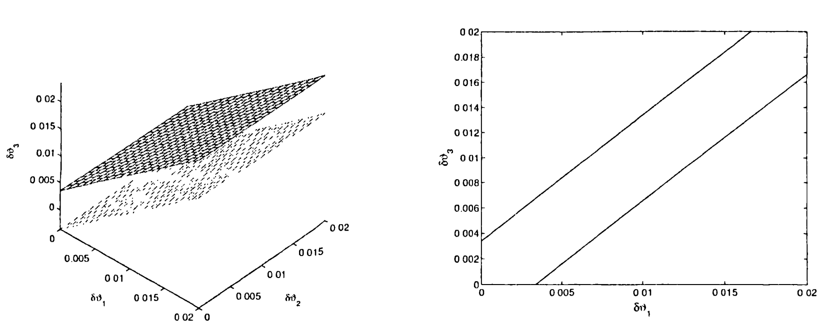

FIGURE 2. The boundary of $\mathcal{N}_{\delta T,0.1}$ from the case I and its projection on $\delta\vartheta_1 \times \delta\vartheta_3$.

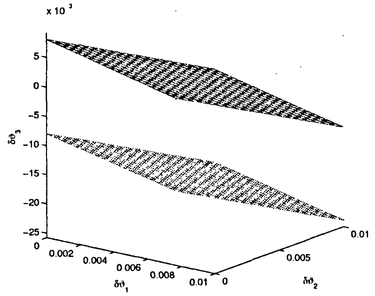

FIGURE 3. The boundary of $\mathcal{N}_{\delta T,0.1}$ from the case III.

The above mentioned conclusion, that the determination of T is independent of the measurement of the straight line $y = 5$, is verified by the case $\sigma_1 = \sigma_3 = 0.1$ and $\sigma_2 = 0.5$ (cf. Table 3, 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 insensitivity region is similar as in the case I. It is the layer in the same direction but with different width equal to 0.0206. Note that $\delta\vartheta_2 > -0.25$ in this case.

Obviously, the straight lines $y = x$ and $y = 10 - x$ have the same weight in the measurement if they have the same accuracy of the measurement. Let us consider $\sigma_1 = 0.5$ and $\sigma_2 = \sigma_3 = 0.1$ or $\sigma_1 = \sigma_2 = 0.1$ and $\sigma_3 = 0.5$ (Table 3, cases III and IV). In both cases $\sqrt{\mathrm{Var}(\widehat{\delta T})} = 0.0656$. An exchange of σ_1 and σ_3 causes similar behavior of the spectral decomposition of $\mathbf{W}_{\delta T}$ in these two cases. Hence the length of semiaxes of $\mathcal{N}_{\delta T,0.1}$ and the maximum tolerable shifts are identical as well as subject to the substitution $\delta\vartheta_1$ and $\delta\vartheta_3$. Evidently, the measurement of f_2 influences the accuracy of the variance of $\widehat{\delta T}$ in these cases. The insensitivity region is also the layer in $\mathbb{R}^3$ given by appropriate eigenvectors $\boldsymbol{v}_i$ and their lengths γ_i, $i = 1, 2, 3$ (cf. Fig. 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..

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