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Confidence Region for Calibration Function Coefficients

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The paper deals with the comparative calibration model, i.e. with a situation when both variables are subject to errors. The calibration function is supposed to be a polynomial. From the statistical point of view, the model after linearization could be represented by the linear errors-in-variables (EIV) model. There are two different ways of using the Kenward and Roger's type approximation to obtain the confidence region for calibration function coefficients. These two confidence regions are compared on a small simulation study. Calibration process and process of measuring with calibrated device are described under the assumption that the measuring errors are normally distributed.

Keywords: Calibration, calibration function parameters, confidence region, measurements with calibrated device.

1. Introduction

Calibration is a very important part of metrology. According to [1] *calibration is an operation that, under specified conditions, in a first step, establishes a relation between the quantity values with measurement uncertainties provided by measurement standards and corresponding indications with associated measurement uncertainties and, in a second step, uses this information to establish a relation for obtaining a measurement result from an indication. Calibration may be expressed by a statement, calibration function, calibration diagram, calibration curve, or calibration table.* It means that, if we have a measuring device and a measurement standard, calibration (process) establishes a relation between the quantity values provided by the measurement standard and corresponding values indicated on the (calibrated) measuring device. Of course, if we measure a quantity by the standard, we obtain only the evidence value (estimate) y of the true quantity value v (expressed in units of the standard). In the same way, if we measure the same quantity by the (calibrated) measuring device, we obtain only the evidence value (estimate) x of the true quantity value μ (expressed in units of the (calibrated) measuring device). The indications (evidence values) can be obtained in the same or different units. In this paper, the theoretical calibration function, $v = f(\mu)$, is understood as a function which expresses the relation between the ideal (true, errorless) values of the same object measured by the calibrated measuring device and the standard, respectively. More precisely, we consider the problem of calibrating the less precise measuring device $\mathscr{X}$ by the more precise measuring device $\mathscr{Y}$. The paper derives the confidence region for calibration function coefficients based on repeated measurements of m different objects (substances, quantities of interest) $V_1, V_2, \ldots, V_m$ realized by two different measuring devices $\mathscr{X}$ and $\mathscr{Y}$, respectively. The accuracy of both measuring devices $\mathscr{X}$ and $\mathscr{Y}$ is unknown, but it is supposed that the squared standard uncertainties σ_x^2 and σ_y^2 are unchanged (but need not be equal) in the whole range of measurements. They are estimated using the MINQUE estimators. The measurements are supposed to be normally distributed and the calibration function is a polynomial of degree k.

The calibration process consists of two parts: (i) creation and evaluation of the calibration model, and (ii) measuring with the calibrated device. In the contribution, we are dealing with creation of the calibration model under some specific but real conditions. In fact, our contribution is about estimation of the calibration function parameters including the problem of determinating the confidence region for these parameters. It turns out that there exist two ways of determinating the desired confidence region using Kenward and Roger's approximation. Using simulations, we compare the behavior of these two confidence regions. It turns out that in the considered situations the statistical performance of both confidence regions is practically the same. Finally, we derive the procedure for measuring with the calibrated device. Given the recorded value x, which is an estimate of the true unknown value μ of the measured object (in units of the less precise measuring device $\mathscr{X}$), we determine the $(1-\alpha)$ confidence interval for v_μ - the true (unknown) errorless value of the same measured object (in units of the more precise measuring device $\mathscr{Y}$).

In this paper, we describe the model of comparative calibration with polynomial calibration function. We derive the best linear unbiased estimators (BLUEs) which are the optimal estimators of the model parameters, and moreover, we

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also derive the approximate $(1-\alpha)$ confidence region for the unknown parameters, as well as for any linear function of the parameters under assumption of normally distributed measurements.

In Section 2 we describe the polynomial calibration model and derive the BLUEs of the model parameters. In Section 3 are derived methods for estimation of the unknown variances (squared uncertainties) of the measurement error. In particular, we consider the minimum norm quadratic unbiased estimator (MINQUE). In Section 4 we present detailed description of the iterative procedure for estimating the model parameters. In Section 5 and Section 6 are described two types of construction of the confidence region for the calibration function parameters based on the Kenward and Rogger's approximation. In Section 7, these two approaches are compared based on using the empirical coverage probabilities by Monte Carlo simulations. Section 8 describes the method of measurements with the calibrated device. The final conclusions and discussion is presented in Section 9.

2. The calibration model and BLUEs of parameters

We assume that we have m different objects (substances, quantities of interest) $V_1, V_2, \ldots, V_m$. Each of these objects is measured with two different measuring devices (device $\mathscr{X}$ and $\mathscr{Y}$, respectively) and we repeat the measurements n times. It is assumed that values measured on both devices are realizations of independent normally distributed random variables.

We shall use the following notation. $X_{i,j}$ is the j-th measurement of object V_i with the device $\mathscr{X}$ and $X_{i,j} \sim N(\mu_i, \sigma_x^2)$, $i = 1,2,\ldots,m$, $j = 1,2,\ldots,n$, where the mean value of $X_{i,j}$ is μ_i — the true errorless value of the object V_i in units of the measuring device $\mathscr{X}$ and σ_x^2 is the dispersion of $X_{i,j}$. Analogously, $Y_{i,j}$ is the j-th measurement of object V_i with the device $\mathscr{Y}$ and $Y_{i,j} \sim N(\nu_i, \sigma_y^2)$, $i = 1,2,\ldots,m$, $j = 1,2,\ldots,n$, where the mean value of $Y_{i,j}$ is ν_i — the true errorless value of the object V_i in units of the measuring device $\mathscr{Y}$ and σ_y^2 is the dispersion of $Y_{i,j}$.

As mentioned above, from the statistical point of view the calibration function expresses the ideal (true, errorless) values of the measurand (the measured object, substance, or quantity) in units of the measuring instrument $\mathscr{Y}$ (here the more precise measuring instrument, the standard) as a function of the true values of the measurand in units of the measuring instrument $\mathscr{X}$ (here the less precise instrument, the calibrated device). In other words, the calibration function expresses the relationship between the ideal (true, errorless) values of measuring the same object (substance, quantity) by two measuring instruments $\mathscr{X}$ and $\mathscr{Y}$, respectively. In our case, we assume that the calibration function is a polynomial of degree k, i.e. $\nu = a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k$.

Let us denote

$$\mathbf{X}_i = \begin{pmatrix} X_{1,i} \\ X_{2,i} \\ \vdots \\ X_{m,i} \end{pmatrix}, \quad i = 1,2,\ldots,n, \quad \mu = \begin{pmatrix} \mu_1 \\ \vdots \\ \mu_m \end{pmatrix}$$

and

$$\mathbf{Y}_i = \begin{pmatrix} Y_{1,i} \\ Y_{2,i} \\ \vdots \\ Y_{m,i} \end{pmatrix}, \quad i = 1,2,\ldots,n, \quad \nu = \begin{pmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_m \end{pmatrix}.$$

The model of calibration is $(\mathbf{X}_1', \mathbf{Y}_1', \ldots, \mathbf{X}_n', \mathbf{Y}_n')' \sim$

$$N\left[(\mathbf{1}_n \otimes \mathbf{I}_{2m}) \begin{pmatrix} \mu \\ \nu \end{pmatrix}, \mathbf{I}_n \otimes \begin{pmatrix} \sigma_x^2\mathbf{I}_m & \mathbf{0} \\ \mathbf{0} & \sigma_y^2\mathbf{I}_m \end{pmatrix}\right]$$

($\otimes$ means the Kronecker product) with the nonlinear constraints on parameters, $\nu = a_0\mathbf{1}_m + a_1\mu + \cdots + a_k\mu^k$, where $\mathbf{1}_m$ is the $m \times 1$ vector $(1,1,\ldots,1)'$, and $\mu^b = (\mu_1^b, \ldots, \mu_m^b)'$. Using the Taylor expansion in proper values $\mathbf{a}_0 = (a_{00}, a_{10}, a_{20}, \ldots, a_{k0})'$ and $\mu_0^b = (\mu_{10}^b, \ldots, \mu_{m0}^b)'$, and neglecting the terms of the second and higher order, and also putting $\delta\mu_i = \mu_i - \mu_{i0}$, $i = 1,2,\ldots,m$, $\delta_\mu = (\delta\mu_1, \ldots, \delta\mu_m)'$, we obtain the linear regression model with (linear) constraints on parameters (see e.g., [2], [3], [4]),

$$\xi = (\mathbf{X}_1' - \mu_0', \mathbf{Y}_1', \ldots, \mathbf{X}_n' - \mu_0', \mathbf{Y}_n')' \sim$$

$$N\left[(\mathbf{1}_n \otimes \mathbf{I}_{2m}) \begin{pmatrix} \delta_\mu \\ \nu \end{pmatrix}, \mathbf{I}_n \otimes \begin{pmatrix} \sigma_x^2\mathbf{I}_m & \mathbf{0} \\ \mathbf{0} & \sigma_y^2\mathbf{I}_m \end{pmatrix}\right], \quad (1)$$

$$\left(\operatorname{diag}\left(a_{10}\mathbf{1}_m + \cdots + ka_{k0}\mu_0^{k-1}\right), -\mathbf{I}_m\right) \begin{pmatrix} \delta_\mu \\ \nu \end{pmatrix} + \left(\mathbf{1}_m, \mu_0, \ldots, \mu_0^k\right)\mathbf{a} = 0 \quad (2)$$

($\operatorname{diag}\left(a_{10}\mathbf{1}_m + \cdots + ka_{k0}\mu_0^{k-1}\right)$ is the diagonal matrix with elements of the vector $\left(a_{10}1_m + \cdots + ka_{k0}\mu_0^{k-1}\right)$ on the diagonal and $\mathbf{a} = (a_0, a_1, \ldots, a_k)'$).

If we denote

$$\beta = (\delta_\mu', \nu')',$$

$$\mathbf{S} = \operatorname{diag}\left(a_{10}\mathbf{1}_m + \cdots + ka_{k0}\mu_0^{k-1}\right),$$

$$\mathbf{B}_1 = (\mathbf{S}, -\mathbf{I}), \quad \mathbf{B}_2 = \left(\mathbf{1}_m, \mu_0, \ldots, \mu_0^k\right),$$

$$\Sigma = \mathbf{I}_n \otimes \begin{pmatrix} \sigma_x^2\mathbf{I}_m & \mathbf{0} \\ \mathbf{0} & \sigma_y^2\mathbf{I}_m \end{pmatrix}, \quad \mathbf{C}^{-1} = \frac{1}{n}\begin{pmatrix} \sigma_x^2\mathbf{I}_m & \mathbf{0} \\ \mathbf{0} & \sigma_y^2\mathbf{I}_m \end{pmatrix},$$

$$\mathbf{A}_1 = \mathbf{A}_1\left(\sigma_x^2, \sigma_y^2\right) = \mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1' = \frac{1}{n}\left(\sigma_x^2\mathbf{S}\mathbf{S} + \sigma_y^2\mathbf{I}\right)$$

$$\overline{\mathbf{X}} = \frac{1}{n}\left(\sum_{i=1}^n X_{1,i}, \ldots, \sum_{i=1}^n X_{m,i}\right)',$$

$$\overline{\mathbf{Y}} = \frac{1}{n}\left(\sum_{i=1}^n Y_{1,i}, \ldots, \sum_{i=1}^n Y_{m,i}\right)',$$

then conditions (2) are

$$(\mathbf{S}, -\mathbf{I}) \begin{pmatrix} \delta_\mu \\ \nu \end{pmatrix} + \mathbf{B}_2\mathbf{a} = \mathbf{0}, \text{ or } \mathbf{B}_1 \begin{pmatrix} \delta_\mu \\ \nu \end{pmatrix} + \mathbf{B}_2\mathbf{a} = \mathbf{0} \quad (3)$$

and according to [2], [3], and [4], the BLUE (best linear unbiased estimator) of vector $(\beta', \mathbf{a}')'$ is

$$\begin{pmatrix} \widehat{\beta} \\ \widehat{\mathbf{a}} \end{pmatrix} = \begin{pmatrix} \mathbf{I}_{2m} - \mathbf{C}^{-1}\mathbf{B}_1'\mathbf{Q}_{11}\mathbf{B}_1 \\ -\mathbf{Q}_{21}\mathbf{B}_1 \end{pmatrix} \begin{pmatrix} \overline{\mathbf{X}} - \mu_0 \\ \overline{\mathbf{Y}} \end{pmatrix},$$

and the covariance matrix of $\widehat{\mathbf{a}}$ is

$$\operatorname{cov}(\widehat{\mathbf{a}}) = -\mathbf{Q}_{22},$$

where

$$\begin{pmatrix} \mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1' & \mathbf{B}_2 \\ \mathbf{B}_2' & \mathbf{0} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{Q}_{11} & \mathbf{Q}_{12} \\ \mathbf{Q}_{21} & \mathbf{Q}_{22} \end{pmatrix}.$$

After a short calculation we finally have (see e.g., [5])

$$\widehat{\mu} = \overline{\mathbf{X}} - \frac{\sigma_x^2}{n}\mathbf{S}\mathbf{Q}_{11}\left(\mathbf{S}\left(\overline{\mathbf{X}} - \mu_0\right) - \overline{\mathbf{Y}}\right), \tag{4}$$

$$\widehat{\nu} = \overline{\mathbf{Y}} + \frac{\sigma_y^2}{n}\mathbf{Q}_{11}\left(\mathbf{S}\left(\overline{\mathbf{X}} - \mu_0\right) - \overline{\mathbf{Y}}\right), \tag{5}$$

$$\widehat{\mathbf{a}} = (\hat{a}_0, \ldots, \hat{a}_k)' = -\mathbf{Q}_{21}\mathbf{B}_1 \begin{pmatrix} \overline{\mathbf{X}} - \mu_0 \\ \overline{\mathbf{Y}} \end{pmatrix} \tag{6}$$

and

$$\operatorname{cov}(\widehat{\mathbf{a}}) = -\mathbf{Q}_{22} = \left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}. \tag{7}$$

We only note that

$$\begin{pmatrix} \overline{\mathbf{X}} - \mu_0 \\ \overline{\mathbf{Y}} \end{pmatrix} \sim N\left(\begin{pmatrix} \delta_\mu \\ \nu \end{pmatrix}, \mathbf{C}^{-1}\right). \tag{8}$$

3. MINQUE ESTIMATORS OF σ_x^2 AND σ_y^2

According to [4], [5], and [6], it can be shown that the MINQUE (minimum norm quadratic unbiased estimator) of the variance components σ_x^2 and σ_y^2 (locally at some appropriate values σ_{x0}^2, σ_{y0}^2) is

$$\begin{pmatrix} \widehat{\sigma}_x^2 \\ \widehat{\sigma}_y^2 \end{pmatrix} = \mathbf{S}_{(M_L\Sigma_0 M_L)^+}^{-1}\mathbf{F}$$

where

$$\mathbf{F} = \begin{pmatrix} \frac{1}{\sigma_{x0}^4}\left[\sum_{j=1}^n \left(X_j - \overline{X}\right)'\left(X_j - \overline{X}\right) + n\left(\overline{X} - \widehat{\mu}\right)'\left(\overline{X} - \widehat{\mu}\right)\right] \\ \frac{1}{\sigma_{y0}^4}\left[\sum_{j=1}^n \left(Y_j - \overline{Y}\right)'\left(Y_j - \overline{Y}\right) + n\left(\overline{Y} - \widehat{\nu}\right)'\left(\overline{Y} - \widehat{\nu}\right)\right] \end{pmatrix},$$

$$\mathbf{S}_{(M_L\Sigma_0 M_L)^+} =$$

$$\begin{pmatrix} \frac{(n-1)m}{\sigma_{x0}^4} + \frac{1}{n^2}\operatorname{tr}\left(\mathbf{S}\mathbf{Q}_{11}\mathbf{S}\mathbf{S}\mathbf{Q}_{11}\mathbf{S}\right) & \frac{1}{n^2}\operatorname{tr}\left(\mathbf{Q}_{11}\mathbf{S}\mathbf{S}\mathbf{Q}_{11}\right) \\ \frac{1}{n^2}\operatorname{tr}\left(\mathbf{Q}_{11}\mathbf{S}\mathbf{S}\mathbf{Q}_{11}\right) & \frac{(n-1)m}{\sigma_{y0}^4} + \frac{1}{n^2}\operatorname{tr}\left(\mathbf{Q}_{11}\mathbf{Q}_{11}\right) \end{pmatrix}.$$

The covariance matrix of $\begin{pmatrix} \widehat{\sigma}_x^2 \\ \widehat{\sigma}_y^2 \end{pmatrix}$ is

$$\mathbf{W}\left(\sigma_{x0}^2, \sigma_{y0}^2\right) = 2\mathbf{S}_{(M_L\Sigma_0 M_L)^+}^{-1}. \tag{9}$$

4. ITERATIVE PROCEDURE FOR ESTIMATING PARAMETERS

To estimate the desired parameters of the calibration function, we apply results described in Section 2 and 3.

1. We compute the initial (appropriate) values of parameters σ_x^2 and σ_y^2 as (realizations of the following random variables)

$$\sigma_{x0}^2 = \frac{1}{mn}\sum_{i=1}^m\sum_{j=1}^n\left(X_{i,j} - \frac{1}{n}\sum_{s=1}^n X_{i,s}\right)^2,$$

$$\sigma_{y0}^2 = \frac{1}{mn}\sum_{i=1}^m\sum_{j=1}^n\left(Y_{i,j} - \frac{1}{n}\sum_{s=1}^n Y_{i,s}\right)^2,$$

then we compute the initial values μ_0 as (realization of the random vector)

$$\mu_0 = \overline{\mathbf{X}},$$

and the vector a_0 as (realization of the random vector)

$$\mathbf{a}_0 = \left(\mathbf{B}_2'\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\overline{\mathbf{Y}}.$$

2. As in Section 2, we obtain the estimators $\widehat{\mu}$ and $\widehat{\nu}$ from (4) and (5), the estimator $\widehat{\mathbf{a}}$ from (6), where

$$\mathbf{Q}_{11} = \left(\mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1'\right)^{-1} - \left(\mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1'\right)^{-1}\mathbf{B}_2\times$$

$$\left(\mathbf{B}_2'\left(\mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1'\right)^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\left(\mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1'\right)^{-1},$$

$$\mathbf{Q}_{12} = \left(\mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1'\right)^{-1}\mathbf{B}_2\left(\mathbf{B}_2'\left(\mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1'\right)^{-1}\mathbf{B}_2\right)^{-1},$$

$$\mathbf{Q}_{21} = \mathbf{Q}_{12}'.$$

3. We put the realization of $\widehat{\mathbf{a}}$ (i.e. the estimate) as the initial value $\mathbf{a}_0 = (a_{00}, a_{10}, \ldots, a_{k0})'$ and calculate the estimators $\widehat{\sigma}_x^2$, $\widehat{\sigma}_y^2$ by the procedure described in Section 3. Thus, we obtain the (approximate) BLUE of $\mu, \nu, \mathbf{a}$ together with the covariance matrix $\operatorname{cov}(\widehat{\mathbf{a}})$.

4. We put the realizations of $\widehat{\sigma}_x^2$, $\widehat{\sigma}_y^2$ (the estimates) as the values σ_{x0}^2 and σ_{x0}^2, respectively, subsequently we put the realization of $\widehat{\mu}$ (i.e. the estimate) as the initial value μ_0 and return to step 2. We have refined the estimates.

We continue with this iteration process (steps 2, 3, and 4) till the subsequent estimates are sufficiently accurate. According to our opinion 4-7 iteration steps are needed.

The MATLAB codes created for this iterative procedure are available on the website[1].

[1] *http://www.math.muni.cz/∼xsirucko/programy/kr.rar*

5. TYPE 1 CONFIDENCE REGION FOR THE CALIBRATION FUNCTION PARAMETERS

For the final estimator of **a**, obtained in (6), it holds

$$\widehat{\mathbf{a}} \sim N\left(\mathbf{a}, \left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\right).$$

In notation of Appendix 1 we have

$$\mathbf{X} = \mathbf{I}, \quad \mathbf{V}\left(\sigma_x^2, \sigma_y^2\right) = \left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1},$$

$$\sigma_1^2 = \sigma_x^2, \quad \sigma_2^2 = \sigma_y^2, \quad \widehat{\sigma}_1^2 = \sigma_{x0}^2, \quad \widehat{\sigma}_2^2 = \sigma_{y0}^2$$

(σ_{x0}^2 and σ_{y0}^2 are from Section 4, point 4). So,

$${}^{(1)}\mathbf{P}_1 = -\frac{1}{n}\mathbf{B}_2'\mathbf{A}_1^{-1}\left(\sigma_{x0}^2, \sigma_{y0}^2\right)\mathbf{S}^2\mathbf{A}_1^{-1}\left(\sigma_{x0}^2, \sigma_{y0}^2\right)\mathbf{B}_2,$$

$${}^{(1)}\mathbf{P}_2 = -\frac{1}{n}\mathbf{B}_2'\mathbf{A}_1^{-2}\left(\sigma_{x0}^2, \sigma_{y0}^2\right)\mathbf{B}_2.$$

Similarly,

$${}^{(1)}\mathbf{U}_{1,1} = \frac{1}{n^2}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2,$$

$${}^{(1)}\mathbf{U}_{1,2} = \frac{1}{n^2}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2,$$

$${}^{(1)}\mathbf{U}_{2,1} = {}^{(1)}\mathbf{U}_{1,2}',$$

$${}^{(1)}\mathbf{U}_{2,2} = \frac{1}{n^2}\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2,$$

$${}^{(1)}\mathbf{R}_{1,1} = \frac{2}{n^2}\Big[\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2$$

$$-\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2\Big],$$

$${}^{(1)}\mathbf{R}_{1,2} = \frac{1}{n^2}\Big[\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2 -$$

$$-\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2 - \mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-2}\mathbf{B}_2 +$$

$$+\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2\Big],$$

$${}^{(1)}\mathbf{R}_{2,2} = \frac{2}{n^2}\left[\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2\left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}\mathbf{B}_2'\mathbf{A}_1^{-2}\mathbf{B}_2 - \mathbf{B}_2'\mathbf{A}_1^{-3}\mathbf{B}_2\right].$$

In the notation of Appendix 1 we have

$$\Phi\left(\sigma_x^2, \sigma_y^2\right) = \left(\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{B}_2\right)^{-1}$$

and

$${}^{(1)}\widehat{\Phi}_A = \Phi\left(\sigma_{x0}^2, \sigma_{y0}^2\right) +$$

$$+2\Phi\left(\sigma_{x0}^2, \sigma_{y0}^2\right)\left\{\sum_{i=1}^{2}\sum_{j=1}^{2}\{\mathbf{W}\}_{i,j}\left({}^{(1)}\mathbf{U}_{i,j} -\right.\right.$$

$$\left.\left. - {}^{(1)}\mathbf{P}_i\Phi(\sigma_{x0}^2, \sigma_{y0}^2)\,{}^{(1)}\mathbf{P}_j - \frac{1}{4}\,{}^{(1)}\mathbf{R}_{i,j}\right)\right\}\Phi\left(\sigma_{x0}^2, \sigma_{y0}^2\right), \quad (10)$$

where $\{\mathbf{W}\}_{i,j}$ is the (i,j)-th element of the matrix $\mathbf{W}(\sigma_{x0}^2, \sigma_{y0}^2)$ given in (9).

According to Appendix 1 we compute ${}^{(1)}A_1$, ${}^{(1)}A_2$, ${}^{(1)}g$, ${}^{(1)}B$, ${}^{(1)}c_1$, ${}^{(1)}c_2$, ${}^{(1)}c_3$, ${}^{(1)}\rho$, ${}^{(1)}u$, and ${}^{(1)}\lambda$. The $(1-\alpha)$ confidence region for vector **a** using the Kenward and Roger's method is

$${}^{(1)}\mathscr{C}_{(1-\alpha)} = \Big\{\mathbf{a}: \ (\widehat{\mathbf{a}}-\mathbf{a})'\,{}^{(1)}\widehat{\Phi}_A^{-1}(\widehat{\mathbf{a}}-\mathbf{a}) \leq$$

$$\frac{k+1}{{}^{(1)}\lambda}F_{k+1,\,{}^{(1)}u}(1-\alpha)\Big\}, \quad (11)$$

where $F_{k+1,\,{}^{(1)}u}(1-\alpha)$ is the $(1-\alpha)$ quantile of the Fisher-Snedecor F distribution with $k+1$ and ${}^{(1)}u$ degrees of freedom.

If inferences are made about a linear combination $\mathbf{l}'\mathbf{a}$ of the elements of **a**, then again according to Appendix 1 we calculate ${}^{(l,1)}A$, ${}^{(l,1)}B$, ${}^{(l,1)}c_1$, ${}^{(l,1)}c_2$, ${}^{(l,1)}c_3$, ${}^{(l,1)}\rho$, ${}^{(l,1)}u$, and ${}^{(l,1)}\lambda$.

The $(1-\alpha)$ confidence region for $\mathbf{l}'\mathbf{a}$ using the Kenward and Roger's method is

$${}^{(l,1)}\mathscr{C}_{(1-\alpha)} = \Big\{\mathbf{l}'\mathbf{a}: \ {}^{(l,1)}\lambda\left(\mathbf{l}'\widehat{\mathbf{a}}-\mathbf{l}'\mathbf{a}\right)\left(\mathbf{l}'\,{}^{(1)}\widehat{\Phi}_A\mathbf{l}\right)^{-1}\left(\mathbf{l}'\widehat{\mathbf{a}}-\mathbf{l}'\mathbf{a}\right) \leq$$

$$F_{1,{}^{(l,1)}u}(1-\alpha)\Big\}. \quad (12)$$

A special case is determination of the $(1-\alpha)$ confidence interval for the value $a_0 + a_1\mu_x + a_2\mu_x^2 + \cdots + a_k\mu_x^k$ for a known value μ_x. In that case is $\mathbf{l} = \mathbf{l}_x = (1, \mu_x, \ldots, \mu_x^k)'$ and according to (12)

$$P\left(\left(\mathbf{l}_x'\widehat{\mathbf{a}}-\mathbf{l}_x'\mathbf{a}\right)^2\left(\mathbf{l}_x'\,{}^{(1)}\widehat{\Phi}_A\mathbf{l}_x\right)^{-1} \leq \right.$$

$$\left.\frac{1}{{}^{(l,1)}\lambda}F_{1,{}^{(l,1)}u}(1-\alpha)\right), \quad (13)$$

i.e.

$$P\left(\mathbf{l}_x'\widehat{\mathbf{a}} - t_{(l,1)_u}(1-\alpha/2)\sqrt{\frac{\mathbf{l}_x'\,{}^{(1)}\widehat{\Phi}_A\mathbf{l}_x}{{}^{(l,1)}\lambda}} \leq \mathbf{l}_x'\mathbf{a} \leq \right.$$

$$\left.\mathbf{l}_x'\widehat{\mathbf{a}} + t_{(l,1)_u}(1-\alpha/2)\sqrt{\frac{\mathbf{l}_x'\,{}^{(1)}\widehat{\Phi}_A\mathbf{l}_x}{{}^{(l,1)}\lambda}}\right) = 1-\alpha, \quad (14)$$

where $t_{(l,1)_u}(1-\frac{\alpha}{2})$ is the $\left(1-\frac{\alpha}{2}\right)$ quantile of Student t distribution with ${}^{(l,1)}u$ degrees of freedom.

6. TYPE 2 CONFIDENCE REGION FOR THE CALIBRATION FUNCTION PARAMETERS

Let us consider the random vector

$$\eta = -\mathbf{S}\left(\overline{\mathbf{X}} - \mu_0\right) + \overline{\mathbf{Y}} = -\mathbf{B}_1 \begin{pmatrix} \overline{\mathbf{X}} - \mu_0 \\ \overline{\mathbf{Y}} \end{pmatrix}. \qquad (15)$$

The mean value of (15) is

$$\mathscr{E}(\eta) = -\mathbf{S}(\mu - \mu_0) + \mathbf{I}\nu = -\mathbf{B}_1 \begin{pmatrix} \delta_\mu \\ \nu \end{pmatrix} = \mathbf{B}_2\mathbf{a}$$

(from condition (2)) and the covariance matrix of (15) is

$$\mathrm{cov}(\eta) = \mathbf{B}_1\mathbf{C}^{-1}\mathbf{B}_1' = \mathbf{A}_1(\sigma_x^2, \sigma_y^2) = \frac{1}{n}(\sigma_x^2\mathbf{S}\mathbf{S} + \sigma_y^2\mathbf{I}).$$

So, for the random vector η holds

$$\eta \sim N(\mathbf{B}_2\mathbf{a}, \mathbf{A}_1).$$

In the notation of Appendix 1, in this section we have

$$\mathbf{X} = \mathbf{B}_2, \quad \mathbf{V}(\sigma_x^2, \sigma_y^2) = \mathbf{A}_1,$$

$$\sigma_1^2 = \sigma_x^2, \quad \sigma_2^2 = \sigma_y^2, \quad \widehat{\sigma}_1^2 = \sigma_{x0}^2, \quad \widehat{\sigma}_2^2 = \sigma_{y0}^2,$$

(σ_{x0}^2 and σ_{y0}^2 are from Section 4, point 4). The REML (restricted maximum likelihood) estimator of $\mathbf{a}$ is the generalized least squares estimator

$$\widehat{\mathbf{a}} = \Phi(\sigma_1^2, \sigma_2^2)\mathbf{B}_2'\mathbf{A}_1^{-1}(\sigma_1^2, \sigma_2^2)\eta$$

with

$$\Phi\left(\sigma_1^2, \sigma_2^2\right) = \left(\mathbf{B}_2'\mathbf{A}_1^{-1}(\sigma_1^2, \sigma_2^2)\mathbf{B}_2\right)^{-1}.$$

The adjusted estimator for small sample covariance matrix of $\widehat{\mathbf{a}}$ recommended by Kenward and Roger [7] is

$$^{(2)}\widehat{\Phi}_A = \Phi\left(\sigma_{x0}^2, \sigma_{y0}^2\right) +$$

$$+2\Phi\left(\sigma_{x0}^2, \sigma_{y0}^2\right)\left\{\sum_{i=1}^{2}\sum_{j=1}^{2}\{\mathbf{W}\}_{i,j}\left(^{(2)}\mathbf{U}_{i,j} - \right.\right.$$

$$\left.\left. - {}^{(2)}\mathbf{P}_i\Phi(\sigma_{x0}^2, \sigma_{y0}^2)\,{}^{(2)}\mathbf{P}_j - \frac{1}{4}\,{}^{(2)}\mathbf{R}_{i,j}\right)\right\}\Phi(\sigma_{x0}^2, \sigma_{y0}^2), \qquad (16)$$

where

$$^{(2)}\mathbf{P}_1 = {}^{(1)}\mathbf{P}_1, \quad {}^{(2)}\mathbf{P}_2 = {}^{(1)}\mathbf{P}_2,$$

$$^{(2)}\mathbf{U}_{1,1} = \frac{1}{n^2}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-1}\mathbf{B}_2,$$

$$^{(2)}\mathbf{U}_{1,2} = \frac{1}{n^2}\mathbf{B}_2'\mathbf{A}_1^{-1}\mathbf{S}^2\mathbf{A}_1^{-2}\mathbf{B}_2,$$

$$^{(2)}\mathbf{U}_{2,1} = {}^{(2)}\mathbf{U}_{1,2}',$$

$$^{(2)}\mathbf{U}_{2,2} = \frac{1}{n^2}\mathbf{B}_2'\mathbf{A}_1^{-3}\mathbf{B}_2,$$

$$^{(2)}\mathbf{R}_{1,1} = {}^{(2)}\mathbf{R}_{1,2} = {}^{(2)}\mathbf{R}_{2,1} = {}^{(2)}\mathbf{R}_{2,2} = \mathbf{0}.$$

According to Appendix 1 (analogously as in Section 5) we compute $^{(2)}A_1$, $^{(2)}A_2$, $^{(2)}g$, $^{(2)}B$, $^{(2)}c_1$, $^{(2)}c_2$, $^{(2)}c_3$, $^{(2)}\rho$, $^{(2)}u$, and $^{(2)}\lambda$.

The $(1-\alpha)$ confidence region for vector $\mathbf{a}$ using the Kenward and Roger's method is now

$$^{(2)}\mathscr{C}_{(1-\alpha)} = \left\{\mathbf{a}:\ (\widehat{\mathbf{a}} - \mathbf{a})'\,{}^{(2)}\widehat{\Phi}_A^{-1}(\widehat{\mathbf{a}} - \mathbf{a}) \le \right.$$

$$\left. \frac{k+1}{^{(2)}\lambda}F_{k+1,\,{}^{(2)}u}(1-\alpha)\right\}. \qquad (17)$$

If inferences are made about the linear combination $\mathbf{l}'\mathbf{a}$ of the elements of $\mathbf{a}$, then again according to Appendix 1 we calculate $^{(l,2)}A$, $^{(l,2)}B$, $^{(l,2)}c_1$, $^{(l,2)}c_2$, $^{(l,2)}c_3$, $^{(l,2)}\rho$, $^{(l,2)}u$, and $^{(l,2)}\lambda$.

The $(1-\alpha)$ confidence region for $\mathbf{l}'\mathbf{a}$ using the Kenward and Roger's method is now

$$^{(l,2)}\mathscr{C}_{(1-\alpha)} = \left\{\mathbf{l}'\mathbf{a}:\ {}^{(l,2)}\lambda\,(\mathbf{l}'\widehat{\mathbf{a}} - \mathbf{l}'\mathbf{a})\left(\mathbf{l}'\,{}^{(2)}\widehat{\Phi}_A\mathbf{l}\right)^{-1}(\mathbf{l}'\widehat{\mathbf{a}} - \mathbf{l}'\mathbf{a}) \le \right.$$

$$\left. F_{1,\,{}^{(l,2)}u}(1-\alpha)\right\}. \qquad (18)$$

So for the value $a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k = \mathbf{l}_\mu'\mathbf{a}$ ($\mathbf{l}_\mu = (1, \mu, \ldots, \mu^k)'$) for a known value μ is

$$P\left(\mathbf{l}_\mu'\widehat{\mathbf{a}} - t_{\,(l,2)u}(1-\alpha/2)\sqrt{\frac{\mathbf{l}_\mu'\,{}^{(2)}\widehat{\Phi}_A\mathbf{l}_\mu}{^{(l,2)}\lambda}} \le \mathbf{l}_\mu'\mathbf{a} \le \right.$$

$$\left.\mathbf{l}_\mu'\widehat{\mathbf{a}} + t_{(l,2)_u}(1-\alpha/2)\sqrt{\frac{\mathbf{l}_\mu'\,{}^{(2)}\widehat{\Phi}_A\mathbf{l}_\mu}{^{(l,2)}\lambda}}\right) = 1-\alpha. \qquad (19)$$

The process of determinating the parameters of the calibration function (the parameter estimation) together with determinating the confidence region for the parameters (and also the confidence region for the whole calibration function) is described as *calibrating the measuring device*.

7. COMPARISON OF TYPE 1 AND TYPE 2 CONFIDENCE REGIONS USING SIMULATIONS

There are two different possibilities to construct the (approximative) $(1-\alpha)$ confidence region for the calibration function parameters $a_0, a_1, \ldots, a_k$, namely (11) (derived in Section 5) and (17) (derived in Section 6). To compare their statistical performances, we carried out a (small) simulation study.

For various parameter sets of the calibration function (polynomial of degree 2, 3, and 4), we realized 10000 repeated measurements of the calibration function and investigated the percentage of the empirical coverage of the true parameters by the $(1-\alpha)$ confidence region (11) (labeled KR1) and by the $(1-\alpha)$ confidence region (17) (labeled KR2). Here, α was in all cases 0.05. Sample results are recorded in Appendix 2. Other simulation results can be found on the website[2]. From the presented simulations it is evident that the performance of both confidence regions (11) and (17) is practically the same.

[2] *http://www.math.muni.cz/∼xsirucko/programy/simulations.pdf*

8. MEASUREMENTS WITH THE CALIBRATED DEVICE

Let us assume that by the measuring device $\mathscr{X}$ (the less precise measuring device, the calibrated measuring device) we have recorded an errorless value μ. We want to determine the (approximate) $(1-\alpha)$ confidence interval for the value $\nu_\mu = a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k$, i.e. the $(1-\alpha)$ confidence interval for the errorless recorded value measured by the measuring device $\mathscr{Y}$ (the more precise measuring device, the standard) using the Kenward and Roger's method.

In that case $\mathbf{l}_\mu = \left(1, \mu, \mu^2, \ldots, \mu^k\right)'$ and the desired $(1-\alpha)$ confidence interval is given by (14) or by (19). If we compute this confidence interval for all μ in a given interval (γ, δ), we obtain a confidence region along the estimated calibration function $\hat{a}_0 + \hat{a}_1\mu + \cdots + \hat{a}_k\mu^k$ in the given interval (γ, δ).

Now, let us determine the confidence interval for $\nu_\mu = a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k$ when (errorless, true) value μ is measured by the measuring device $\mathscr{X}$, but the realization of the measurement (the registered value, evidence value) is x. It means we have realized the measurement $X \sim N(\mu, \sigma_x^2)$. It is well known that if $X \sim N(\mu, \sigma_x^2)$ and S^2 is an estimator of σ_x^2 for which it holds $\frac{w}{\sigma_x^2}S^2 \sim \chi_w^2$ (χ_w^2 is χ^2 distribution with w degrees of freedom), while X and S^2 are independent, then the following holds true

$$\frac{X-\mu}{S} \sim t_w.$$

It means that the dispersion is $\mathscr{D}(S^2) = \frac{2\sigma_x^4}{w}$ and the degrees of freedom are $w = \frac{2\sigma_x^4}{\mathscr{D}(S^2)}$. If we substitute S^2 by the MINQUE estimator $\widehat{\sigma}_x^2$, then the degrees of freedom are given approximately as

$$w \doteq \frac{2\widehat{\sigma_x^4}}{\left\{\mathbf{W}(\sigma_{x0}^2, \sigma_{y0}^2)\right\}_{1,1}},$$

where $W(\sigma_{x0}^2, \sigma_{y0}^2)$ is given in (9).

The $(1-\gamma)$ confidence interval for μ is

$$\left(x - \widehat{\sigma}_x t_w(1-\gamma/2), x + \widehat{\sigma}_x t_w(1-\gamma/2)\right),$$

i.e.

$$P\left\{X - \widehat{\sigma}_x t_w(1-\gamma/2) < \mu < X + \widehat{\sigma}_x t_w(1-\gamma/2)\right\} \doteq 1-\gamma.$$

Our main aim is to find the confidence interval for $\nu_\mu = a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k$ (the errorless (true) value measured on the standard) if the reading on the calibrated measuring device is x. Let us denote

$$d = \operatorname*{argmin}_{s \in (x - \widehat{\sigma}_x t_w(1-\gamma/2), x + \widehat{\sigma}_x t_w(1-\gamma/2))} \{\hat{a}_0 + \hat{a}_1 s + \hat{a}_2 s^2 + \cdots + \hat{a}_k s^k\},$$

$$h = \operatorname*{argmax}_{s \in (x - \widehat{\sigma}_x t_w(1-\gamma/2), x + \widehat{\sigma}_x t_w(1-\gamma/2))} \{\hat{a}_0 + \hat{a}_1 s + \hat{a}_2 s^2 + \cdots + \hat{a}_k s^k\},$$

then, by using the Bonferroni inequality, we finally get the approximate $(1-\alpha-\gamma)$ confidence interval for $\nu_\mu = a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k$

$$P\Bigg\{\hat{a}_0 + \hat{a}_1 d + \cdots + \hat{a}_k d^k - t_w(1-\alpha/2)\times$$
$$\sqrt{\frac{1}{{}^{(l,i)}\lambda}(1\ d\ d^2\ \ldots\ d^k)\ {}^{(i)}\widehat{\Phi}_A(1\ d\ d^2\ \ldots\ d^k)'} \leq$$
$$\leq \nu_\mu = a_0 + a_1\mu + a_2\mu^2 + \cdots + a_k\mu^k \leq$$
$$\leq \hat{a}_0 + \hat{a}_1 h + \cdots + \hat{a}_k h^k + t_w(1-\alpha/2)\times$$
$$\sqrt{\frac{1}{{}^{(l,i)}\lambda}(1\ h\ h^2 \ldots\ h^k)\ {}^{(i)}\widehat{\Phi}_A(1\ h\ h^2 \ldots\ h^k)'}\Bigg\}$$
$$\geq 1-\alpha-\gamma.$$

In our case, the index i can be equal to 1 or 2.

9. CONCLUSIONS

We derived the comparative calibration model where the calibration function is a (complete) polynomial of a given degree. This model is an errors-in-variables model and after linearization could be represented as a linear regression model with linear constraints on parameters. The optimal linear estimators (BLUEs) of the unknown calibration function parameters are shown. The (approximate) $(1-\alpha)$ confidence region for the whole unknown parameter vector and also for any linear function of the parameters is derived using results obtained by Kenward and Roger [7]. This derivation was done in two ways, and simulations indicate that the performance of both ways is practically the same. Further deeper investigation is needed to explain this fact, which is beyond the scope of this paper. The whole contribution is based on the assumption of normally distributed measuring errors. Further research in the issues continues in considering also type B uncertainties of measurements.

APPENDIX 1 — SMALL SAMPLE INFERENCE FOR FIXED EFFECTS

Let us derive the confidence region for the whole parameter $\mathbf{a}$ and also for an arbitrary linear combination $\mathbf{l}'\mathbf{a}$ by using the method suggested by Kenward and Roger [7].

Consider the general Gaussian linear model for s observations $\xi_{s,1}$,

$$\xi \sim N(\mathbf{X}\mathbf{a}; \mathbf{V}),$$

where $\mathbf{X}$ is $s \times (k+1)$ matrix with rank $k+1$, $\mathbf{V}$ is a known covariance matrix, $\mathbf{a}$ is a $(k+1)$-dimensional vector of unknown parameters, and the elements of the covariance matrix $\mathbf{V}(\sigma_1^2, \sigma_2^2)$ are assumed to be functions of two parameters σ_1^2 and σ_2^2. We assume that the first two partial derivatives $\frac{\partial \mathbf{V}}{\partial \sigma_i^2}$, $\frac{\partial^2 \mathbf{V}}{\partial \sigma_i^2 \partial \sigma_j^2}$, $i, j \in \{1,2\}$ exist.

The REML (restricted maximum likelihood) estimator of $\mathbf{a}$ is the generalized least squares estimator

$$\widehat{\mathbf{a}} = \Phi\left(\sigma_1^2, \sigma_2^2\right)\mathbf{X}'\left(\mathbf{V}\left(\sigma_1^2, \sigma_2^2\right)\right)^{-1}\xi$$

with

$$\Phi(\sigma_1^2,\sigma_2^2)=\left(\mathbf{X}'\left(\mathbf{V}\left(\sigma_1^2,\sigma_2^2\right)\right)^{-1}\mathbf{X}\right)^{-1}.$$

The REML estimator of **a** is unbiased. Kenward and Roger [7] recommend to use an adjusted estimator of the small sample covariance matrix of $\widehat{\mathbf{a}}$

$$\widehat{\Phi}_A=\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)+2\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\left\{\sum_{i=1}^{2}\sum_{j=1}^{2}\{\mathbf{W}\}_{i,j}(\mathbf{U}_{i,j}-\right.$$

$$\left.\mathbf{P}_i\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\mathbf{P}_j-\frac{1}{4}\mathbf{R}_{i,j})\right\}\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2),$$

where for $i=1,2$

$$\mathbf{P}_i=\mathbf{X}'\frac{\partial\mathbf{V}^{-1}}{\partial\sigma_i^2}\bigg|_{\substack{\sigma_1^2=\widehat{\sigma}_1^2\\ \sigma_2^2=\widehat{\sigma}_2^2}}\mathbf{X}, \tag{20}$$

$$\mathbf{U}_{i,j}=\mathbf{X}'\frac{\partial\mathbf{V}^{-1}}{\partial\sigma_i^2}\bigg|_{\substack{\sigma_1^2=\widehat{\sigma}_1^2\\ \sigma_2^2=\widehat{\sigma}_2^2}}\mathbf{V}\frac{\partial\mathbf{V}^{-1}}{\partial\sigma_j^2}\bigg|_{\substack{\sigma_1^2=\widehat{\sigma}_1^2\\ \sigma_2^2=\widehat{\sigma}_2^2}}\mathbf{X},$$

$$\mathbf{R}_{i,j}=\mathbf{X}'\mathbf{V}^{-1}\frac{\partial^2\mathbf{V}}{\partial\sigma_i^2\partial\sigma_j^2}\bigg|_{\substack{\sigma_1^2=\widehat{\sigma}_1^2\\ \sigma_2^2=\widehat{\sigma}_2^2}}\mathbf{V}^{-1}\mathbf{X}$$

and $\{\mathbf{W}\}_{i,j}$ is the (i,j)-th element of the matrix $\mathbf{W}(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)$ given in (9).

Inferences are to be made simultaneously about the (whole) vector **a**. Kenward and Roger in [7] showed that the statistics

$$\frac{1}{k+1}(\widehat{\mathbf{a}}-\mathbf{a})'\widehat{\Phi}_A^{-1}(\widehat{\mathbf{a}}-\mathbf{a})\sim\frac{1}{\lambda}F_{k+1,u}$$

has approximately $\frac{1}{\lambda}F_{k+1,u}$ distribution, where λ and u are calculated as follows:

$$A_1=\sum_{i=1}^{2}\sum_{j=1}^{2}\{\mathbf{W}(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\}_{i,j}\times$$

$$\times\operatorname{tr}\left(\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\mathbf{P}_i\right)\operatorname{tr}\left(\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\mathbf{P}_j\right),$$

$$A_2=\sum_{i=1}^{2}\sum_{j=1}^{2}\{\mathbf{W}(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\}_{i,j}\times$$

$$\times\operatorname{tr}\left(\mathbf{P}_i\Phi\left(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2\right)\mathbf{P}_j\Phi\left(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2\right)\right),$$

$$g=\frac{(k+2)A_1-(k+5)A_2}{(k+3)A_2},\quad B=\frac{1}{2(k+1)}(A_1+6A_2),$$

$$c_1=\frac{g}{3(k+1)+2(1-g)},\quad c_2=\frac{k+1-g}{3(k+1)+2(1-g)},$$

$$c_3=\frac{k+3-g}{3(k+1)+2(1-g)},$$

$$\rho=\frac{(1+c_1B)(1-\frac{1}{k+1}A_2)^2}{(k+1)(1-c_2B)^2(1-c_3B)},$$

and finally,

$$u=4+\frac{k+3}{(k+1)\rho-1},$$

$$\lambda=\frac{u}{u-2}\left(1-\frac{1}{k+1}A_2\right).$$

The $(1-\alpha)$ confidence region for vector **a** using the Kenward and Roger's method is

$$\mathscr{C}_{(1-\alpha)}=\left\{\mathbf{a}:\ (\widehat{\mathbf{a}}-\mathbf{a})'\widehat{\Phi}_A^{-1}(\widehat{\mathbf{a}}-\mathbf{a})\le\right.$$

$$\left.\frac{k+1}{\lambda}F_{k+1,u}(1-\alpha)\right\}.$$

If inferences are made about the linear combination $\mathbf{l}'\mathbf{a}$ of the elements of **a** (e.g., we are interested in the $(1-\alpha)$ confidence interval for $\mathbf{l}'\mathbf{a}$), then according to Kenward and Roger in [7]

$$(\widehat{\mathbf{a}}-\mathbf{a})'\mathbf{l}\left(\mathbf{l}'\widehat{\Phi}_A\mathbf{l}\right)^{-1}\mathbf{l}'(\widehat{\mathbf{a}}-\mathbf{a})\sim\frac{1}{{}^{(l)}\lambda}F_{1,{}^{(l)}u},$$

where ${}^{(l)}\lambda$ and ${}^{(l)}u$ are calculated as follows:

$${}^{(l)}A=\frac{1}{(\mathbf{l}'\Phi(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2)\mathbf{l})^2}\sum_{i=1}^{2}\sum_{j=1}^{2}\{\mathbf{W}\left(\widehat{\sigma}_1^2,\widehat{\sigma}_2^2\right)\}_{i,j}\times$$

$$\times\left(\mathbf{l}'\Phi\mathbf{P}_i\Phi\mathbf{l}\right)\left(\mathbf{l}'\Phi\mathbf{P}_j\Phi\mathbf{l}\right),$$

$${}^{(l)}B=\frac{7}{2(k+1)}\,{}^{(l)}A,$$

$${}^{(l)}c_1=\frac{-3}{3(k+1)(k+3)+2(k+6)},$$

$${}^{(l)}c_2=\frac{3+(k+1)(k+3)}{3(k+1)(k+3)+2(k+6)},$$

$${}^{(l)}c_3=\frac{(k+3)^2+3}{3(k+1)(k+3)+2(k+6)},$$

$${}^{(l)}\rho=\frac{(1+\,{}^{(l)}c_1\,{}^{(l)}B)(k+1-\,{}^{(l)}A)}{(k+1)^3(1-\,{}^{(l)}c_2\,{}^{(l)}B)^2(1-\,{}^{(l)}c_3\,{}^{(l)}B)},$$

and finally,

$${}^{(l)}u=\frac{4(k+1)\,{}^{(l)}\rho+k-1}{(k+1)\,{}^{(l)}\rho-1},$$

$${}^{(l)}\lambda=\frac{{}^{(l)}u}{{}^{(l)}u-2}\,\frac{k+1-\,{}^{(l)}A}{k+1}.$$

The $(1-\alpha)$ confidence interval for $\mathbf{l}'\mathbf{a}$ using the Kenward and Roger's method is

$${}^{(l)}\mathscr{C}_{(1-\alpha)}=\left\{\mathbf{l}'\mathbf{a}:\ {}^{(l)}\lambda(\mathbf{l}'\widehat{\mathbf{a}}-\mathbf{l}'\mathbf{a})\left(\mathbf{l}'\widehat{\Phi}_A\mathbf{l}\right)^{-1}(\mathbf{l}'\widehat{\mathbf{a}}-\mathbf{l}'\mathbf{a})\le\right.$$

$$\left.F_{1,{}^{(l)}u}(1-\alpha)\right\}.$$

APPENDIX 2 — SIMULATION RESULTS

The simulation results presented in the tables are explained in Section 7.

Table 1. Polynomial of degree 2, $f_2(x) = 0.25 + 0.5x + 0.05x^2$

$\mu = (0;2.5;5)'$	KR1	KR2	$\mu = (0;1;\ldots;9)'$	KR1	KR2
$\sigma_X = 0.125, \sigma_Y = 0.0625$			$\sigma_X = 0.125, \sigma_Y = 0.0625$		
n=2	0.8763	0.8763	n=2	0.9263	0.9264
n=3	0.9246	0.9246	n=3	0.9376	0.9376
n=4	0.9361	0.9361	n=4	0.9407	0.9409
n=5	0.9409	0.9409	n=5	0.9470	0.9470
n=10	0.9466	0.9466	n=10	0.9499	0.9500
n=20	0.9501	0.9501	n=20	0.9511	0.9511
$\sigma_X = 0.25, \sigma_Y = 0.125$			$\sigma_X = 0.25, \sigma_Y = 0.125$		
n=2	0.8925	0.8925	n=2	0.9268	0.9268
n=3	0.9209	0.9209	n=3	0.9406	0.9407
n=4	0.9279	0.9279	n=4	0.9429	0.9430
n=5	0.9365	0.9365	n=5	0.9434	0.9435
n=10	0.9432	0.9432	n=10	0.9480	0.9481
n=20	0.9518	0.9518	n=20	0.9456	0.9456
$\sigma_X = 0.5, \sigma_Y = 0.25$			$\sigma_X = 0.5, \sigma_Y = 0.25$		
n=2	0.9412	0.9412	n=2	0.9174	0.9178
n=3	0.9306	0.9306	n=3	0.9288	0.9288
n=4	0.9272	0.9272	n=4	0.9332	0.9333
n=5	0.9283	0.9283	n=5	0.9353	0.9354
n=10	0.9416	0.9416	n=10	0.9458	0.9458
n=20	0.9447	0.9447	n=20	0.9461	0.9461
$\sigma_X = 1, \sigma_Y = 0.5$			$\sigma_X = 1, \sigma_Y = 0.5$		
n=2	0.9481	0.9481	n=2	0.9066	0.9072
n=3	0.9328	0.9328	n=3	0.9093	0.9096
n=4	0.9268	0.9268	n=4	0.9200	0.9202
n=5	0.9302	0.9302	n=5	0.9219	0.9220
n=10	0.9293	0.9293	n=10	0.9364	0.9364
n=20	0.9353	0.9353	n=20	0.9409	0.9409

Table 2. Polynomial of degree 2, $g_2(x) = 2 + 0.3x + 0.01x^2$

$\mu = (0;25;50)'$	KR1	KR2	$\mu = (0;10;\ldots;90)'$	KR1	KR2
$\sigma_X = 1.25, \sigma_Y = 0.625$			$\sigma_X = 1.25, \sigma_Y = 0.625$		
n=2	0.8692	0.8692	n=2	0.9249	0.9250
n=3	0.9212	0.9212	n=3	0.9364	0.9364
n=4	0.9340	0.9340	n=4	0.9417	0.9418
n=5	0.9434	0.9434	n=5	0.9454	0.9455
n=10	0.9488	0.9488	n=10	0.9482	0.9484
n=20	0.9516	0.9516	n=20	0.9531	0.9531
$\sigma_X = 2.5, \sigma_Y = 1.25$			$\sigma_X = 2.5, \sigma_Y = 1.25$		
n=2	0.8865	0.8865	n=2	0.9210	0.9211
n=3	0.9257	0.9257	n=3	0.9386	0.9388
n=4	0.9332	0.9332	n=4	0.9445	0.9447
n=5	0.9361	0.9361	n=5	0.9489	0.9490
n=10	0.9464	0.9464	n=10	0.9468	0.9469
n=20	0.9491	0.9491	n=20	0.9476	0.9476
$\sigma_X = 5, \sigma_Y = 2.5$			$\sigma_X = 5, \sigma_Y = 2.5$		
n=2	0.9473	0.9473	n=2	0.9230	0.9236
n=3	0.9376	0.9376	n=3	0.9349	0.9353
n=4	0.9345	0.9345	n=4	0.9430	0.9431
n=5	0.9401	0.9401	n=5	0.9407	0.9411
n=10	0.9462	0.9462	n=10	0.9466	0.9468
n=20	0.9505	0.9505	n=20	0.9475	0.9475
$\sigma_X = 10, \sigma_Y = 5$			$\sigma_X = 10, \sigma_Y = 5$		
n=2	0.9508	0.9508	n=2	0.9253	0.9260
n=3	0.9363	0.9363	n=3	0.9302	0.9370
n=4	0.9381	0.9381	n=4	0.9328	0.9329
n=5	0.9362	0.9362	n=5	0.9368	0.9368
n=10	0.9366	0.9366	n=10	0.9437	0.9437
n=20	0.9466	0.9466	n=20	0.9468	0.9469

Table 3. Polynomial of degree 3, $f_3(x) = -0.8 + 2.46x - 0.38x^2 + 0.025x^3$

$\mu = (1;3.5;6;8.5)'$	KR1	KR2	$\mu = (0;1;\ldots;10)'$	KR1	KR2
$\sigma_X = 0.125, \sigma_Y = 0.0625$			$\sigma_X = 0.125, \sigma_Y = 0.0625$		
n=2	0.8731	0.8731	n=2	0.9228	0.9230
n=3	0.9153	0.9153	n=3	0.9368	0.9370
n=4	0.9342	0.9342	n=4	0.9429	0.9429
n=5	0.9420	0.9420	n=5	0.9439	0.9441
n=10	0.9431	0.9431	n=10	0.9447	0.9447
n=20	0.9509	0.9509	n=20	0.9475	0.9475
$\sigma_X = 0.25, \sigma_Y = 0.125$			$\sigma_X = 0.25, \sigma_Y = 0.125$		
n=2	0.8684	0.8684	n=2	0.9145	0.9146
n=3	0.9070	0.9070	n=3	0.9298	0.9299
n=4	0.9321	0.9321	n=4	0.9352	0.9353
n=5	0.9382	0.9382	n=5	0.9418	0.9418
n=10	0.9422	0.9422	n=10	0.9480	0.9480
n=20	0.9463	0.9463	n=20	0.9462	0.9462
$\sigma_X = 0.5, \sigma_Y = 0.25$			$\sigma_X = 0.5, \sigma_Y = 0.25$		
n=2	0.8583	0.8583	n=2	0.9074	0.9075
n=3	0.8979	0.8979	n=3	0.9203	0.9205
n=4	0.9195	0.9195	n=4	0.9243	0.9244
n=5	0.9231	0.9231	n=5	0.9311	0.9311
n=10	0.9388	0.9388	n=10	0.9441	0.9442
n=20	0.9460	0.9460	n=20	0.9465	0.9466
$\sigma_X = 1, \sigma_Y = 0.5$			$\sigma_X = 1, \sigma_Y = 0.5$		
n=2	0.8997	0.8997	n=2	0.8610	0.8619
n=3	0.8822	0.8822	n=3	0.8776	0.8784
n=4	0.8717	0.8717	n=4	0.8943	0.8948
n=5	0.8759	0.8759	n=5	0.9032	0.9036
n=10	0.9073	0.9073	n=10	0.9219	0,9219
n=20	0.9322	0.9322	n=20	0.9294	0.9295

Table 4. Polynomial of degree 3, $g_3(x) = 0.00023x^3 - 0.035x^2 + 2.2x + 1$

$\mu = (10;35;60;85)'$	KR1	KR2	$\mu = (0;10;\ldots;100)'$	KR1	KR2
$\sigma_X = 1.25, \sigma_Y = 0.625$			$\sigma_X = 1.25, \sigma_Y = 0.625$		
n=2	0.8778	0.8778	n=2	0.9242	0.9243
n=3	0.9219	0.9219	n=3	0.9415	0.9415
n=4	0.9376	0.9376	n=4	0.9414	0.9414
n=5	0.9412	0.9412	n=5	0.9461	0.9461
n=10	0.9433	0.9433	n=10	0.9481	0.9482
n=20	0.9520	0.9520	n=20	0.9457	0.9457
$\sigma_X = 2.5, \sigma_Y = 1.25$			$\sigma_X = 2.5, \sigma_Y = 1.25$		
n=2	0.8776	0.8776	n=2	0.9147	0.9150
n=3	0.9136	0.9136	n=3	0.9354	0.9354
n=4	0.9310	0.9310	n=4	0.9354	0.9356
n=5	0.9375	0.9375	n=5	0.9393	0.9359
n=10	0.9458	0.9458	n=10	0.9452	0.9454
n=20	0.9479	0.9479	n=20	0.9489	0.9489
$\sigma_X = 5, \sigma_Y = 2.5$			$\sigma_X = 5, \sigma_Y = 2.5$		
n=2	0.8683	0.8683	n=2	0.9010	0.9011
n=3	0.8973	0.8973	n=3	0.9155	0.9159
n=4	0.9235	0.9235	n=4	0.9200	0.9204
n=5	0.9218	0.9218	n=5	0.9297	0.9298
n=10	0.9382	0.9382	n=10	0.9457	0.9457
n=20	0.9442	0.9442	n=20	0.9413	0.9414
$\sigma_X = 10, \sigma_Y = 5$			$\sigma_X = 10, \sigma_Y = 5$		
n=2	0.9058	0.9058	n=2	0.8633	0.8639
n=3	0.8856	0.8856	n=3	0.8773	0.8777
n=4	0.8796	0.8796	n=4	0.8911	0.8915
n=5	0.8900	0.8900	n=5	0.9045	0.9047
n=10	0.9098	0.9098	n=10	0.9215	0.9215
n=20	0.9306	0.9306	n=20	0.9346	0.9347

Table 5. Polynomial of degree 4, $f_4(x) = -0.45 + 0.8x + 0.35x^2 - 0.07x^3 + 0.0037x^4$

$\mu = (0;2.5;\ldots;10)'$	KR1	KR2	$\mu = (0;1;\ldots;11)'$	KR1	KR2
$\sigma_X = 0.125, \sigma_Y = 0.0625$			$\sigma_X = 0.125, \sigma_Y = 0.0625$		
n=2	0.8658	0.8658	n=2	0.9204	0.9206
n=3	0.9157	0.9157	n=3	0.9342	0.9344
n=4	0.9295	0.9295	n=4	0.9358	0.9358
n=5	0.9345	0.9345	n=5	0.9381	0.9384
n=10	0.9466	0.9466	n=10	0.9445	0.9446
n=20	0.9475	0.9475	n=20	0.9496	0.9496
$\sigma_X = 0.25, \sigma_Y = 0.125$			$\sigma_X = 0.25, \sigma_Y = 0.125$		
n=2	0.8500	0.8500	n=2	0.8995	0.8996
n=3	0.9108	0.9108	n=3	0.9210	0.9211
n=4	0.9242	0.9242	n=4	0.9253	0.9254
n=5	0.9241	0.9241	n=5	0.9332	0.9333
n=10	0.9333	0.9333	n=10	0.9423	0.9423
n=20	0.9412	0.9412	n=20	0.9457	0.9457
$\sigma_X = 0.5, \sigma_Y = 0.25$			$\sigma_X = 0.5, \sigma_Y = 0.25$		
n=2	0.8658	0.8658	n=2	0.8859	0.8859
n=3	0.9025	0.9025	n=3	0.8991	0.8992
n=4	0.9134	0.9134	n=4	0.9084	0.9086
n=5	0.9169	0.9169	n=5	0.9176	0.9177
n=10	0.9211	0.9211	n=10	0.9268	0.9268
n=20	0.9296	0.9296	n=20	0.9376	0.9376
$\sigma_X = 1, \sigma_Y = 0.5$			$\sigma_X = 1, \sigma_Y = 0.5$		
n=2	0.9334	0.9334	n=2	0.8297	0.8306
n=3	0.9121	0.9121	n=3	0.8628	0.8634
n=4	0.9086	0.9086	n=4	0.8782	0.8790
n=5	0.9114	0.9114	n=5	0.8951	0.8955
n=10	0.9172	0.9172	n=10	0.9068	0.9068
n=20	0.9247	0.9247	n=20	0.9146	0.9146

Table 6. Polynomial of degree 4, $g_4(x) = 5 - 2.47x + 0.175x^2 - 0.0027x^3 + 0.000013x^4$

$\mu = (0;25;\ldots;100)'$	KR1	KR2	$\mu = (0;10;\ldots;110)'$	KR1	KR2
$\sigma_X = 1.25, \sigma_Y = 0.625$			$\sigma_X = 1.25, \sigma_Y = 0.625$		
n=2	0.8605	0.8605	n=2	0.9193	0.9200
n=3	0.9157	0.9157	n=3	0.9388	0.9392
n=4	0.9316	0.9316	n=4	0.9464	0.9469
n=5	0.9356	0.9356	n=5	0.9443	0.9446
n=10	0.9482	0.9482	n=10	0.9537	0.9537
n=20	0.9494	0.9494	n=20	0.9479	0.9479
$\sigma_X = 2.5, \sigma_Y = 1.25$			$\sigma_X = 2.5, \sigma_Y = 1.25$		
n=2	0.8527	0.8527	n=2	0.9159	0.9162
n=3	0.9090	0.9090	n=3	0.9341	0.9348
n=4	0.9254	0.9254	n=4	0.9443	0.9447
n=5	0.9399	0.9399	n=5	0.9397	0.9403
n=10	0.9423	0.9423	n=10	0.9501	0.9503
n=20	0.9482	0.9482	n=20	0.9495	0.9495
$\sigma_X = 5, \sigma_Y = 2.5$			$\sigma_X = 5, \sigma_Y = 2.5$		
n=2	0.8356	0.8356	n=2	0.9092	0.9105
n=3	0.8823	0.8823	n=3	0.9256	0.9259
n=4	0.9079	0.9079	n=4	0.9296	0.9303
n=5	0.9158	0.9158	n=5	0.9392	0.9394
n=10	0.9372	0.9372	n=10	0.9442	0.9442
n=20	0.9431	0.9431	n=20	0.9494	0.9494
$\sigma_X = 10, \sigma_Y = 5$			$\sigma_X = 10, \sigma_Y = 5$		
n=2	0.8794	0.8794	n=2	0.8549	0.8565
n=3	0.8529	0.8529	n=3	0.8895	0.8900
n=4	0.8592	0.8592	n=4	0.8976	0.8978
n=5	0.8606	0.8606	n=5	0.9105	0.9106
n=10	0.8962	0.8962	n=10	0.9285	0.9289
n=20	0.9214	0.9214	n=20	0.9432	0.9433

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REFERENCES

[1] Joint Committee for Guides in Metrology (JCGM). (2012). *International vocabulary of metrology — Basic and general concepts and associated terms (VIM)*. 3rd edition, 2008 version with minor corrections. JCGM 200:2012.

[2] Kubáček, L. (2012). *Foundations of Estimation Theory*. Elsevier.

[3] Fišerová, E., Kubáček, L., Kunderová, P. (2007) *Linear Statistical Models: Regularity and Singularities*. Prague, Czech Republic: Academia.

[4] Kubáček, L., Kubáčková, L. (2000) *Statistics and Metrology*. (In Czech). Olomouc, Czech Republic: Palacký University Olomouc. (in Czech)

[5] Wimmer, G., Palenčár, R., Witkovský, V., Ďuriš, S. (2015). *Vyhodnotenie kalibrácie meradiel: Štatistické metódy pre analýzu neistôt v metrológii (Evaluation of the Calibration of the Measuring Instruments: Statistical Methods for the Analysis of Uncertainties in Metrology)*. Bratislava, Slovak Republic: Slovak University of Technology in Bratislava (STU). (in Slovak)

[6] Rao, C.R., Kleffe, J. (1988) *Estimation of Variance Components and Applications*. North Holland.

[7] Kenward, M.G., Roger, J.H. (1997) Small sample inference for fixed effects from restricted maximum likelihood *Biometrics*, 53, 983–997.

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