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Abstract. The paper builds the comparative calibration model with a polynomial calibration function. The model allows to consider possibly correlated data and combines the type A as well as type B unceranities of measurements. From statistical point of view the model after linearization could be represented by the linear errors-in-variables model (EIV).

1. Introduction

We suggest a procedure for fitting the calibration function. From 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 $\mathcal{Y}$ (typically the less precise measuring instrument, the calibrated device) as a function of the true values of the measurand in units of the measuring instrument $\mathcal{X}$ (typically the more precise instrument, the standard). 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 $\mathcal{X}$ and $\mathcal{Y}$, respectively. The calibration function is supposed to be a polynomial of degree p. Here we consider a model that allows to incorporate possibly correlated data and combines the type A as well as type B uncertaities of the measurements (for more details on metrological interpretation see the international standard [1]). Combined are the current stage-of-knowledge probability distributions about values attributed to measurands and the statistical techniques based on using the EIV model. This model allows using Monte Carlo Methods [2] or characteristic function approach [5] to estimate the parameters, its state-of-knowledge distributions, the approximate coverage intervals for the parameters and also properly evaluate measurements with the calibration device, what is beyond the scope of the contribution.

2. Measurement procedure

Throughout the paper we shall assume that the following assumptions and restrictions for the calibration model hold true: For building the calibration model we perform a pre-planned calibration experiment with replicated measurements made by both instruments $\mathcal{X}$ (the more precise one) and $\mathcal{Y}$ (the less precise one), on a set of m suitably chosen objects (substances, quantities of interest), say $V_1, V_2, \ldots, V_I$, such that their true values μ_i, $i = 1, 2, \ldots, I$, in units of instrument $\mathcal{X}$, span its (that is of instrument $\mathcal{X}$) appropriate calibration range. The measurements are made repeatedly N times for each object measured by the measuring instrument $\mathcal{X}$ and N times for each object measured by the measuring instrument $\mathcal{Y}$.

For the more precise instrument $\mathcal{X}$ the measurement result $x_{i,n}$ is a realization the $n-$th measuring the $i-$th quantity, i.e. the realization of the random variable

$$\xi_{X_{i,n}} = \mu_i + T_{i,n} + \sum_{k=1}^{K} \Delta_{i,n,k}^{(X,1)} + \sum_{j=1}^{J} \Delta_j^{(X,2)},\ i = 1, \ldots, I, \quad n = 1, ..., N \tag{1}$$

where

μ_i are the true (unknown) values of considered quantities of interest in units of the more precise measuring device $\mathcal{X}$, $\quad i = 1, ..., m,$

$T_{i,n}$ are independent random variables representing our knowledge about the measurement errors, with known zero-mean distributions (typically normal or t-distribution) and given standard deviations u_t, obtained from type A evaluations,

$\Delta_{i,n,k}^{(X,1)}$, $i = 1, 2, ..., I,\ n = 1, 2, ..., N,\ k = 1, 2, ..., K$, are corrections due to $n-$th measurement the $i-$th object with the measuring device $\mathcal{X}$ with known distributions, zero mean and known standard uncertainties $u_{\Delta_k^{(X,1)}}$ (type B measurements).

$\Delta_j^{(X,2)}$, $\quad j = 1, 2, ..., J$ are corrections common to all measurements realized with the measuring device $\mathcal{X}$ with known distributions, zero mean and known standard uncertainties $u_{\Delta_j^{(X,2)}}$ (type B measurements)

All corrections including the measuremets $\mu_i + T_{i,n}$ are independently distributed. The distribution of $\xi_{X_{i,n}}$, $i = 1, \ldots, I,\ n = 1, ..., N$ is the state-of-knowlwdge distribution (see [1]).

Similarly the less precise instrument $\mathcal{Y}$ the measurement result $y_{i,n}$ is a realization the $n-$th measuring the $i-$th quantity, i.e. the realization of the random variable

$$\xi_{Y_{i,n}} = \nu_i + R_{i,n} + \sum_{m=1}^{M} \Delta_{i,n,m}^{(Y,1)} + \sum_{r=1}^{R} \Delta_j^{(Y,2)},\ i = 1, \ldots, I, \quad n = 1, ..., N \tag{2}$$

where

ν_i are the true (unknown) values of considered quantities of interest in units of the less precise (calibrated) measuring device $\mathcal{Y}$, $\quad i = 1, ..., I,$

$R_{i,n}$ are independent random variables representing our knowledge about the measurement errors, with known zero-mean distributions (typically normal or t-distribution) and given standard deviations u_R, obtained from type A evaluations.

$\Delta_{i,n,m}^{(Y,1)}$, $\ i = 1, 2, ..., I,\ n = 1, 2, ..., N,\ m = 1, 2, ..., M$, are corrections due to $n-$th measurement the $i-$th object with the measuring device $\mathcal{Y}$ with known distributions, zero mean and known standard uncertainties $u_{\Delta_m^{(Y,1)}}$ (type B measurements).

$\Delta_r^{(Y,2)}$, $\quad r = 1, 2, ..., R$ are corrections common to all measurements realized with the measuring device $\mathcal{Y}$ with known distributions, zero mean and known standard uncertainties $u_{\Delta_r^{(Y,2)}}$ (type B measurements)

All corrections including in the measuremets $R_{i,n}$ are independently distributed. The distribution of $\xi_{Y_{i,n}}$, $i = 1, \ldots, I,\ n = 1, ..., N$ is again the state-of-knowledge distribution (see [1]). Let us denote $\boldsymbol{T}_n = (T_{1,n}, ..., T_{I,n})'$, $\boldsymbol{\mu} = (\mu_1, ..., \mu_I)'$, $\boldsymbol{\nu} = (\nu_1, ..., \nu_I)'$, $R_n = (R_{1,n}, ..., R_{I,n})'$, $n = 1, 2, ..., N$, $\mathbf{1} = (1, 1, ..., 1)' \in \mathcal{R}^I$, $\boldsymbol{\xi}_{X_n} = (\xi_{X_{1,n}}, \xi_{X_{2,n}}, ..., \xi_{X_{I,n}})'$, $\boldsymbol{\xi}_{Y_n} = (\xi_{Y_{1,n}}, \xi_{Y_{2,n}}, ..., \xi_{Y_{I,n}})'$, $i = 1, ..., I$, $n = 1, 2, ..., N$, $\boldsymbol{\mu} = (\mu_1, \mu_2, ..., \mu_I)'$, $\boldsymbol{\nu} = (\nu_1, \nu_2, ..., \nu_I)'$, $\boldsymbol{\Delta}_{n,k}^{(X,1)} = (\Delta_{1,n,k}^{(X,1)}, \Delta_{2,n,k}^{(X,1)}, ..., \Delta_{I,n,k}^{(X,1)})'$, $n = 1, 2, ..., N$, $k = 1, 2, ..., K$, $\boldsymbol{\Delta}_{n,m}^{(Y,1)} = (\Delta_{1,n,m}^{(Y,1)}, \Delta_{2,n,m}^{(Y,1)}, ..., \Delta_{I,n,m}^{(Y,1)})'$, $n = 1, 2, ..., N$, $m = 1, 2, ..., M$.

The model of measurement can be written as

$$\boldsymbol{\xi}_{X_n}=\boldsymbol{\mu}+\boldsymbol{T}_n+\sum_{k=1}^{K}\boldsymbol{\Delta}_{n,k}^{(X,1)}+\sum_{j=1}^{J}\Delta_j^{(X,2)}\mathbf{1},\quad \boldsymbol{\xi}_{Y_n}=\boldsymbol{\nu}+\boldsymbol{R}_n+\sum_{m=1}^{M}\boldsymbol{\Delta}_{n,m}^{(Y,1)}+\sum_{r=1}^{R}\Delta_l^{(Y,2)}\mathbf{1},\ \ n=1,...,N, \tag{3}$$

We denote $u_{x_1}^2$ the known value $u_t^2+\sum_{k=1}^{K}u^2_{\Delta_k^{(X,1)}}$ and $u_{y_1}^2$ the known value $u_R^2+\sum_{m=1}^{M}u^2_{\Delta_m^{(Y,1)}}$. Further let $\sum_{j=1}^{J}u^2_{\Delta_j^{(X,2)}}=u_{x_2}^2$ and $\sum_{r=1}^{R}u^2_{\Delta_r^{(Y,2)}}=u_{y_2}^2$. So the random vector $\boldsymbol{\xi}_{X_n}$, $n=1,2,...,N$ has its mean value $\mathcal{E}(\boldsymbol{\xi}_{X_n})=\boldsymbol{\mu}$, covariance matrix $cov(\boldsymbol{\xi}_{X_n})=u_{x_1}^2\boldsymbol{I}_{I,I}+u_{x_2}^2\boldsymbol{E}_{I,I}$ ($\boldsymbol{E}=\mathbf{11}'$) and $cov(\boldsymbol{\xi}_{X_t},\boldsymbol{\xi}_{X_u})=u_{x_2}^2\boldsymbol{E}\ \ t\neq u$.

Similarly the random vector $\boldsymbol{\xi}_{Y_n}$, $n=1,2,...,N$ has its mean value $\mathcal{E}(\boldsymbol{\xi}_{Y_n})=\boldsymbol{\nu}$, covariance matrix $cov(\boldsymbol{\xi}_{Y_n})=u_{y_1}^2\boldsymbol{I}_{I,I}+u_{y_2}^2\boldsymbol{E}_{I,I}$ and $cov(\boldsymbol{\xi}_{Y_t},\boldsymbol{\xi}_{Y_u})=u_{y_2}^2\boldsymbol{E},\ \ t\neq u$.

The calibration function is supposed to be a polynomial of degree p, i.e.

$$\nu(\mu_i)=\sum_{j=0}^{p}\ {}_{(0)}\alpha_j\mu_i^j a_0+\sum_{j=0}^{p}\ {}_{(1)}\alpha_j\mu_i^j a_1+...+\sum_{j=0}^{p}\ {}_{(p)}\alpha_j\mu_i^j a_p,\quad i=1,2,...,I \tag{4}$$

where parameters ${}_{(0)}\alpha_j,\ {}_{(1)}\alpha_j,...,\ {}_{(p)}\alpha_j,\ j=1,2,...,p$ are known, parameters $a_0,a_1,...,a_p$ are (unknown) coefficients (parameters) of the calibration function.

3. The calibration model

The vector of all measurements is $\boldsymbol{\xi}'=(\boldsymbol{\xi}_{X_1},\boldsymbol{\xi}_{Y_1},\boldsymbol{\xi}_{X_2},\boldsymbol{\xi}_{Y_2},\ldots,\boldsymbol{\xi}_{X_N},\boldsymbol{\xi}_{Y_N})'$ with the mean value

$$\mathcal{E}(\boldsymbol{\xi})=\mathbf{1}_{N,1}\otimes\begin{pmatrix}\boldsymbol{\mu}\\ \boldsymbol{\nu}\end{pmatrix}=(\mathbf{1}_{N,1}\otimes\boldsymbol{I}_{2I,2I})\begin{pmatrix}\boldsymbol{\mu}\\ \boldsymbol{\nu}\end{pmatrix},$$

($\otimes$ means the Kronecker product) and covariance matrix

$$\boldsymbol{\Sigma}=cov(\boldsymbol{\xi})=\boldsymbol{I}_{N,N}\otimes\begin{pmatrix}u_{x_1}^2\boldsymbol{I}_{I,I} & \mathbf{0}\\ \mathbf{0} & u_{y_1}^2\boldsymbol{I}_{I,I}\end{pmatrix}+\boldsymbol{E}_{N,N}\otimes\begin{pmatrix}u_{x_2}^2\boldsymbol{E}_{I,I} & \mathbf{0}\\ \mathbf{0} & u_{y_2}^2\boldsymbol{E}_{I,I}\end{pmatrix}$$

(a known matrix). The (unknown) parameters $\boldsymbol{\mu},\boldsymbol{\nu},\boldsymbol{a}=(a_0,a_1,...,a_k)'$ are bounded with a nonlinear system of conditions (4). This calibration model is an *errors-in-variables model*, see [3]. We shall linearize the system (4) of nonlinear conditions in proper values ${}^{(k)}\mu_1,\ {}^{(k)}\mu_2,...,\ {}^{(k)}\mu_I,\ {}^{(k)}\nu_1,\ {}^{(k)}\nu_2,$ $...,\ {}^{(k)}\nu_I,\ {}^{(k)}a_0,\ {}^{(k)}a_1,...,\ {}^{(k)}a_p$ using Taylor expansion. Let us denote ${}^{(k)}\Delta\mu_1=\mu_1-{}^{(k)}\mu_1,\ {}^{(k)}\Delta\mu_2=\mu_2-{}^{(k)}\mu_2,...\ {}^{(k)}\Delta\mu_I=\mu_I-{}^{(k)}\mu_I,\ {}^{(k)}\Delta\nu_1=\nu_1-{}^{(k)}\nu_1,\ {}^{(k)}\Delta\nu_2=\nu_2-{}^{(k)}\nu_2,...,\ {}^{(k)}\Delta\nu_I=\nu_I-{}^{(k)}\nu_I,\ {}^{(k)}\Delta a_0=a_0-{}^{(k)}a_0,\ {}^{(k)}\Delta a_1=a_1-{}^{(k)}a_1,...,\ {}^{(k)}\Delta a_p=a_p-{}^{(k)}a_p$. After neglecting the terms of 2−nd an higher order and denoting ${}^{(k)}\boldsymbol{\mu}'=({}^{(k)}\mu_1,...,\ {}^{(k)}\mu_I)',\ {}^{(k)}\boldsymbol{\nu}'=({}^{(k)}\nu_1,...,\ {}^{(k)}\nu_I)',\ {}^{(k)}\boldsymbol{\Delta\mu}'=({}^{(k)}\Delta\mu_1,...,\ {}^{(k)}\Delta\mu_I)',\ {}^{(k)}\boldsymbol{\Delta\nu}'=({}^{(k)}\Delta\nu_1,...,\ {}^{(k)}\Delta\nu_I)',\ {}^{(k)}\boldsymbol{\Delta a}'=({}^{(k)}\Delta a_0,...,\ {}^{(k)}\Delta a_p)',\ {}^{(k)}\boldsymbol{\xi}=(\boldsymbol{\xi}_{X_1}-{}^{(k)}\boldsymbol{\mu},\boldsymbol{\xi}_{Y_1}-{}^{(k)}\boldsymbol{\nu},\ldots,\boldsymbol{\xi}_{X_N}-{}^{(k)}\boldsymbol{\mu},\boldsymbol{\xi}_{Y_N}-{}^{(k)}\boldsymbol{\nu})'$, we finally obtain the regression model with type-II (linear) conditions [4] with parameters ${}^{(k)}\boldsymbol{\Delta\mu},\ {}^{(k)}\boldsymbol{\Delta\nu},\ {}^{(k)}\boldsymbol{\Delta a}$

$$\mathcal{E}(\ {}^{(k)}\boldsymbol{\xi})=(\mathbf{1}_{N,1}\otimes\boldsymbol{I}_{2I,2I})\begin{pmatrix}{}^{(k)}\boldsymbol{\Delta\mu}\\ {}^{(k)}\boldsymbol{\Delta\nu}\end{pmatrix}=\boldsymbol{X}\begin{pmatrix}{}^{(k)}\boldsymbol{\Delta\mu}\\ {}^{(k)}\boldsymbol{\Delta\nu}\end{pmatrix}, \tag{5}$$

$$\boldsymbol{\Sigma}=cov(\ {}^{(k)}\boldsymbol{\xi})=\boldsymbol{I}_{I,I}\otimes\begin{pmatrix}u_{x_1}^2\boldsymbol{I}_{I,I} & \mathbf{0}\\ \mathbf{0} & u_{y_1}^2\boldsymbol{I}_{I,I}\end{pmatrix}+\boldsymbol{E}_{I,I}\otimes\begin{pmatrix}u_{x_2}^2\boldsymbol{E}_{I,I} & \mathbf{0}\\ \mathbf{0} & u_{y_2}^2\boldsymbol{E}_{I,I}\end{pmatrix} \tag{6}$$

and with a system of linear conditions (with proper matrices ${}^{(k)}\boldsymbol{B}_1, {}^{(k)}\boldsymbol{B}_2$ and vector ${}^{(k)}\boldsymbol{b}$)

$$ {}^{(k)}\boldsymbol{b} + ({}^{(k)}\boldsymbol{B}_1 \vdots - \boldsymbol{I}_{I,I}) \begin{pmatrix} {}^{(k)}\boldsymbol{\Delta\mu} \\ {}^{(k)}\boldsymbol{\Delta\nu} \end{pmatrix} + {}^{(k)}\boldsymbol{B}_2 \, {}^{(k)}\boldsymbol{\Delta a} = \boldsymbol{0}. \tag{7} $$

This model is a linear approximation of the original model. As we are closer with values ${}^{(k)}\mu_1, {}^{(k)}\mu_2, ..., {}^{(k)}\mu_I, {}^{(k)}\nu_1, {}^{(k)}\nu_2, ..., {}^{(k)}\nu_I, {}^{(k)}a_0, {}^{(k)}a_1, ..., {}^{(k)}a_p$ to the true values $\boldsymbol{\mu}, \boldsymbol{\nu}, \boldsymbol{a}$, the more acurate are the estimates $\widehat{\boldsymbol{\mu}}, \widehat{\boldsymbol{\nu}}, \widehat{\boldsymbol{\theta}}$. In the $k-$th iteration step ($k = 1, 2, ...$) are the estimators ${}^{(k)}\widehat{\boldsymbol{\mu}} = {}^{(k-1)}\boldsymbol{\mu} + {}^{(k-1)}\widehat{\boldsymbol{\Delta\mu}}$, ${}^{(k)}\widehat{\boldsymbol{\nu}} = {}^{(k-1)}\boldsymbol{\nu} + {}^{(k-1)}\widehat{\boldsymbol{\Delta\nu}}$, ${}^{(k)}\widehat{\boldsymbol{a}} = {}^{(k-1)}\boldsymbol{a} + {}^{(k-1)}\widehat{\boldsymbol{\Delta a}}$.

4. The BLUE of the calibration model parameters

The BLUE of the parameters of (calibration) model (5) with (linear) constraints on parameters (7) is (according to [4])

$$ \begin{pmatrix} \begin{pmatrix} {}^{(k)}\widehat{\boldsymbol{\Delta\mu}} \\ {}^{(k)}\widehat{\boldsymbol{\Delta\nu}} \end{pmatrix} \\ {}^{(k)}\widehat{\boldsymbol{\Delta a}} \end{pmatrix} = - \begin{pmatrix} (\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}(\boldsymbol{B}_1 \vdots - \boldsymbol{I})' \, {}^{(k)}\boldsymbol{Q}_{11} \\ {}^{(k)}\boldsymbol{Q}_{21} \end{pmatrix} {}^{(k)}\boldsymbol{b} + $$

$$ \begin{pmatrix} \boldsymbol{I} - (\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}(\boldsymbol{B}_1 \vdots - \boldsymbol{I})' \, {}^{(k)}\boldsymbol{Q}_{11}(\boldsymbol{B}_1 \vdots - \boldsymbol{I}) \\ {}^{(k)}\boldsymbol{Q}_{11}(\boldsymbol{B}_1 \vdots - \boldsymbol{I}) \end{pmatrix} (\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{\Sigma}^{-1} \, {}^{(k)}\boldsymbol{\xi}, $$

where

$$ \begin{pmatrix} {}^{(k)}\boldsymbol{Q}_{11} & {}^{(k)}\boldsymbol{Q}_{12} \\ {}^{(k)}\boldsymbol{Q}_{21} & {}^{(k)}\boldsymbol{Q}_{22} \end{pmatrix} = \begin{pmatrix} ({}^{(k)}\boldsymbol{B}_1 \vdots - \boldsymbol{I}_{I,I})(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}({}^{(k)}\boldsymbol{B}_1 \vdots - \boldsymbol{I}_{I,I})' & {}^{(k)}\boldsymbol{B}_2 \\ {}^{(k)}\boldsymbol{B}_2' & \boldsymbol{0} \end{pmatrix}^{-1}. $$

The covariance matrix of ${}^{(k)}\widehat{\boldsymbol{\Delta a}}$ is

$$ cov({}^{(k)}\widehat{\boldsymbol{\Delta a}}) = {}^{(k)}\boldsymbol{B}_2' \left(({}^{(k)}\boldsymbol{B}_1 \vdots \boldsymbol{I})(\boldsymbol{X}'\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}({}^{(k)}\boldsymbol{B}_1 \vdots \boldsymbol{I})' \right)^{-1} {}^{(k)}\boldsymbol{B}_2. $$

5. Conclusions

Introduced was the model of polynomial calibration. The characteristic function approach [5] is able to estimate the parameters, their state-of-knowledge distributions, the approximate coverage intervals for the parameters and also properly evaluate measurements with the calibration device. This approach is an alternative approach to Monte Carlo Methods [2]. But description of this method is beyond the scope of the contribution.

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