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UNCERTAINTY IN POLYNOMIAL CALIBRATION

The article deals with formulation of measurement uncertainty for polynomial calibration functions. The uncertainty of values calculated from calibration function has contributions from classical influence quantities as well as uncertainty of calibrations parameters. The dependence between the calibrations parameters can be expressed by covariances. The covariance terms have to be taken into account in uncertainty calculation.

uncertainty, polynomial, calibration, least squares method, covariance matrix, residual variance

Preface

In metrological practice in the calibration of measuring instruments linear behavior is usually assumed. Occasionally a linear function is not suitable and linearization is not possible. In such cases a non-linear function is used to approximate the points measured.

The selection of suitable non-linear function is not easy. In the ideal case the approximation function is similar to function derived from theory. This may be impossible in many cases. Then it is possible to use a polynomial function. The advantage of this approach is the possibility to use linear regression methods and simple mathematical apparatus. Additionally this mathematical apparatus is contained in standard software for personal computers.

Principle

In the process of the calibration a relationship between values of the standard and the instrument is established. If this relationship is not linear and there is no reason to prefer another function, a polynomial can be used to fit the data.

The selection of the polynomial order is subjective. As guidance the value of the residual variance can be used. The residual scatter decreases with increasing polynomial order. In the case of non-linear relationship this decrease is steep at the beginning. If the variance changes negligibly on further increasing of the polynomial order, this polynomial can be used for calibration evaluation. The decision, whether the consecutive variances are significantly different can be made by tests, e.g. Fisher F-test [5].

It should be noted that the stability of the parameters of the polynomial is relatively low due to mutual correlation. The polynomial is used as an interpolation function only. The effort for interpretation of the values of parameters is not effective. A small change in the structure of experimental points may lead to completely different values of parameters, although the fit of the points is similar.

Least squares method

In this case the mathematical model is the equation:

$$f = b_0 + b_1 x + b_2 x^2 + b_3 x^3 .$$

In the calibration measurements it is usual to make more measurements than the number of function parameters. A minimum number of data points is usually recommended, corresponding to three times the number of adjusted parameters – for a linear function 6 points are recommended. For each measurement point an equation can be written, where the residual ε is also given.

$$y_i = b_0 + b_1 x_i + b_2 x_i^2 + b_3 x_i^3 + \varepsilon_i .$$

For n points *n* equations can be written. If they are written in a matrix form, we get:

$$\begin{pmatrix} y_1 \\ y_2 \\ . \\ . \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ . & . & . & . \\ . & . & . & . \\ 1 & x_n & x_n^2 & x_n^3 \end{pmatrix} \times \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ . \\ . \\ \varepsilon_n \end{pmatrix} .$$

Or in matrix notation

$$\mathbf{y} = \mathbf{X.b} + \boldsymbol{\varepsilon} .$$

In the least squares method such vector **b** is sought to yield minimum value of the term $\sum \varepsilon_i^2$ [1, 3, 4]. Parameter vector calculated from the following equation fulfils this condition:

$$\mathbf{b} = \left(\mathbf{X}^\mathbf{T}\mathbf{X}\right)^{-1}\mathbf{X}^\mathbf{T}\mathbf{y} .$$

In parallel with the calculation of vector **b** it is possible to calculate the values of the elements of the covariance matrix:

$$\mathbf{C} = \boldsymbol{\sigma}^2\left(\mathbf{X}^\mathbf{T}\mathbf{X}\right)^{-1} .$$

The variance σ^2 can be estimated from the residual variance s_R^2 according to the equation

$$s_R^2 = \frac{\sum\left(y_i - f\left(x_i\right)\right)^2}{n-k} ,$$

where k is the number of adjusted parameters.

The covariance matrix is symmetrical. In the main diagonal it contains the variances s_{ii} of the individual parameters. The off-diagonal elements contain individual covariances s_{ij} between the parameters. The covariance matrix for a polynomial of the III order looks like this:

$$\mathbf{C} = \sigma^2\left(\mathbf{X}^{\mathbf{T}}\mathbf{X}\right)^{-1} = \begin{pmatrix} s_{00} & s_{01} & s_{02} & s_{03} \\ s_{10} & s_{11} & s_{12} & s_{13} \\ s_{20} & s_{21} & s_{22} & s_{23} \\ s_{30} & s_{31} & s_{32} & s_{33} \end{pmatrix}.$$

Uncertainty calculation

If the mathematical model of the measurement of *f* is known, then the uncertainty can be calculated according to the document [2] using the basic equation,

$$u_f^2 = \sum_{i=1}^{k}\sum_{j=1}^{k}\left(\frac{\partial f}{\partial x_i}\right)\left(\frac{\partial f}{\partial x_j}\right)u_{ij},$$

which is for practical reasons used in the form:

$$u_f^2 = \sum_{i=1}^{n}\left[\left(\frac{\partial f}{\partial x_i}\right)^2 \cdot u_{ii}\right] + 2\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}\cdot u_{ij}.$$

This equation is sometimes called law of uncertainty propagation. The first term relates to diagonal elements of the covariance matrix, the second term to the off-diagonal ones.

After application of the law of uncertainty propagation to our mathematical model we get an equation applicable for calculation of the standard uncertainty.

$$u_f^2 = (1u_{00})^2 + (x\,u_{11})^2 + \left(x^2u_{22}\right)^2 + \left(x^3u_{33}\right)^2 + \\ + 2\left(xu_{01} + x^2u_{02} + x^3u_{03} + x^3u_{12} + x^4u_{13} + x^5u_{23}\right).$$

This uncertainty relates to the value calculated from the regression function and has the character of type A uncertainty. Type B uncertainty can be obtained after evaluation of contributions of all influence quantities. These uncertainties are combined as follows

$$u_c = \sqrt{u_A^2 + u_B^2}.$$

To yield combined standard uncertainty u_c and after multiplication with coverage factor k we get expanded uncertainty U, which is added to the measured value to yield the measurement result.

$$U = k.u_c.$$

For coverage factor value k =2 is used usually.

Example

The procedure is best illustrated on an example. The data are taken from a real measurement, where the conductivity of a solution is calculated from measured conductance. For simplicity the conductance and conductivity will be noted as x and y.

In the first step a linear function was used for regression. For the calculation of parameters the procedure described above was used. The graph is not interesting. The individual points lie almost exactly at the calibration line, see Fig. 1.

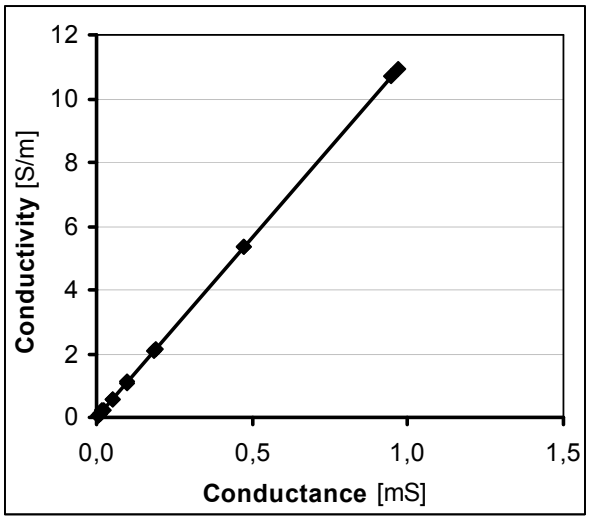

Fig. 1. Calibration line

More information can be drawn from a graph where the residuals (differences between experimental and calculated values) are plotted against independent variable (Fig. 2, together wit expanded uncertainties). All deviations are at once easy to see, as the calibration function is projected into the x-axis.

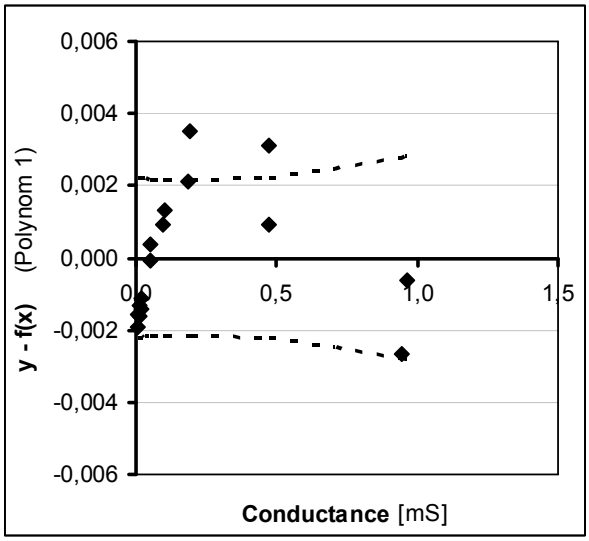

Fig. 2. Dispersion of residuals around the straight line

For calculation of uncertainty the above equations were used, which for a line give the formula:

$$U = \sqrt{\left(s_{00} + x_i^2.s_{11} + 2.x_i.s_{01}\right) + u_B^2}.$$

It is clear from the graph that the residuals are not randomly distributed and the calibration function is not linear. Some points are even outside the limits of the expanded uncertainty.

After that, a polynomial of the third order was used. The residuals graph is more illustrative (Fig. 3).

Residuals are evenly distributed around the regression line (here shown as x-axis) and this functional dependence can be used for calibration.

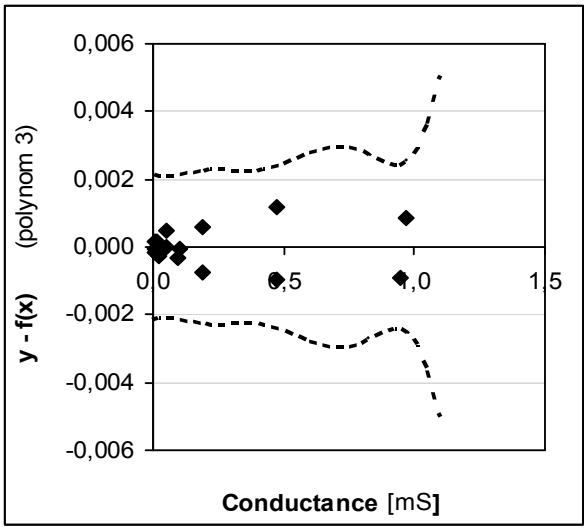

Fig. 3. Dispersion of residuals around polynomial III

The expanded uncertainty is also given in the graph. It can be clearly seen that the uncertainty **depends** on the structure of experimental data and it is not possible to claim the same uncertainty for the whole calibration interval.

Finally, the intermediate data for the matrix calculation are given for those who want to reproduce the calculation.

Summary

Higher order polynomials can be used for calibration. The function should be regarded as a regression function and the parameters should not be given any physical meaning. Due to strong covariance between the parameters, it must be taken into account in calculation of uncertainty. Uncertainty from regression is of type A. In graphical display it is useful to depict the residuals instead of function values.

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