

## 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:

$$f = b_0 + b_1x + b_2x^2 + b_3x^3.$$

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  $\varepsilon$  is also given.

$$y_i = b_0 + b_1x_i + b_2x_i^2 + b_3x_i^3 + \varepsilon_i.$$

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

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

Or in matrix notation

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

In the least squares method such vector  $\mathbf{b}$  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:

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

In parallel with the calculation of vector  $\mathbf{b}$  it is possible to calculate the values of the elements of the covariance matrix:

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

The variance  $\sigma^2$  can be estimated from the residual variance  $s_R^2$  according to the equation

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

where  $k$  is the number of adjusted parameters.



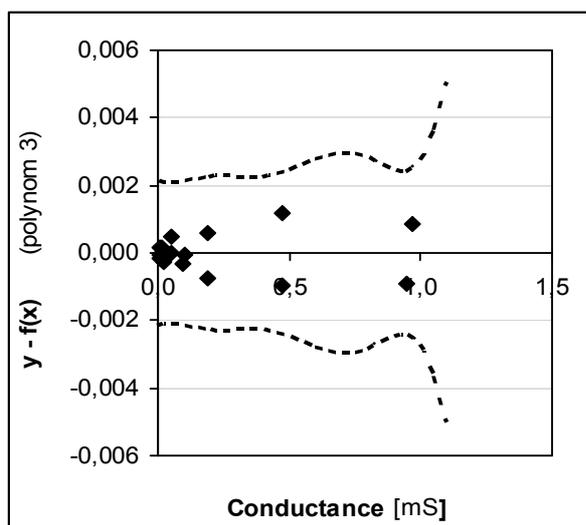


Fig. 3. Dispersion of residuals around polynomial III

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.

## References

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