Using of Monte Carlo simulation to investigate of the correlation influences to the thermocouple deviation function uncertainty

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Abstract. For proper use of thermocouples in every day laboratory calibration is important to know the deviation function from the thermocouple standard EN 60584-1. In practise, the polynomial of first, second and third order are used for an interpolation calculation. Evaluation of uncertainty is often based on least squared method where no correlation is involved. In reality, each calibration point is correlated by using of same equipment and traceability. This paper will show the influence of different levels of correlation to the uncertainty propagation of interpolation. The evaluation is based on real thermocouple and Monte Carlo simulation method.

1. Introduction
In the temperature laboratories, there are several procedures based on European standards (eg. EN 60584) used for parameters of the calibration equations calculations. In these standards the basic polynomials for the calculations are defined. The main reason of this investigation is showing of the influence of correlation in calibration data. This correlation is based on usage of same equipment (e.g. multimeter, cable, ice point) or traceability source.

All applied methods will be explained on the data obtained from the thermocouple calibration. The thermocouple is a device consisting of two different conductors (usually metal alloys) that produce a voltage proportional to a temperature difference between either ends of the pair of conductors [1, 2]. All the calculations were made in the SW package MATLAB® version 2011a.

2. Used Methods
Calibration of the sensor is performed only in a few defined points of the sensors working range, but they are used for measuring of the temperature in a whole range. The standardised function to describe the relation between thermoelectric voltage $E$ and temperature $t$ is described by equation

$$E_{\text{ref}} = \sum_{i=0}^{n} c_i (t_{90})^i,$$

where $E_{\text{ref}}$ is reference function, $n$ and $c_i$ are tabled coefficient according to [1] and $t_{90}$ is temperature according to international temperature scale ITS-90. Each thermocouple is different and his behaviour is described by deviation function in the form

$$E - E_{\text{ref}} = \sum_{i=1}^{m} a_i t_{90}^i,$$

where $E$ is measured thermoelectric voltage, $a_i$ is adjustable coefficient and $m$ is order of the model.

Most commonly used are polynomials of the first, second or third order.

This is the reason for application of the methods, which take into account all measured points, and mistake caused by wrong choice of the points for fitting is minimized. Among the simplest methods...
include Method of Least Squares of its modification Weighted Least Square Method. More information about these methods can be found for example in [3, 4 and 5].

2.1. Weighted Least Square Method
Weighted Least Square Method (WLS) is used for finding of the accurate orders of deviation function for various type of thermometer. This method represents a modification of the Method of Least Squares, so this method will be described firstly.

The Method of Least Squares (MLS) is a procedure to determine the best fit line to data, the proof uses simple calculus and linear algebra. For calculations are used data sets, which obtain independent variable \( x \) (in our case reference temperature \( t_{90} \)) and dependent variable \( y \) (values of the deviation function).

Fitting curve \( f(x, \Theta) \) has the deviation \( e \) from each data point

\[
e_i = y_i - f(x_i, \Theta).
\]

Here, symbol \( \Theta \) means the set of adjustable parameters. The symbol in bold character means vector.

According to the method of least squares, the best fitting curve minimize this deviation, known also as 

\[
\text{SSE} = \sum_{i=1}^{n} (y_i - f(x_i, \Theta))^2.
\]

WLS represents a modification of above described MLS. Into the calculation enters another term – vector or matrix of weights \( W \). These values set to each pair of the data some weight. Weighted Least Square Method affects the points, which are used for the calculation of new regression function. The higher the value of weight, the greater the influence of this point in the regression is. The equation (4) than can be written as follows

\[
\Theta = \arg \min e^T W e = \arg \min \sum_{i=1}^{n} (y_i - f(x_i, \Theta))^2.
\]

A lot of possibilities exist for weights determination. Most common way is a calculation of the standard deviation \( \sigma \). In presented case are weights determined otherwise – as weights are considered uncertainties \( u \) of calibration.

In the normalised form it can be written as

\[
W_i = \frac{1}{\max_i w_i^2}.
\]

2.2. Statistical Evaluation
For the statistical evaluation of the results, three criterions are used [5]. First one, SSE, was already explained in the previous text. Second used criterion is R-square value. This statistic measures how successful the fit is in explaining the variation of the data. R-square is defined as the ratio of the sum of squares of the regression (SSR) and the total sum of squares (SST). SSR is defined as

\[
SSR = \sum_{i=1}^{n} w_i (\hat{y}_i - \bar{y})^2.
\]

SST is also called the Sum of squares about the mean, and is defined as

\[
SST = \sum_{i=1}^{n} w_i (y_i - \bar{y})^2.
\]

Given these definitions, R-square is expressed as

\[
R - square = \frac{SSR}{SST}.
\]

R-square can take on any value between 0 and 1, with a value closer to 1 indicating that a greater proportion of variance is accounted for by the model.

Last criterion used for statistical evaluation is RMSE (Root Mean Square Error) defined as follows (calculation is based on MLS)

\[
RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y - f(x_i))^2}.
\]

2.3. Monte Carlo Method
Monte Carlo simulation was devised as an experimental probabilistic method to solve difficult deterministic problems since computers can easily simulate a large number of experimental trials that have random outcomes. When applied to uncertainty estimation, random numbers are used to randomly sample parameters' uncertainty space instead of point calculation carried out by conventional methods.
So the application of Monte Carlo simulation in the uncertainty estimation of different states of a system seems to offer a more realistic approach. The method can handle both small and large uncertainties in the input quantities. Complex partial differentiations to determine the sensitivity coefficients are not necessary. It also takes care of input covariance or dependencies automatically [6, 7]. The last point is the main reason for using of this method here.

3. Results

The data used for this evaluation were acquired from real calibration of type S thermocouple. Calibration was performed in fixed points of In, Zn, Al, Ag, Au and Cu. The data are shown in figure 1.

Each calibration point is evaluated according to the standard uncertainty calculation for expansion coefficient \( k=2 \) with normal probability distribution. The approach of WLS and MLS will give the first look on the deviation function. By using of statistical evaluation methods in chapter 2.2 was the structure of the model (value of \( m \) and probability of existing of the parameters \( \Theta \)). The model is

\[
E - E_{\text{ref}} = a_1 t_90^2 + a_2,
\]

(11)

Figure 2 shows the 95% probability bounds for interpolation calculation by means of MLS method. The main problem is the influence of cross-correlation between the calibration points. The uncertainty budget shows, that the correlation value depends on used equipment and is in the range from 0.2 to 0.7. That is why the Monte Carlo method was used for simulating of this influence. The covariance matrix of

\[
C = \begin{pmatrix}
1 & \cdots & r \\
\vdots & \ddots & \vdots \\
r & \cdots & 1
\end{pmatrix}.
\]

(12)

The value of \( r \) was using 0, 0.25, 0.5, 0.75 and 1. For no correlation the results are the same as in figure 2. This is the proof that both methods are equivalent.

In left part of figure 3 is shown the comparison of MLS (green) and Monte Carlo method (yellow). The right part shows the decreasing of the uncertainty by means of both MLS and WLS methods. The results with different values of \( r \) are shown in following figure.
It is clearly visible, that correlation increase the uncertainty value. An interesting results is, that the overall uncertainty in the interpolated range is lower than uncertainty at each point (depends on the correlation coefficient). This is often valid in fixed point calibration, where the consisteny of the data and more calibration points create best possible condition for interpolation evaluation.

4. Conclusion
This paper was devoted to find the influence of correlation to the interpolation uncertainty. The comparison of interpolation uncertainty of MLS and WLS on real data were performed. The Monte Carlo methods was used to evaluate different correlation values between calibrated data. The calculated uncertainty is increased with increasing correlation. This will cause the underestimating of the fit uncertainty by standard method.

5. References
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