DIFFERENT APPROACHES COMPARISON OF THE TEMPERATURE DATA EVALUATION

L. Kňazovická, [1,2], R. Strnad[1]

[1]Czech Metrology Institute, Okružní 31, 638 00 Brno, Czech Republic

[2]Department of Computing and Control Engineering, Institute of Chemical Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic

Abstract

This paper is devoted to an evaluation of the data obtained by the calibration of the platinum resistance thermometers and thermocouples.

Measured data are used for calibration model parameters calculation based on standards EN 60751, ITS-90 and EN 60584.

According to the mentioned standards, only a few points are necessary for the calculation of the parameters. Whole set of measured calibration data usually consists of more measured points, and remaining points should be used for verification of the calculated model. A mistake can be done easily, when wrong points for calculation are chosen. To prevent this fact, all measured point should be included into the calculation.

A method based on least square fitting allows using whole set of the measured data for calibration model coefficient calculation. This approach allows minimizes the error and provide more objective results.

Usually used methods will be described and comparison with the evaluation based on least square fitting will be presented.

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 missed or outlined calibration data.

All applied methods will be explained on the data coming 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, and case of thermocouple data evaluation will be presented in this paper.

2 Mathematical Background

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. Values of deviation function are not linear with the temperature, but it is always a function with some, not exactly defined behavior. For practical purpose, the standard polynomial function is used. Most common used polynomials are polynomials of the 2nd order.

For estimation of the calibration curve are usually used only 3 measured points, instead of the whole available data set. This fact may lead to the non-correct fit of the data, because of wrong choice of the 3 required data.

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. Application of well-known Method of Least Squares and its weighted form provides strong tool for this kind of fitting.

2.1 Method of least Square and Weighted Least Square Method

Weighted Least Square Method (WLS) is used for finding of the best fit of the deviation function. This method is simple and is described in a lot of sources [3, 4]. Even if application of this method is not very complicated, it provides a strong tool for function approximation. 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. Data sets, obtain independent variable x (in our case reference temperature t_{90}) and dependent variable y (values of the deviation function), are used for calculations. Fitting curve f(x, **Θ**) has the deviation *e* from each data point

$$e_i = y_i - f(x_i, \boldsymbol{\Theta}). \tag{1}$$

Here, symbol **Θ** 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 SSE – Sum of Squares Error.

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

To obtain the least square error, unknown coefficients must yield zero first derivatives.

$$\frac{\partial e}{\partial \Theta} = 0 \tag{3}$$

These equations can be solved as a set of linear equation for unknown parameters. Important fact for this method is that for the final fit calculations all used point have the same weight.

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 (2) than can be written as follows

$$\widehat{\boldsymbol{\Theta}} = \arg\min e^T W e. \tag{4}$$

A lot of possibilities exist for weights determination. Most common way is a calculation of the standard deviation (**σ**), and uses one of these forms:

$$W_i = \frac{1}{\sigma_i} \quad \text{or} \quad W_i = \frac{1}{\sigma_i^2} \tag{5}$$

In presented case are weights determined otherwise – as weights are considered uncertainties of calibration

$$W_i = \frac{1}{u_i}. \tag{6}$$

2.2 Robust Approach

The main disadvantage of least-squares fitting is its sensitivity to outliers (extreme values which are a valid part of a data set).

It is usually assumed that the response errors follow a normal distribution, and that extreme values are rare. Still, extreme values called outliers do occur.

Outliers have a large influence on the fit, squaring the residuals magnifies the effects of these extreme data points. To minimize the influence of outliers, data can be fitted by using robust least-squares regression Least Absolute Residuals (LAR). The LAR method finds a curve that minimizes the absolute difference of the residuals, rather than the squared differences. Therefore, extreme values have a minor influence on the fit. The common criteria are as follows

$$\widehat{\boldsymbol{\Theta}} = \arg\min \sum_{i=1}^{n} (|y_i - f(x_i, \boldsymbol{\Theta})|)^p, \tag{7}$$

where $p \geq 1$. In this paper we will use p=1.

2.3 Statistical Evaluation

For the results statistical evaluation, three criterions are used. First one, SSE, was already explained in the previous section.

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

$$SSR = \sum_{i=1}^{n} w_i(\hat{y}_i - \bar{y})^2. \quad (8)$$

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

$$SST = \sum_{i=1}^{n} w_i(y_i - \bar{y})^2 \quad (9)$$

Given these definitions, R-square is expressed as

$$R - square = \frac{SSR}{SST}. \quad (10)$$

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)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y - f(x_i)\right)^2} \quad (11).$$

3 Results

In this part, comparison of the four mentioned methods will be presented. Calculations were made on the data, obtained during calibration of the thermocouple, type S. Calibration was performed in fixed point of In, Zn, Al, Ag, Au and Cu. For the final fit, polynomial of the 2nd order is used. Used data set contains one outlined value – measured value in fixed point of Zn (231,9 °C). Influence of this outline point to the result of fitting will be described for each mentioned approach. Data are presented in Table 1, values listed in uncertainty column are used for weight calculation according to Eq. 6.

Table 1: MEASURED DATA USED FOR FITTING

Temperature t_{90} °C	Deviation from reference, according ČSN EN 60584-1 ($E - E_{ref}$) mV	Uncertainty U_c mV
156,5985	-2,7	1,4
231,928	10,0	1,0
419,527	3,9	1,8
660,323	17,0	1,6
961,78	38,8	2,3
1064,18	51,7	8,0
1084,62	51,7	2,4

First, Method of Least Squares was applied to the data (Figure 1). This method calculates the fitting curve from all data and each point has the same weight for the final calculation in a way to have as small as possible SSE value (Table 2). Because MLS represents non-robust fitting approach, this method is not suitable for outliers detection.

Second method applied to the data is WLS (Figure 2). Difference between MLS and WLS in fitting calculation is that WLS take into account also weights. This allows affecting the calculation in a way that measured points with higher uncertainty have a lower influence to the final calculation than points with lower uncertainty. But calculation of the uncertainty depends on many things, and it does not provide the reliable way for detection of the outliers.

Robust approach allows us to detect the outliers. Even if these points are still valid part of the data set, outliers are not taking into calculation of the final data fit. Results from this approach are presented in Figure 3 and Figure 4. Figure 3 shows results, when robust approach is applied together with MLS. From the results can be seen, that final curve fits the data very well, and outliers has a minimal influence in a fit calculation.

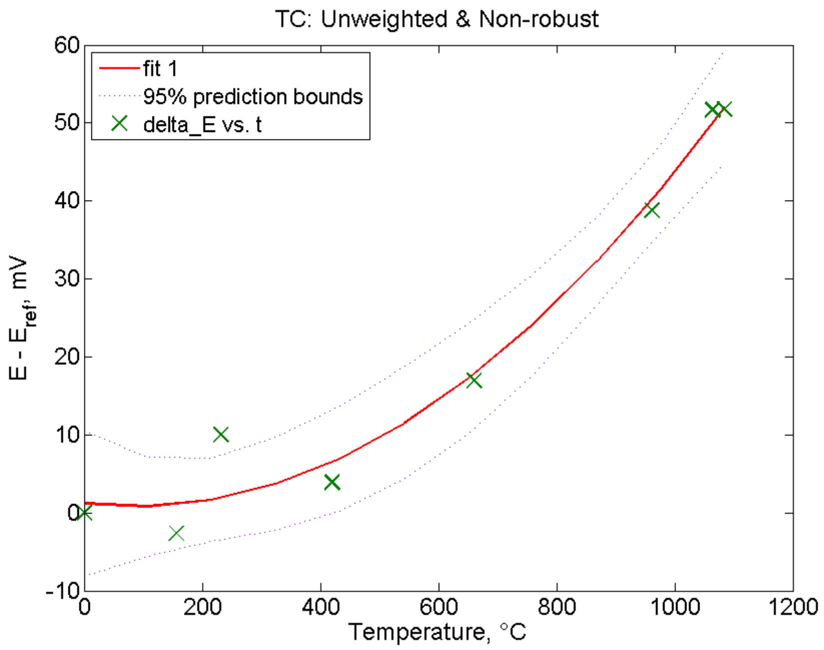

Figure 1: MLS fitting of the data

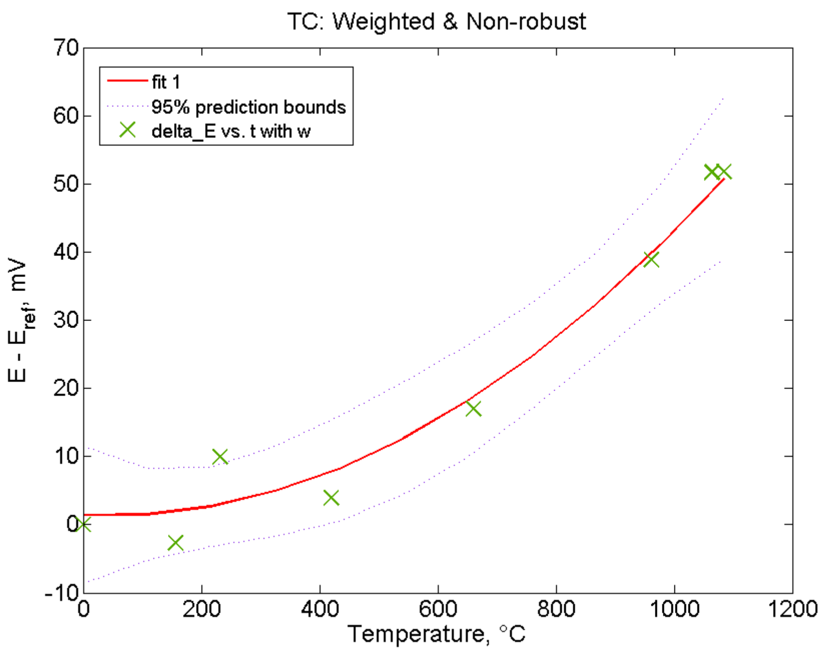

Figure 2: WLS fitting of the data

For a comparison, robust approach in combination with WLS is presented in Figure 4. This approach provides very similar results as the previous one.

Results are also compared with objective statistical criterions (Table 2). The value of SSE is higher in the non-robust WLS. The reason of this fact is, that value with a higher uncertainty have a smaller weight and this point doesn`t affect the fit as much as the other values with the higher weight.

Robust methods can identify the outliers, and the knowledge of the weights isn`t necessary. Because the outliers have very low influence on this calculation, the value of the SSE is higher than SSE of non-robust methods.

In all figures are also shown confidence intervals. They describe the interval in which a measurement falls corresponding to a given probability. This interval of interest is symmetrically placed around the mean, and for all cases is this value equal to 95 %.

From the presented results is clear, that robust methods are very good for laboratory measurements and data evaluation, because they are able to identify the outliers. Also the confidence interval is smaller. Statistical criterions for this kind of data provide very high values in case of SSE and RMSE and very low values on case of R-square. This is caused by their definition, because they are calculated from all points, without any weights or detection of the outliers. For this kind of the data, and also for other type of sensors is recommended to use *weighted robust approach*.

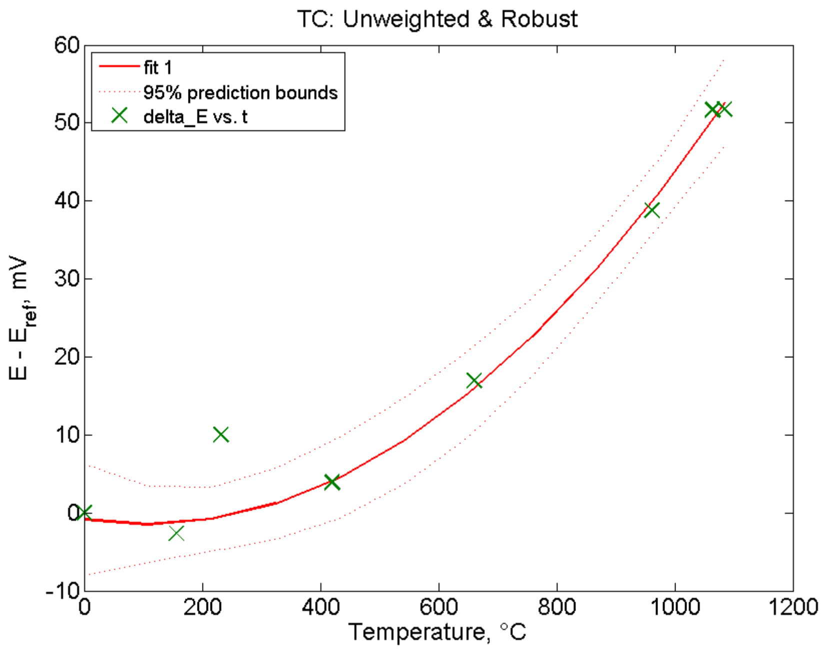

Figure 3: Robust unweighted fit of the data

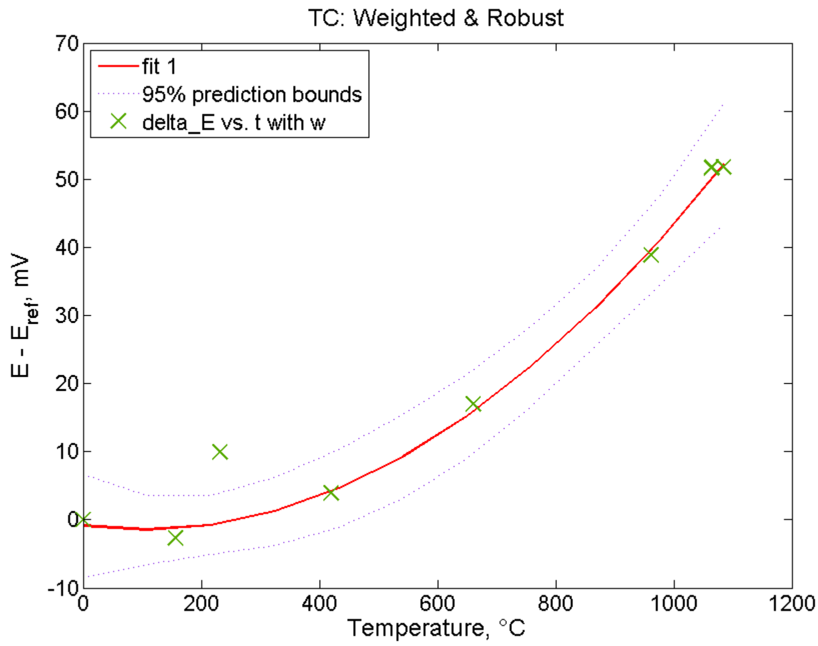

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Figure 4: Robust weighted fit of the data

Table 2: STATISTICAL EVALUATION OF THE DATA

	Unweight & Non-robust	**Unweight & Robust**	**Weighted & Non-robust**	**Weighted & Robust**
SSE	152,3	173,4	1987	2398
R-square	0,956	0,949	0,925	0,909
RMSE	5,5	5,9	19,9	21,9

4 Conclusion

This paper was devoted to four different approaches in the evaluation of the temperature calibration data. The paper was focused on the data contains outliers, which are common in real measured data.

Method of Least Squares was applied first for the fitting of the data, because only simply calculations are needed. This method uses all points for the fitting without any difference, and because of that this method doesn't provide appropriate results for the fitting data with outliers.

Weighted methods provide better results, than MLS, because to each point is assign certain weight, which affects calculation. Points with lower weight doesn`t have such a big influence on the fitting as a points with higher weight. That's the reason, why this kind of methods is suitable for the data fitting.

Robust approach allows finding outlying values even if they are not known. These values have only low influence in the calculations results. According to the results from the statistical analysis, these methods doesn`t provide optimal values of the statistical criterions. This can be shown from the Table 2. When robust approach is used, fitted line crossed only the "correct" values, and that is very important for final evaluation of the calibration and determination of the calibration equation.

That is the main reason, why usage of robust and weighted approach is recommended for the fitting of the data obtained during the temperature sensors calibration.

References

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Lenka Kňazovická
Thermal Properties Department, Czech Metrology Institute, lknazovicka@cmi.cz

Radek Strnad
Thermal Properties Department, Czech Metrology Institute, rstrnad@cmi.cz