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Evaluating Uncertainties in Interpolations Between Calibration Data for Thermocouples

J. V. Pearce · P. M. Harris · J. C. Greenwood

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Abstract Two methods for evaluating thermocouple calibration uncertainty over the temperature range of the calibration are presented, when the thermocouple is calibrated at only a few temperatures. The evaluation of the uncertainty at fixed-point temperatures is well established, but it is often not clear how the uncertainty arising from interpolation between fixed points can be determined. We present a conventional method, based on that described in the "Guide to the expression of uncertainty in measurement" (GUM), and a numerically-based Monte Carlo method, for quantifying the calibration uncertainty arising from the use of an interpolating polynomial defined by calibration data. The two methods are compared and found to be in excellent agreement, but the Monte Carlo method is, in general, more flexible, e.g., when measurements are described by non-normal distributions.

Keywords Calibration · Fixed point · Interpolation · Thermocouple · Uncertainty

1 Background

During a calibration, the measuring junction of a thermocouple is immersed in a controlled environment at an accurately known temperature, e.g., [1] normally a fixed point as defined by ITS-90 [2]. The calibration data are presented in terms of the difference between the thermocouple *electromotive force* (emf) measured at the fixed point and the corresponding value provided by the IEC reference function [3] at that temperature. This difference is referred to as the *deviation* from the reference function.

To fully characterize the thermocouple output, the emf at other temperatures is determined by interpolation between the calibration data. A common and economical means of interpolating is to use a so-called interpolating polynomial that is fully

J. V. Pearce (✉) · P. M. Harris · J. C. Greenwood
National Physical Laboratory, Hampton Road, TW11 0LW Teddington, UK
e-mail: jonathan.pearce@npl.co.uk

defined by the calibration data. Values of the coefficients of the polynomial are found by solving the simultaneous equations arising from the requirement that the calibration data must lie on the curve. However, since the measured deviation at each of the fixed points is subject to measurement uncertainty, then so is the resulting interpolating polynomial.

In this article, two methods are described for evaluating the uncertainty associated with estimates of the emf obtained from an interpolating polynomial: a conventional method based on the law of propagation of uncertainty [4], and a Monte Carlo method [5] that generates many interpolating polynomials arising from a large number of simulated deviation values at each fixed-point temperature and employs a statistical analysis of the results. Both the methods are applied to a particular scheme employed at NPL to calibrate Pt/Pt-Rh (specifically, Type R) thermocouples from 0 °C to 1100 °C.

We begin by defining the measurement model and developing the GUM solution before introducing two distinct error models (describing, respectively, no correlation and partial correlation associated with the measured deviation values). Next, we outline the Monte Carlo method and present results for both error models using the two approaches before presenting some concluding remarks.

2 Thermocouple Measurement Model

By convention, the interpolating polynomial associated with a thermocouple calibration is defined in terms of a power series of degree n in the calibration temperature, x, where n corresponds to the number of fixed points:

$$p(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_2 x^2 + a_1 x. \tag{1}$$

The polynomial is constrained to pass through the origin (since the ideal thermocouple output at the ice point (0 °C) is 0 μV) and through each of the calibration points. Therefore, for a given set of calibration data $\{(x_i,\ y_i) : i = 1, 2, \ldots, n\}$,

$$p(x_i) = y_i, \tag{2}$$

where y_i is the emf deviation measured at temperature x_i. Together, Eqs. 1 and 2 define a system of equations that is linear in the coefficients a_k $(k = 1, 2, \ldots, n)$:

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1^n & x_1^{n-1} & x_1^{n-2} & \ldots & x_1^2 & x_1 \\ x_2^n & x_2^{n-1} & x_2^{n-2} & \ldots & x_2^2 & x_2 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ x_n^n & x_n^{n-1} & x_n^{n-2} & \ldots & x_n^2 & x_n \end{bmatrix} \begin{bmatrix} a_n \\ a_{n-1} \\ \vdots \\ a_1 \end{bmatrix} \tag{3}$$

which can be solved for a_k to construct the interpolating function $p(x)$. Because the function is constrained to go through the calibration data, it can exhibit large excursions or oscillations between the fixed points, which are not likely to represent the real thermocouple output in those temperature ranges. It is these excursions that contribute most to the uncertainty in the interpolated value between calibration points.

Define the vector quantities $\boldsymbol{Y} = (Y_1, \ldots, Y_n)^{\mathrm{T}}$ and $\boldsymbol{A} = (A_1, \ldots, A_n)^{\mathrm{T}}$ with the measured data $\boldsymbol{y} = (y_1, \ldots, y_n)^{\mathrm{T}}$ regarded as a realization of $\boldsymbol{Y}$ and the corresponding estimates $\boldsymbol{a} = (a_1, \ldots, a_n)^{\mathrm{T}}$ of the polynomial coefficients a realization of $\boldsymbol{A}$. Furthermore, suppose the values $\boldsymbol{x} = (x_1, \ldots, x_n)^{\mathrm{T}}$ of the fixed-point temperatures are known with no associated uncertainty. The linear system of Eq. 3 defines the measurement model,

$$\boldsymbol{CA} = \boldsymbol{Y} \tag{4}$$

relating $\boldsymbol{Y}$, input quantities in the model, to $\boldsymbol{A}$, output quantities in the model, with

$$\boldsymbol{C} = \begin{bmatrix} x_1^n & x_1^{n-1} & x_1^{n-2} & \ldots & x_1^2 & x_1 \\ x_2^n & x_2^{n-1} & x_2^{n-2} & \ldots & x_2^2 & x_2 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ x_n^n & x_n^{n-1} & x_n^{n-2} & \ldots & x_n^2 & x_n \end{bmatrix}.$$

Formally, $\boldsymbol{Y}$ and $\boldsymbol{A}$ are related by the (multivariate) measurement function,

$$\boldsymbol{A} = \boldsymbol{C}^{-1}\boldsymbol{Y}. \tag{5}$$

For reasons of numerical stability, explicit calculation of the matrix inverse $\boldsymbol{C}^{-1}$ is not recommended and such systems of equations are usually solved by factorization techniques.

2.1 Standard GUM Uncertainty Framework

Applying a generalization [6] of the law of propagation of uncertainty [4] to the measurement model (Eq. 4) gives

$$\boldsymbol{C}\boldsymbol{U}_{\boldsymbol{a}}\boldsymbol{C}^{T} = \boldsymbol{U}_{\boldsymbol{y}}, \tag{6}$$

where $\boldsymbol{U}_{\boldsymbol{y}}$ and $\boldsymbol{U}_{\boldsymbol{a}}$ are, respectively, the covariance matrices of dimension $n \times n$ associated with $\boldsymbol{y}$ and $\boldsymbol{a}$. $\boldsymbol{U}_y$ contains the variances $u^2(y_i)$ (squared standard uncertainties) associated with the elements y_i of $\boldsymbol{y}$ on its diagonal and the covariances $\mathrm{cov}(y_i, y_j)$ associated with pairs of elements elsewhere, and similarly for $\boldsymbol{U}_a$. Equation 6 defines a linear system of equations that can be solved for $\boldsymbol{U}_a$ in terms of $\boldsymbol{U}_y$ and $\boldsymbol{C}$.

Let Y denote the emf provided by the interpolating polynomial defined by coefficients $\boldsymbol{A}$ corresponding to a general value x of temperature, with $y = p(x)$ and $\boldsymbol{a}$ regarded as realizations of Y and $\boldsymbol{A}$ and x known with no associated uncertainty. Equation 1 defines the measurement function,

$$Y = \boldsymbol{c}\boldsymbol{A}, \tag{7}$$

relating $\boldsymbol{A}$, input quantities in the measurement function, to Y, the output quantity, with

$$\boldsymbol{c} = \begin{bmatrix} x^n & x^{n-1} & x^{n-2} & \cdots & x^2 & x \end{bmatrix}. \tag{8}$$

Application of the law of propagation of uncertainty to the measurement function (Eq. 7) gives

$$u^2(y) = \boldsymbol{c}\boldsymbol{U}_{\boldsymbol{a}}\boldsymbol{c}^{\mathrm{T}} \tag{9}$$

for the standard uncertainty $u(y)$ associated with the estimate y of Y.

Finally, if it is assumed that Y can be characterized by the normal distribution $\mathrm{N}(y,\ u^2(y))$, a coverage interval for Y corresponding to 95 % coverage probability is given by $y \pm 1.96u(y)$. The central limit theorem is often used to justify characterizing the output quantity by such a normal distribution, and assumes that there are a "sufficient" number of input quantities and that there is not a "dominant" input quantity described by a non-normal distribution.

2.2 Case 1: Errors Are Not Correlated

In the case that the measurement errors associated with each y_i are uncorrelated, Y and y are related through the following simple error model describing the measurement of the emf corresponding to the ith fixed-point temperature:

$$Y_i = y_i + E_i, \quad i = 1, 2 \ldots n \tag{10}$$

where E_i describes a random error quantity with expectation zero and variance σ_i^2.

In this case, the covariance matrix $\boldsymbol{U}_y$ associated with $\boldsymbol{y}$ is the diagonal matrix,

$$\boldsymbol{U}_{\boldsymbol{y}} = \mathrm{diag}\left(\sigma_1^2, \sigma_2^2, \ldots, \sigma_n^2\right). \tag{11}$$

Equations 6 and 9 are then used to evaluate the standard uncertainty associated with the interpolated value y provided by the interpolating polynomial corresponding to the value x of temperature.

2.3 Case 2: Errors Are Correlated

In the case, the measurement errors associated with each y_i are correlated, Y and y are related through the error model,

$$Y_i = y_i(1 + E_0) + E_i, \quad i = 1, 2 \ldots n \tag{12}$$

where E_0 describes a systematic error quantity with expectation zero and variance σ_0^2 (expressed as a fraction) and E_i describes a random error quantity with expectation

zero and variance σ_i^2 (expressed in units corresponding to emf squared). The quantities E_0 and E_i are furthermore assumed to be mutually independent.

It follows that the variance of Y_i is

$$\mathrm{Var}(Y_i) = y_i^2\sigma_0^2 + \sigma_i^2, \tag{13}$$

and the covariance of Y_i and Y_j $(i \neq j)$ is

$$\mathrm{Cov}(Y_i, Y_j) = y_i y_j \sigma_0^2, \tag{14}$$

and so

$$\begin{aligned} \boldsymbol{U}_y &= \begin{bmatrix} y_1^2\sigma_0^2 + \sigma_1^2 & y_1y_2\sigma_0^2 & y_1y_3\sigma_0^2 & \cdots & y_1y_{n-1}\sigma_0^2 & y_1y_n\sigma_0^2 \\ y_2y_1\sigma_0^2 & y_2^2\sigma_0^2 + \sigma_2^2 & y_2y_3\sigma_0^2 & \cdots & y_2y_{n-1}\sigma_0^2 & y_2y_n\sigma_0^2 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ y_ny_1\sigma_0^2 & y_ny_2\sigma_0^2 & y_ny_3\sigma_0^2 & \cdots & y_ny_{n-1}\sigma_0^2 & y_n^2\sigma_0^2 + \sigma_n^2 \end{bmatrix} \\ &= \sigma_0^2 \boldsymbol{y}\boldsymbol{y}^{\mathrm{T}} + \mathrm{diag}\left(\sigma_1^2, \sigma_2^2, \cdots, \sigma_n^2\right). \end{aligned} \tag{15}$$

Equations 6 and 9 are then used, as in case 1, to evaluate the standard uncertainty associated with the interpolated value y provided by the interpolating polynomial corresponding to the value x of temperature.

3 Monte Carlo Method for Evaluating Uncertainty

The Monte Carlo method is particularly suited to applications where the underlying assumptions of the central limit theorem do not apply or the model is non-linear or numerical. Use of this method is entirely consistent with the GUM; however, to provide detailed guidance on the method, the first supplement [5] has recently been published.

In our implementation, for each Monte Carlo trial, the error models, represented by Eqs. 10 and 12, were used to simulate sets of measurement errors by making random draws from the distributions used to characterize the error quantities. At each fixed-point temperature the simulated errors were combined with the corresponding IEC value, i.e., the thermocouple emf for zero deviation, and the coefficients of the interpolating polynomial were then determined. For each trial, we evaluated the polynomial over a wide range of temperatures (see, e.g., Fig. 1) and at each temperature determined the (symmetrical) limits bounding 95 % of the evaluated values (see, e.g., Fig. 2).

3.1 Evaluation Example

In this example, we consider calibration at the fixed points Zn (419.527 °C), Ag (961.78 °C), and Cu (1084.62 °C).

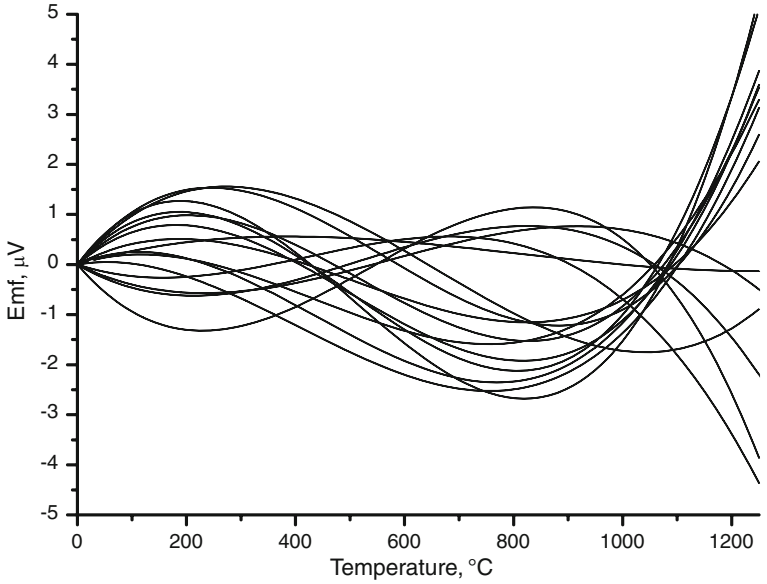

Fig. 1 Polynomials obtained from 15 Monte Carlo trials

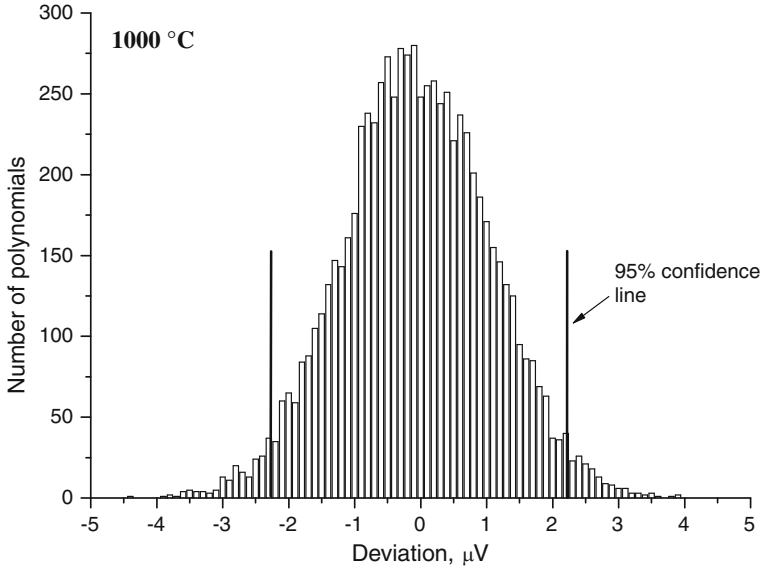

Fig. 2 Histogram (scaled frequency distribution) of polynomial values at a given temperature for 20,000 Monte Carlo trials, showing the 95 % limits

3.1.1 Case 1: Uncorrelated Errors

In this case, the errors in the measured values at each fixed point are *uncorrelated*, and the error quantities associated with each measurement are normally distributed with standard deviations given in Table 1.

These parameters are those formerly used by NPL to evaluate thermocouple calibration uncertainties for a Type R thermocouple at Zn, Ag, and Cu fixed points.

3.1.2 Case 2: Correlated Errors

The current scheme employed at NPL recognizes that in practice there is one significant measurement error that, for any given thermocouple, produces a strong correlation between fixed points, namely, the thermoelectric homogeneity. This error arises from changes in chemical composition or physical condition along the length of the thermocouple wires in regions where there are temperature gradients. Ignoring this correlation tends to substantially overestimate the uncertainty due to interpolation.

The correlation arises because the homogeneity at one temperature is representative of the homogeneity at another temperature [7]. Previous work has established that the uncertainty due to inhomogeneity at a particular temperature is a multiple of the emf at that temperature, e.g., for new Type R thermocouples the emf can be multiplied by 0.02 % to obtain the contribution in the "worst case" [8]. (For comparison, for Pt/Pd thermocouples this value is close to 0.005 % [9].) The parameters for the uncertainty evaluation discussed in this article are summarized in Table 2. Two different probability distributions, normal (N) and uniform (R), both having the same standard deviation,

Table 1 Parameters for the evaluation of uncertainty with uncorrelated errors at Zn, Ag, and Cu fixed points

Fixed point:	Zn	Ag	Cu
Temperature (°C)	$x_1 = 419.527$	$x_2 = 961.78$	$x_3 = 1084.62$
emf (μV)	$y_1 = 3611.30$	$y_2 = 10003.43$	$y_3 = 11640.43$
Standard uncertainty (μV)	$u(y_1) = 0.67$	$u(y_2) = 1.28$	$u(y_3) = 1.45$

Table 2 Parameters for the evaluation of uncertainty, with correlated errors, for thermocouple calibration at Zn, Ag, and Cu fixed points

Fixed point:	Zn	Ag	Cu
Temperature (°C)	$x_1 = 419.527$	$x_2 = 961.78$	$x_3 = 1084.62$
emf (μV)	$y_1 = 3611.30$	$y_2 = 10003.43$	$y_3 = 11640.43$
Uncorrelated component, E_i (μV)	$E_1 \in \mathrm{N}(0, \sigma_1^2)$	$E_2 \in \mathrm{N}(0, \sigma_2^2)$	$E_3 \in \mathrm{N}(0, \sigma_3^2)$
	$\sigma_1 = 0.53$	$\sigma_2 = 0.54$	$\sigma_3 = 0.54$
Correlated component, E_0/1	(2a)$E_0 \in N(0, r^2/3)$		
	(2b)$E_0 \in R(-r, r)$		
	$r = 0.0002$		

are considered for the (common) systematic error quantity, E_0, labelled "2a" and "2b" in the table. Note that for routine calibrations performed at NPL a uniform distribution (2b) is assumed.

4 Results and Discussion

The case of uncorrelated errors, described by the parameters given in Table 1, has been evaluated using the methods described above. The results are summarized in Fig. 3. As expected, these results demonstrate the equivalence of the two methods, because the measurement functions are linear and all quantities involved in the measurement are described by normal distributions.

For the case of correlated errors, the Monte Carlo approach was used to evaluate the expanded uncertainty for both choices of a normally distributed and uniformly distributed systematic error quantity as described by the parameters in Table 2. Since the conventional method makes no use of the distributions used to characterize the error quantities, only the standard deviations of those distributions, the method returns the same results for the two choices. The results are also summarized in Fig. 3. These results demonstrate, for this example, the equivalence of the conventional and Monte Carlo approaches for normally distributed error distributions. However, the Monte Carlo results are clearly different when a uniform distribution is chosen for the systematic error quantity.

The example demonstrates what happens when the central limit theorem no longer holds—in this case due to a small number of contributions with one of the contributions characterized by a significant uniform distribution. The histogram of interpolated

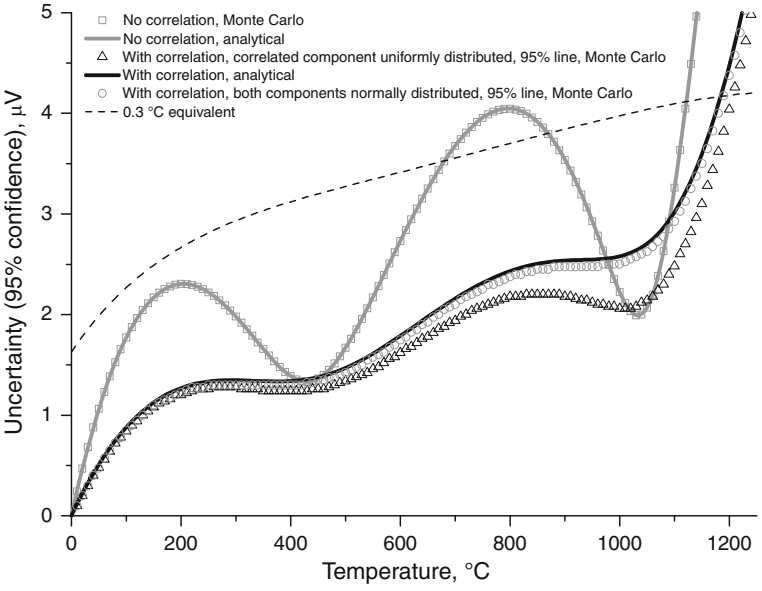

Fig. 3 Comparison of results for a Type R thermocouple (10^6 Monte Carlo trials, 95 % coverage probability)

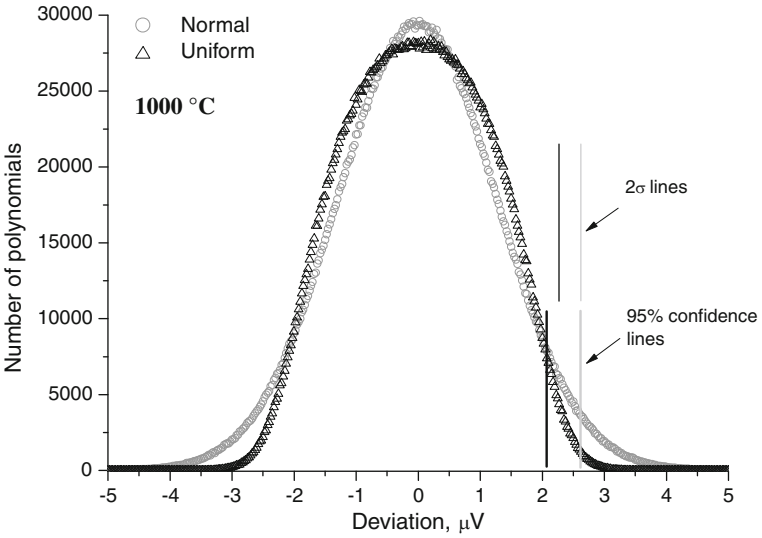

Fig. 4 Comparison of distributions of emfs (10^7 Monte Carlo trials) at a temperature of 1000 °C, in the case that measurements are correlated. *Gray circles* correlated component drawn from normal distribution, *black triangles* correlated component drawn from uniform distribution

values shown in Fig. 4 clearly demonstrates that the resulting output distribution is *not* Gaussian.

5 Conclusion

A conventional and a Monte Carlo methods have been presented to quantify the uncertainty arising from interpolation of calibrations between defined fixed points, given the uncertainty at the fixed points themselves. The methods are illustrated by considering the calibration of thermocouples. Here, the interpolation method considered is an interpolating polynomial, which is completely defined by the calibration data at the fixed points.

By assuming that the *underlying* measured values are zero at all fixed points, the methods provide an estimate of the effect arising from the uncertainty of measurement during the calibration, and the uncertainty in the resulting interpolation. The conventional and Monte Carlo methods were employed under two circumstances characterized by uncorrelated and partially correlated measurement errors. When the measured values are uncorrelated and normally distributed, the conventional and Monte Carlo results agree completely. However, when there is correlation associated with the measured values, the Monte Carlo results are not equivalent to the conventional results if the measured values are drawn from a non-normal distribution.

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