Sensors & Transducers, Vol. 245, Issue 6, October 2020, pp. 27-35

www.sensorsportal.com

Sensors & Transducers

Published by IFSA Publishing, S. L., 2020
http://www.sensorsportal.com

Intrinsically Non-Overfitting, Nonlinear Multivariate Calibration: Application to Thermocouples

[*] Luis RODRIGUES, Jorge FERREIRA, Daniel MARQUES, Fernando SILVA and Nelson MARTINS

University of Aveiro, TEMA - Centre for Mechanical Technology and Automation,
Campus Universitário de Santiago, 3810-193 Aveiro, Portugal
Tel.: +351 234 370 200
[*] E-mail: lrodrigues@ua.pt

Received: 30 July 2020 /Accepted: 25 September 2020 /Published: 30 October 2020

Abstract: The paper presents an original and empirically validated method for nonlinear multivariate data correction and sensor calibration, inspired by a Lagrangian approach. Being analytical and non-iterative, the method is extremely efficient, computationally. It is also very precise and accurate, since the precision truncation errors of iterative methods are avoided, and the resulting correcting function fits the calibration dataset with zero residual errors. Being inherently infinitely differentiable, the method avoids the discontinuities of piecewise approaches. The method accounts for typical nonlinearities in the response curves of most analog sensors and transducers, as well as nonlinear influences from the explanatory covariates. It is also virtually immune to over-fitting. A major application of this approach is temperature compensation of analog sensors, transducers, voltage references, and piezo oscillators. This is particularly relevant for metrological applications outside laboratory-controlled environments – e.g., strain gauge networks for outdoor structural health monitoring. A practical application for thermocouples is demonstrated, where the adverse influences of the *cold junction* potential and the temperature-induced drift of a voltage reference are, simultaneously, compensated. A simple and practical regression method for calculating the transfer function parameter matrix will be demonstrated and its implementation will be shown. A practical methodology for acquiring a representative calibration dataset is proposed.

Keywords: Multivariate, Nonlinear, Non-overfitting, Sensor calibration, Signal correction, Temperature compensation.

1. Introduction

Ideally, to attain the greatest measurement precision and accuracy, all the variables that account for the degradation of a signal should be measured and corrected for. Naturally, this is only possible for deterministic (i.e., non-random) influences. A prime example of a common adverse influence is temperature: virtually all analog sensors and transducers are susceptible to this variable, particularly relevant in applications outside the controlled environment of a laboratory.

Nowadays, the use of multivariate calibration methods is relatively common in analytical chemistry [1] (thanks, in great part, to recent advances in machine learning methods). But it is still seldom applied in engineering metrology. This is certainly due to practical complications, among which are the difficulty of identifying and analytically describing (or quantifying) the influence of relevant variables on the

signal, and the considerable labor of acquiring calibration data sets for all the relevant combinations of conditions.

Machine learning methods directly address these difficulties. However, these tend to overfit the data. That is, they are prone to excessive granularity, i.e., improperly resolving the noise, inevitably present in any signal. By contrast, the herein proposed method is virtually immune to this undesirable behavior. Fig. 1 attempts to illustrate the basic differences between the *classical* analytical methods and the newest machine learning approaches, and their preferential application field, as a function of the complexity of the system being modeled – i.e., the number of covariates and the intricacy of their convolutions.

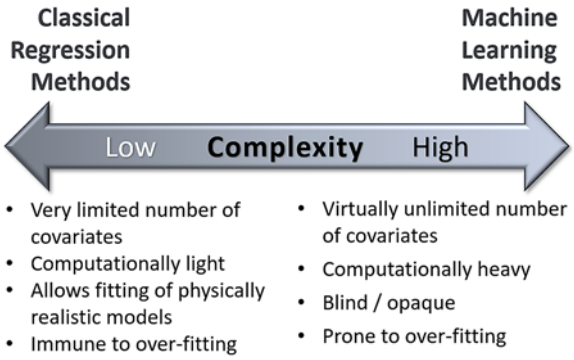

Fig. 1. Differences between the classical analytical approaches and the more recent machine learning methods.

For relatively *simple* systems, with two or three covariates, the classical regression methods are, generally, more adequate. The proposed method falls into this category. The sophistication and power of machine learning techniques and neural networks can be, in these cases, not only unwarranted but counterproductive [2].

Our method is non-iterative, thus being computationally very efficient, which can be critically relevant in applications where energy-efficiency is crucial (like, e.g., low-power autonomous remote data logging). Also, being purely analytical, numerical precision truncation errors are intrinsically minimized. It also accounts for non-linearities in a smooth continuous fashion, without resorting to piecewise approaches.

Thermocouples are a prime candidate for the application of this approach. It can be used to compensate for the influences of the *cold junction*, while simultaneously accounting for the nonlinear response of these sensing devices (without costly piecewise calibrations) and the temperature-induced drift of a voltage reference, as will be demonstrated.

1.1. Multivariate Dependence: The General Case

If the major sources of error that deterministically affect a given signal are known and can be precisely measured, it is possible to define a transfer function that returns a good estimation of the true value:

$$y \approx \hat{y} := f(\chi_1, \chi_2, \ldots, \chi_n) \equiv \hat{y}(\mathbf{x}), \tag{1}$$

where y is the value to be measured, $\hat{y}$ its dependent estimator and $\mathbf{x}$ is the vector (or set) of c_i independent explanatory or predictor measured signals (i.e., covariates) [1–3].

Crucially for the current application, the estimator $\hat{y}(\mathbf{x})$ must have injective properties, i.e., it should only return a unique value for every unique covariate vector $\mathbf{x}$ (i.e., parametric functions are inherently excluded):

$$\forall \mathbf{x}, \exists! \, \hat{y}(\mathbf{x}) \tag{2}$$

Topologically, the continuous scalar $\hat{y}(\mathbf{x})$ function can be regarded as a $(n+1)$-dimensional surface defined in an n-dimensional vector space. For the current purposes, $\hat{y}(\mathbf{x})$ will be defined as a polynomial surface, which can be written in the generalized form of a scalar product of two tensors:

$$\hat{y}(\mathbf{x}) = \mathbf{A} \cdot \mathbf{X}, \tag{3}$$

where $\mathbf{A}$ is the tensor that contains the scalar coefficients a_{ij} that uniquely defines the calibration surface (akin to a metric tensor), and $\mathbf{X}$ is the tensor that defines the polynomial nature of the multivariate covariate space.

Expression (3) will be defined, for the current purpose, as the summation:

$$\hat{y}(\mathbf{x}) = \sum_{j=0}^{N-1} \sum_{i=0}^{M-1} a_{ij} \chi_1^i \chi_2^j \tag{4}$$

Please note that – in the particular scope of the current paper – matrix indices start at zero and not at one, contrary to the usual convention. This is done purely for notational clarity and elegance (i.e., making the indices equal to the exponents).

1.2. Simplified Two-dimensional Special Case

Although the proposed approach could be, virtually, generalized to an arbitrary number of covariates or explanatory variables, it will henceforth be limited to only two, for the sake of presentation simplicity. However simplistic, this bivariate approach can be remarkably sufficient in a great number of practical cases. For instance, in the context of engineering metrology, the temperature is typically one of the main causes of measurement deviation, affecting the response of analog sensors and transducers, and influencing voltage references and oscillator/clock frequencies. Whenever impractical or unfeasible to conduct the measurements in a temperature-controlled environment, the quality of measurement can be severely impacted. In these

circumstances, accurately measuring the temperature and controlling for it, by applying an adequate bivariate correction, can make a decisive difference between invalid and valid results.

Additionally, it is assumed that both the sensor response curve and the influence of its single covariate have a simple curvature in the working domain – i.e., no inflections. Therefore, they can be adequately approximated by a 2nd-degree polynomial. In our experience, this simplification is realistically adequate for a great number of practical applications and, more specifically, for thermocouples (whenever this simplification is not acceptable – i.e., curvature with inflection – a piecewise solution could be adopted). This assumption will further limit the exponent degree of the approximating bivariate transfer function to 4.

The use of a polynomial transfer function has several desirable advantages: (*a*) it is inherently injective; (*b*) it is continuous and infinitely differentiable (i.e., C^{∞} smooth); (*c*) it is extremely efficient in terms of computation; (*d*) it is capable of adequately fitting arbitrarily non-linear responses and convolutions, given enough exponent degree; (*e*) polynomial regression algorithms are easy to implement and very efficient; (*f*) last but not least, overfitting is easily kept under control (by limiting the exponent degree to an adequate minimum).

Limiting the analysis to a two-dimensional covariate space allows the clarification of the meaning of **A** and **X** in (3), by explicitly expanding (4):

$$\mathbf{A}^{(2)} = \begin{bmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{bmatrix} \tag{5}$$

$$\mathbf{X}^{(2)} = \begin{bmatrix} 1 & \chi_2 & \chi_2^2 \\ \chi_1 & \chi_1\chi_2 & \chi_1\chi_2^2 \\ \chi_1^2 & \chi_1^2\chi_2 & \chi_1^2\chi_2^2 \end{bmatrix} \tag{6}$$

For notational simplicity reasons (which will become evident further on), the following variable nomenclature for the two degrees of freedom of our model will be, henceforth, adopted:

$$\chi_1 \equiv \sigma \quad \chi_2 \equiv \tau$$

Let *s* and *t* be, respectively, the *raw* error-containing signal and the explanatory covariate (e.g., temperature). With this naming convention, the previous expressions immediately become less cluttered (albeit less general):

$$\mathbf{X} = \begin{bmatrix} 1 & \tau & \tau^2 \\ \sigma & \sigma t & \sigma\tau^2 \\ \sigma^2 & \sigma^2\tau & \sigma^2\tau^2 \end{bmatrix} \tag{7}$$

$$\hat{y}(\sigma,\tau) = \sum_{j=0}^{2}\sum_{i=0}^{2} a_{ij}\sigma^i\,\tau^j \tag{8}$$

2. A Lagrangian Solution

A practical and efficient procedure for calculating the set of a_{ij} coefficients of matrix **A** will be described, inspired by a classical noniterative polynomial regression technique.

2.1. The Conventional Approach

The *least-squares method* is the most usual conventional approach for obtaining polynomial regressions. It finds the *best* statistical fit of a polynomial function to a particular dataset, by minimizing the sum *S* of the squares of the residual errors e_i, which are the difference between the actual value y_i and the value returned by the approximating function $\hat{y}(\mathbf{x}_i)$ [4–7]:

$$S = \sum_{i=1}^{N} \varepsilon_i^2 \equiv \sum_{i=1}^{N} [y_i - \hat{y}(\mathbf{x}_i)]^2 \tag{9}$$

This minimization is usually achieved by applying iterative algorithms like, e.g., the *Gauss-Newton* and *Gauss-Seidel*. These methods can effectively be used to obtain the aforementioned a_{ij} coefficients, directly from the multidimensional problem space.

Implementations of these iterative algorithms are readily and broadly available, since they are included in numerous software platforms (e.g., *Matlab®, Mathematica®, Mathcad®, Maple®,* etc.). In fact, these were used for the initial validation of the herein proposed multivariate calibration technique.

However, despite the formidable technological advances in computing power, these algorithms can be computationally taxing and somewhat cumbersome to implement in simple microcontroller-based solutions, which are still relevant for some applications where cost, power consumption, and autonomy are key aspects (e.g., compact battery-powered dataloggers).

There are no alternatives to iterative error minimization algorithms for finding the best-approximating function to *overdetermined* datasets (i.e., when there are more data points than the minimum needed to define the approximating curve/function). However, it is possible to obtain a less computationally demanding noniterative fitting solution if the number of input points is kept exactly sufficient for defining the approximating function (e.g., three points for a 2nd-degree polynomial).

2.2. Lagrange Interpolating Functions

Before delving into the deeper details of the proposed method, an introduction to the fundamental concepts of Lagrange's interpolation technique that will be applied is pertinent.

There exists a unique N^{th} degree polynomial that passes exactly through a given set of N+1 $[x_i\, y_i]$ nodes:

$$y(x) = \sum_{i=0}^{N} a_i x^i \tag{10}$$

Which is equivalent to say that there exists a unique set of $\{a_0, a_1 \ldots a_N\}$ coefficients that satisfies:

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^N \\ 1 & x_1 & x_1^2 & \cdots & x_1^N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N & x_N^2 & \cdots & x_N^N \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_N \end{bmatrix} \tag{11}$$

Solving this system of equations – by, e.g., Gauss elimination – will give us the unknown a_i coefficients. However, this is computationally costly. Instead, a series of Lagrange basis L_i functions is defined, such that:

$$y(x) = \sum_{i=0}^{N} y_i L_i(x), \tag{12}$$

where $L_i(x)$ are polynomials of degree N that weigh the known y_i values, in a way that satisfies the fundamental condition:

$$L_i(x_j) \equiv \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases} \tag{13}$$

The L_i functions are defined as:

$$L_i(x) := \prod_{\substack{j=0 \\ j \neq i}}^{N} \frac{x - x_j}{x_i - x_j} \tag{14}$$

The numerator $(x - x_j)$ guarantees that $L_i(x) = 0$ when x is equal to any of the x_j values, except when $x = x_i$, in which case the numerator becomes equal to the denominator, assuring the fundamental $L_i(x_i) = 1$ condition.

Putting it all together, the final expression of the Lagrange interpolating polynomial can be written:

$$(x) = \sum_{i=0}^{N} y_i \prod_{\substack{j=0 \\ j \neq i}}^{N} \frac{x - x_j}{x_i - x_j} \tag{15}$$

Extracting the set of $\{a_0, a_1 \ldots a_N\}$ polynomial coefficients from (15) – i.e., expressing (15) as a power series, in the guise of expression (10) – for the particular case of N=2, yields the following:

$$a_0 = w_0 x_1 x_2 + w_1 x_0 x_2 + w_2 x_0 x_1 \tag{16}$$

$$\begin{aligned} a_1 = -w_0(x_1 + x_2) - \\ w_1(x_0 + x_2) - \\ w_2(x_0 + x_1), \end{aligned} \tag{17}$$

$$a_2 = w_0 + w_1 + w_2, \tag{18}$$

where the weights w_0, w_1, and w_2 are given by:

$$w_0 = \frac{y_0}{(x_0 - x_1)(x_0 - x_2)}, \tag{19}$$

$$w_1 = \frac{y_1}{(x_1 - x_0)(x_1 - x_2)}, \tag{20}$$

$$w_2 = \frac{y_2}{(x_2 - x_0)(x_2 - x_1)} \tag{21}$$

Rewriting (16) to (21) in a more compact notation:

$$a_0 = \sum_{i=0}^{2} w_i \prod_{\substack{j=0 \\ j \neq i}}^{2} x_j, \tag{22}$$

$$a_1 = -\sum_{i=0}^{2} w_i \sum_{\substack{j=0 \\ j \neq i}}^{2} x_j, \tag{23}$$

$$a_2 = \sum_{i=0}^{2} w_i, \tag{24}$$

$$w_i = y_i \div \prod_{\substack{j=0 \\ j \neq i}}^{2} (x_i - x_j) \tag{25}$$

Alternatively, if the a_i coefficients are interpreted as components of a vector:

$$\mathbf{a} := [a_0 \quad a_1 \quad a_2]^{\mathrm{T}} \tag{26}$$

then, Eq. (22) to Eq. (25) can be written as:

$$\mathbf{a} = \sum_{i=0}^{2} y_i \begin{bmatrix} \prod_{\substack{j=0 \\ j \neq i}}^{2} x_j \\ -\sum_{\substack{j=0 \\ j \neq i}}^{2} x_j \\ 1 \end{bmatrix} \div \prod_{\substack{j=0 \\ j \neq i}}^{2} (x_i - x_j) \tag{27}$$

which, besides being notationally less redundant, allows us to succinctly write the polynomial interpolator as an inner product:

$$y(x) = \mathbf{a} \cdot \mathbf{x} \equiv \mathbf{a}\mathbf{x}^{\mathbf{T}} \equiv \langle \mathbf{a}, \mathbf{x} \rangle, \tag{28}$$

where

$$\mathbf{x} = [1 \quad x \quad x^2]^{\mathrm{T}} \tag{29}$$

Additionally, expressions (22) to (25) can also be combined in the following (arguably less elegant) scalar equation:

$$a_i = \sum_{j=0}^{2} y_j \frac{\delta_{i0} \prod_{\substack{k=0 \\ k\neq j}}^{2} x_k - \delta_{i1} \sum_{\substack{k=0 \\ k\neq j}}^{2} x_k + \delta_{i2}}{\prod_{\substack{k=0 \\ k\neq j}}^{2} (x_j - x_k)}, \quad (30)$$

where the symbol *d* is the *Kronecker delta* function:

$$\delta_{ij} := \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$$

2.3. Bivariate Lagrange Regression

The Lagrange interpolation is, intrinsically, a univariate method which does not lend itself to be generalized to higher dimensions. However, in the conditions of our particular case, it is possible to decompose a bivariate regression problem into two separate univariate ones, as will be demonstrated.

Let us expand and rearrange Eq. (8) in the following manner:

$$\begin{aligned} \hat{y}(\sigma,\tau) = & \ (a_{00} + a_{01}\tau + a_{02}\tau^2) + \\ & + \ (a_{10} + a_{11}\tau + a_{12}\tau^2)\ \sigma + \\ & + \ (a_{20} + a_{21}\tau + a_{22}\tau^2)\ \sigma^2 \end{aligned} \quad (31)$$

Looking at (31), the bivariate interpolation function $\hat{y}(s,t)$ can be interpreted as a univariate polynomial in *s*, whose coefficients are given, in turn, by three P_i univariate polynomials in *t*:

$$\hat{y}(\sigma,t) = P_0(\tau) + P_1(\tau)\,\sigma + P_2(\tau)\,\sigma^2 \quad (32)$$

The procedure to find the values of the a_{ij} coefficients of the bivariate interpolator $\hat{y}(s,t)$ starts by acquiring an averaged signal $s(y_i,t_j)$ for each of the nine combinations of three discrete calibration standards $\{y_0, y_1, y_2\}$ (e.g., three reference temperatures) and three averaged discrete values for the controlled covariate $\{t_0, t_1, t_2\}$ (e.g. three *cold junction* temperatures), thus obtaining the following calibration matrix:

$$\mathbf{S} := \begin{bmatrix} \bar{\sigma}(y_0,\bar{t}_0) & \bar{\sigma}(y_0,\bar{\tau}_1) & \bar{\sigma}(y_0,\bar{\tau}_2) \\ \bar{\sigma}(y_1,\bar{\tau}_0) & \bar{\sigma}(y_1,\bar{\tau}_1) & \bar{\sigma}(y_1,\bar{\tau}_2) \\ \bar{\sigma}(y_2,\bar{\tau}_0) & \bar{\sigma}(y_2,\bar{\tau}_1) & \bar{\sigma}(y_2,\bar{\tau}_2) \end{bmatrix} \quad (33)$$

which, for notational simplicity, will be written as:

$$\mathbf{S} \equiv \begin{bmatrix} \sigma_{00} & \sigma_{01} & \sigma_{02} \\ \sigma_{10} & \sigma_{11} & \sigma_{12} \\ \sigma_{20} & \sigma_{21} & \sigma_{22} \end{bmatrix} \quad (34)$$

Next, using Lagrange interpolation, three intermediate 2nd-degree polynomials that interpolate the correct(ed) value $\hat{y}$ as a function of the measured average signal *s*, for each of the discrete controlled covariate values $\{t_0, t_1, t_2\}$, are calculated:

$$\hat{y}(\bar{\sigma}) = \begin{cases} b_{00} + b_{01}\bar{\sigma} + b_{02}\bar{\sigma}^2 & \text{if } \tau = \bar{\tau}_0 \\ b_{10} + b_{11}\bar{\sigma} + b_{12}\bar{\sigma}^2 & \text{if } \tau = \bar{\tau}_1, \\ b_{20} + b_{21}\bar{\sigma} + b_{22}\bar{\sigma}^2 & \text{if } \tau = \bar{\tau}_2 \end{cases} \quad (35)$$

where the nine b_{ij} intermediate coefficients can be obtained by the application of an adequate derivation of the set of Eq. (22) to Eq. (25) to the previously acquired set of nine calibration points (s_{ij}, y_i):

$$b_{i0} = \sum_{j=0}^{2} w_{ij} \prod_{\substack{k=0 \\ k\neq j}}^{2} \sigma_{ki}, \quad (36)$$

$$b_{i1} = -\sum_{j=0}^{2} w_{ij} \sum_{\substack{k=0 \\ k\neq j}}^{2} \sigma_{ki}, \quad (37)$$

$$b_{i2} = \sum_{j=0}^{2} w_{ij}, \quad (38)$$

$$w_{ij} = y_j \div \prod_{\substack{k=0 \\ k\neq j}}^{2} (\sigma_{jk} - \sigma_{ki}) \quad (39)$$

Alternatively, the equivalent single expression – derived from Eq. (30) – can be employed:

$$b_{ij} = \sum_{k=0}^{2} y_k \frac{\delta_{j0} \prod_{\substack{l=0 \\ l\neq k}}^{2} \sigma_{li} - \delta_{j1} \sum_{\substack{l=0 \\ l\neq k}}^{2} \sigma_{li} + \delta_{j2}}{\prod_{\substack{l=0 \\ l\neq k}}^{2} (\sigma_{jl} - \sigma_{li})} \quad (40)$$

Lastly, the nine a_{ij} coefficients of the final bivariate polynomial interpolator $\hat{y}(s,t)$ are obtained by finding the three $P_i(t)$ univariate sub-polynomials of Eq. (28), which can be done by interpolating how the previously calculated b_{ij} intermediate coefficients vary in the continuous subspace of the *t* covariate. This is accomplished by, once again, appropriately deriving from (22) to (25), this time using the nine (t_i, b_{ij}) pairs previously calculated with (36) to (39), or with (40):

$$a_{i0} = \sum_{j=0}^{2} v_{ij} \prod_{\substack{k=0 \\ k\neq j}}^{2} \tau_k, \quad (41)$$

$$a_{i1} = -\sum_{j=0}^{2} v_{ij} \sum_{\substack{k=0 \\ k\neq j}}^{2} \tau_k, \quad (42)$$

$$a_{i2} = \sum_{j=0}^{2} v_{ij}, \quad (43)$$

$$v_{ij} = b_{ji} \div \prod_{\substack{k=0 \\ k\neq j}}^{2} (\tau_j - \tau_k) \quad (44)$$

Like previously, the equivalent single expression – again based on Eq. (30) – can also be employed:

$$a_{ij} = \sum_{k=0}^{2} b_{ji} \frac{\delta_{j0} \prod_{\substack{l=0 \\ l\neq k}}^{2} \tau_l - \delta_{j1} \sum_{\substack{l=0 \\ l\neq k}}^{2} \tau_l + \delta_{i2}}{\prod_{\substack{l=0 \\ l\neq k}}^{2} (\tau_k - \tau_l)} \quad (45)$$

Additionally, it is possible to consolidate all the previous steps – (36) to (45) – in a single expression:

$$\mathbf{A} = \sum_{i=0}^{2} \frac{\begin{bmatrix} \prod_{\substack{k=0 \\ k\neq i}}^{2} \sigma_{ki} \\ -\sum_{\substack{k=0 \\ k\neq i}}^{2} \sigma_{ki} \\ 1 \end{bmatrix} \cdot \begin{bmatrix} \prod_{\substack{j=0 \\ j\neq i}}^{2} \tau_j \\ -\sum_{\substack{j=0 \\ j\neq i}}^{2} \tau_j \\ 1 \end{bmatrix}^T}{\prod_{\substack{j=0 \\ j\neq i}}^{2} [(\tau_i - \tau_j) \prod_{\substack{k=0 \\ k\neq j}}^{2} (\sigma_{jk} - \sigma_{ki})]}, \quad (46)$$

which allows us to obtain the matrix of coefficients **A** directly from the calibration matrix **S**. However, expression (46) might not be as practical to implement as the previously presented set of equations.

This completes the derivation of the method. In conclusion, Eq. (46) – or expressions (40) and (45) – define the transformation (or mapping) of a 3×3 matrix of 3D points (or vectors) – in the current context, a set of nine averaged raw values returned by a sensor (s_{ij}, i,j = 0, 1, 2) for all the combinations of three calibration standards (y_i, i = 0, 1, 2) and three discrete controlled values of an error-inducing covariate (t_j, j = 0, 1, 2) – to a 3×3 matrix of scalar values (a_{ij}, i,j = 0, 1, 2), which are the coefficients of a bivariate function that defines a 4th-degree polynomial surface that contains the nine 3D calibration points without residuals. For the present purposes, the key characteristic of this polynomial surface is that the third dimension is injectively dependent on the other two (independent) degrees of freedom. Concretely, the calibrated value $\hat{y}$ is injectively dependent on the raw sensor signal s and the controlled error-inducing covariate t:

$$(\bar{\sigma}_{ij}, \bar{\tau}_j, y_i) \mapsto a_{ij} : \hat{y}(\sigma, \tau) = \sum_{j=0}^{2} \sum_{i=0}^{2} a_{ij} \sigma^i \tau^j \quad (47)$$

3. Practical Application: Calibration of Thermocouple Temperature Sensors

Although applicable to any type of analog sensor or transducer, the proposed method is particularly indicated for thermocouple compensation. Here are some of the main reasons [2]:

1) Although considered sufficiently linear for many applications, thermocouples cannot be assumed to have a linear response when high accuracy is required, especially if the operating temperature range is relatively wide; the common solution consists of using piecewise linear interpolations; however, this method requires a relatively large set of calibration points and can be computationally wasteful if taken to the limit;

2) The nonlinear response curve of a thermocouple is relatively smooth and has, at most, one major inflection point; in many typical applications, there are no relevant inflections inside the operational temperature range, meaning that the curve can be successfully approximated by a low degree polynomial; but, if inflections do occur, two alternative solutions can be employed: (*a*) increasing the polynomial degree and/or (*b*) definition of distinct piecewise temperature domains (*splining*);

3) The major external influence on the signal is the electric potential occurring at the *cold junction(s)* (i.e., the unavoidable bimetal contacts at the contact points with the signal acquisition electronics); this effect can be effectively compensated with the help of an additional temperature sensor;

4) Since the physical phenomenon giving origin to the *cold junction* potential is the same as the one occurring at the sensing junction, it shares the same properties, i.e., smooth response with simple curvature (i.e., few or no inflections);

5) As the *cold junction* temperature sensor is usually placed close to the acquisition equipment electronics – and, particularly, the voltage reference used by the analog-to-digital (ADC) converter – the signal from this sensor can be used to compensate for the combination of both the *cold junction* potential and the eventual temperature-dependent reference voltage drift (i.e., effectively combining two covariates into just one).

3.1. In Practice: A Real Example

The procedure performed to calibrate a set of thermocouples connected to a data logger, in the range [-25 ºC; 0 ºC] with *cold junction* temperatures in the interval [18 ºC; 42 ºC], using the proposed calibration method will be now described.

For this purpose, three temperature standards will be used: two composed of eutectic aqueous saline solutions and one of pure water. These three standards provide the necessary three calibration temperatures which, in combination with three discrete *cold junction* temperatures, allow us to obtain the nine points of the calibration matrix needed for a 4th-degree nonlinear bivariate calibration.

Fig. 2 shows the three temperature standards used. The eutectic solutions were tinted with a residual amount of food-grade coloring, to facilitate the respective identification. They are, respectively, from left to right: an aqueous eutectic solution of 23.3 % (by mass) sodium chloride, with a fusion temperature of approximately -21.1 °C [8] (yellow); an eutectic aqueous solution of 19.7 % (by mass) of potassium chloride, with a fusion temperature of approximately -10.6 °C [9] (blue); and pure (distilled) water:

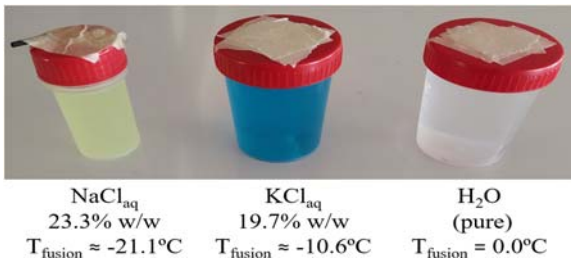

Fig. 2. The three temperature standards used in the thermocouple calibration.

The calibration will make use of the fact that, given appropriate conditions, the temperature of the liquid-phase will remain practically constant at the fusion temperature during the phase transition – as illustrated in Fig. 3 – due to the abrupt increase in entropy.

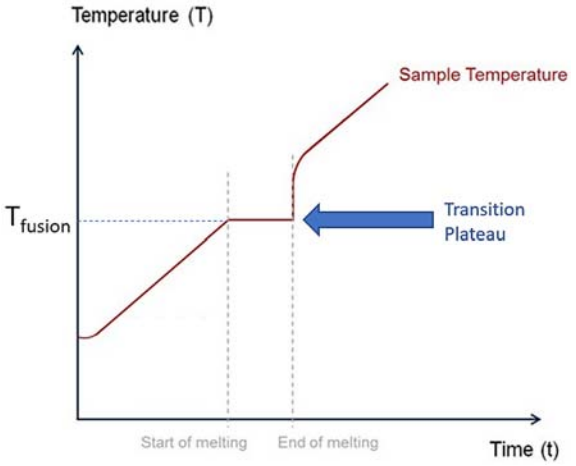

Fig. 3. The temperature of the liquid phase remains constant during fusion.

The procedure starts by placing the standards in a freezer chest, as shown in Fig. 4. The standards start to freeze from the outside in, which is essential for the procedure.

As soon as one of the standards has formed an adequately thick layer of ice on the periphery, it is removed from the freezer (being the first one the pure water, followed by the KCl eutectic and, finally, by the NaCl).

After stirring the liquid core, to homogenize the temperature, the bundle of thermocouples under calibration (*type-T*, in our case) is securely held in the geometric center of the cylindrical container, where the liquid phase is surrounded by the solid (ice) phase, as shown in Fig. 5.

The container is, in turn, placed in the center of a thermally insulated enclosure (in this case, a polystyrene foam box).

Fig. 4. The temperature standards are placed in a freezer chest.

Fig. 5. The bundle of thermocouples under calibration is placed in the center of the calibration standard.

The enclosure is closed shut with a weight over the lid – as shown in Fig. 6 – to keep it as insulated from ambient temperature as possible, while the thermocouple signals are recorded with the data logger.

Fig. 6. The insulating enclosure is closed shut with the help of a weight on its lid, while the signals are acquired.

The data logger hardware is also placed in a thermally insulated enclosure and its temperature is controlled with the help of a resistive element and a small fan, which are driven by an external micro-controller. It is assumed that the electronic components of the data logger are, for all practical purposes, in thermal equilibrium with the electric terminals of the thermocouples, which constitute the *cold junction*, in this case. In this manner, both the *cold junction* temperature and the temperature of the electronic components (which affect the voltage references) are compensated using the signal of a single temperature sensor. In our case, this temperature sensor is an active medium-precision thermistor, whose signal is also recorded by the same data logger. Fig. 7 shows the data logger in its temperature-controlled enclosure.

The calibration procedure is repeated for three different actively stabilized *cold junction* (and voltage reference) temperatures, in the range [18ºC; 42ºC]. This range is representative of the typical *cold junction* temperatures that might occur in our non-climatized laboratory.

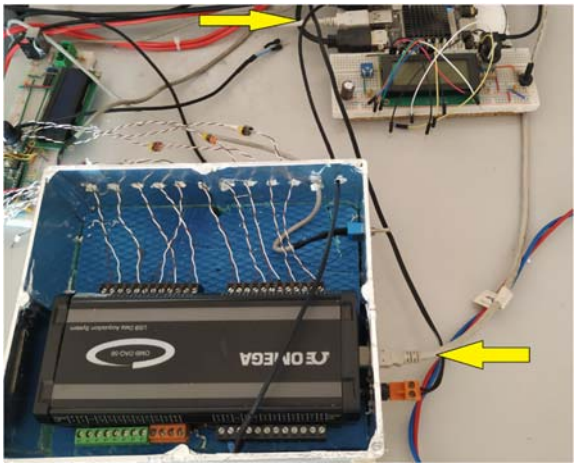

Fig. 7. The data logger is placed in a temperature-controlled enclosure.

The acquired values were the uncalibrated *raw* values returned by the multiplexed 12-bit analog-to-digital converter (ADC) of the data logger (after amplification and signal conditioning). The correction procedure will, inherently, provide an output in proper temperature units (note: converting the ADC values into temperatures units beforehand would add an unnecessary truncation error to the final results).

Fig. 8 represents, graphically, the calibration dataset acquired with the described procedure, from an arbitrarily chosen random thermocouple. The nine representative points were obtained by averaging at least 10 measurements, with an interval of about 6 seconds between consecutive acquisitions, which totals about 1 minute for each temperature combination (hot and *cold junction* values).

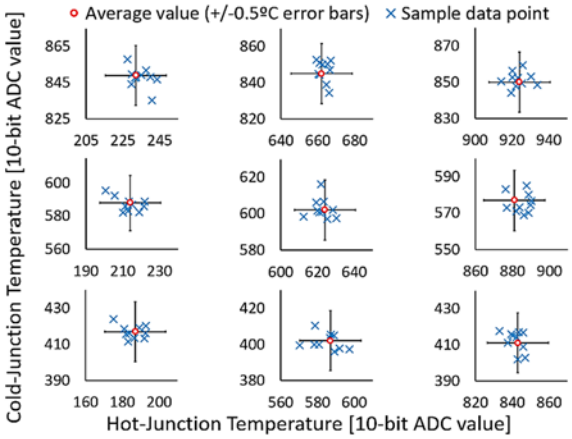

Fig. 8. The example dataset used in the demonstration, acquired from a randomly chosen thermocouple.

Clear outliers were rejected. The standard deviation of all points – represented as error bars in Fig. 8 – was about ~0.17 °C. The rejection threshold was heuristically defined as ±0.5 °C (i.e., approximately three times the standard deviation), which is about half the typical accuracy of a *type-T* thermocouple.

Table 1 shows the calibration matrix **S**, containing the nine calibration points s_{ij}, obtained by averaging the recorded values for three different temperature standards T_{std} and three values of the controlled *cold junction* temperature t. The calibration was targeted at measuring temperatures in the range [-25 ºC; 0 ºC] with *cold junction* temperatures in the typical interval [18 ºC; 42 ºC]. The three discrete controlled *cold junction* temperatures (acquired with a medium-precision thermistor) were, approximately, ~18.0 ºC, ~30.0 ºC, and ~42.0 ºC.

Table 1. Calibration matrix **S** (s_{ij} values).

T_{std} [ºC]	$t \cong 407$	$t \cong 589$	$t \cong 843$
0.0	843	881	924
-10.6	587	624	662
-21.1	187	214	232

(s and t values in ADC arbitrary units)

Table 2 shows the resultant matrix **A**, containing the nine a_{ij} calibration coefficients, calculated from the input values shown in Table 1, using Eq. (46).

Table 2. Matrix **A** (a_{ij} calibration coefficients).

-2.306×10^{1}	-1.798×10^{-3}	1.929×10^{-6}
1.608×10^{-2}	-2.293×10^{-5}	9.778×10^{-9}
2.076×10^{-5}	8.453×10^{-9}	-6.626×10^{-12}

Fig. 9 shows the calibration surface generated with Eq. (47), using the a_{ij} coefficients shown in Table 2. The surface contains the nine calibration points – represented as red circles – with *zero residuals*.

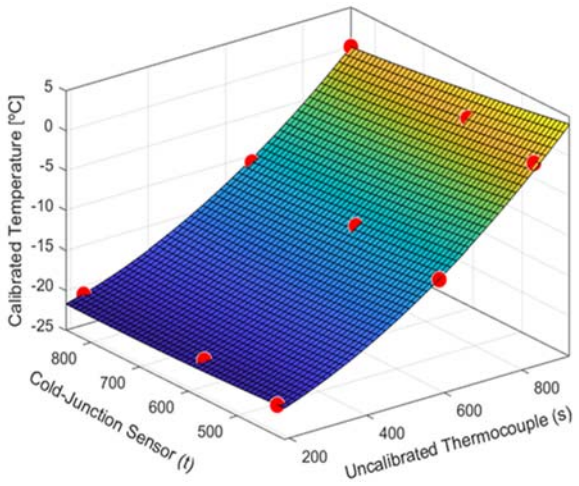

Fig. 9. Interpolated surface containing the 9 calibration points, represented as red circles.

4. Conclusions

The present method has the potential to augment both the accuracy and precision of, virtually, any electronic measurement system based on analog sensors and/or transducers. Being nonlinear, the method allows for better modeling of the typically nonlinear response of analog electronic devices. Being bivariate, it allows compensation for an external or environmental detrimental influence (typically temperature).

Our practical experience has consistently confirmed the validity, practicability, and usefulness of the proposed method for improving the measurement quality of – specifically – thermocouples. These are inexpensive and fast-responding sensors, capable of covering very broad ranges of temperatures. However, they are notoriously lacking in precision. Besides the electrical noise that plagues their low-level signal, they have significantly nonlinear responses. Also contributing to their lack of precision is the absolute necessity to compensate for the *cold junction* voltage, which needs to be measured with precision for best results. The fact that this voltage also varies nonlinearly with temperature adds complications. Addressing these drawbacks, the proposed method allows for the compensation of this nonlinear detrimental influence on the signal.

The accurate measurement of temperature by electronic means has always presented a challenge. Accurate temperature reference standards are not abundant and/or accessible, which makes it difficult to calibrate nonlinear sensors. The wider the calibration range, the more difficult it becomes. A nonlinear calibration method is, in these cases, practically mandatory, as it becomes unfeasibly onerous to conduct a piecewise linear approach.

Despite their relatively unwieldy appearance, the herein presented system of equations – which performs the essential transformation of the calibration dataset into the signal-correcting function parameters – is extremely straightforward to implement. It is also very much less computationally taxing than the more conventional iterative alternatives. These assertions are supported by our experience. For instance, this method has been successfully implemented in microcontroller code, within the development of a data logging device.

Acknowledgments

This work was supported by the R&D project «UFA+EE – Research and Development of Autonomous and Energy-Efficient Cold Units», in a partnership between the University of Aveiro and Tensai, S. A., and co-funded by the European Structural and Investment Funds, Portugal 2020, 03/SI/2017, POCI-01-0247-FEDER-033755.

References

[1]. H. Martens, T. Naes, Multivariate Calibration, *John Wiley & Sons*, 1992.

[2]. L. S. Rodrigues, *et al*., Practical Multivariate Data Correction and Sensor Calibration Methods, *IEEE Sensors Journal*, Vol. 20, Issue 13, 2020, pp. 7283-7291.

[3]. L. S. Rodrigues, Analytical Method for Smooth Interpolation of Two-Dimensional Scalar Fields, in "Estudo Geral" – Digital Repository for the Scientific Production of the University of Coimbra, September 2015, http://hdl.handle.net/10316/38850.

[4]. A. Araújo, Polynomial regression with reduced over-fitting - The PALS technique, *Measurement*, Vol. 124, August 2018, pp. 515-521.

[5]. D. S. Young, Handbook of Regression Methods, *CRC Press*, 2018, ISBN 1351650742.

[6]. R. R. Rhinehart, Nonlinear Regression Modeling for Engineering Applications: Modeling, Model Validation, and Enabling Design of Experiments, *John Wiley & Sons*, 2016.

[7]. J. Devore, A Modern Introduction to Probability and Statistics: Understanding Why and How, *Journal of the American Statistical Association*, Vol. 101, 2006.

[8]. R. J. Bodnar, Revised equation and table for determining the freezing point depression of H_2O-NaCl solutions, *Geochimica and Cosmochimica Acta*, Vol. 57, Issue 3, Feb. 1993, pp. 683–684.

[9]. R. J. Bakker, Package FLUIDS. Part 4: thermodynamic modelling and purely empirical equations for H_2O-NaCl-KCl solutions, *Mineralogy and Petrology*, Vol. 105, May 2012, pp. 1–29.