A MONTE CARLO ANALYSIS OF THE EFFECTS OF COVARIANCE ON PROPAGATED UNCERTAINTIES

Ronald Ainsworth

Hart Scientific, American Fork UT, USA

ABSTRACT

Reports of calibration typically provide total combined uncertainties at each individual calibration point with no information describing the correlation among those uncertainties. This affects the ability of the user of the report of calibration to make an accurate determination of propagated uncertainty values. Although covariance is known to affect propagated uncertainties, in those cases where there is insufficient information to evaluate the covariance it is generally taken to be zero even when the assumption is unlikely to be true. When correlation coefficients are allowed to vary from zero, the resulting shape of the propagated uncertainty curve varies depending on the specific combination of correlation coefficient values. When combinations of correlation coefficients are chosen at random a wide range of propagated uncertainty curves are obtained. This type of Monte Carlo simulation is not intended to recreate the physical insight withheld by the provider of the report of calibration however it does demonstrate the magnitude of the problem faced by the user of the calibration certificate. In particular the paper discusses the impact that the absence of correlation coefficient information has on the propagation of uncertainty curves for an Au/Pt thermocouple calibration. Furthermore this paper discusses the possibility of a maximum likelihood estimator for propagation of uncertainty curves where information about the degree of correlation among uncertainties is not provided. The simulations show that uncertainty in the degree of correlation between the variances of calibration points may have a demonstrably significant impact on the overall uncertainty of the calibration.

1. INTRODUCTION

The calibration of a temperature sensor generally requires measuring the sensor at known temperatures and the fitting of measured data to an applicable function used to interpolate between the measured datum points. SPRT calibration data are fit to the functions described by the ITS-90, thermocouple calibration data may be fit to functions such as those described in [1] and [2], and similarly there are curves which apply to PRTs and thermistors.

The true values of the calibration data are unknown quantities, however the range of values in which the true value is believed to be contained is quantified by a standard deviation-like quantity referred to as a standard uncertainty. Uncertainties are used to describe the state of mind of the metrologist and to reflect the knowledge of the metrologist regarding the dispersion of values represented by a particular measurement. Uncertainties in the calibration data result in uncertainty in the interpolation function fit to the calibration data. This effect is called the propagation of uncertainty.

Just as there is a curve which interpolates between measured values, there is also a curve which interpolates between the associated uncertainties of the measured values. This curve is defined in part by the variance-covariance matrix of the uncertainties of the measured quantities. The diagonal elements of this matrix are the variances (the squares of the standard uncertainties) of each measured value. The rest of the matrix is filled in by the covariance of each uncertainty (i.e. two unique standard uncertainties multiplied by their associated correlation coefficient.) The shape of the propagation of uncertainty curve and therefore the uncertainties assigned to the interpolated calibration values depend on our knowledge of the correlation between individual uncertainties. Unfortunately most calibration certificates provide only the k=2 uncertainties with no information regarding the degree of correlation among those uncertainties. In this situation only the diagonal elements of the variance-covariance matrix are known. This lack of knowledge implies an additional uncertainty that deserves evaluation and leads to a dispersion of possible curves to choose from. Therefore it is desirable to choose a propagation of uncertainty curve that represents an unbiased maximum likelihood estimate of the propagated uncertainty.

2. EXAMPLES OF CORRELATED UNCERTAINTIES

Metrologists preparing reports of calibration may have access to much useful information for evaluating covariance. Take for example the calibration of an Au/Pt thermocouple. Uncertainty components that may be correlated between calibration points are indicated in Table 1.

Table 1: Example of some Type B Thermocouple Uncertainties and possible subjective degrees of correlation

Uncertainties for Thermocouple Calibration at Individual Fixed Points	Degree of Correlation With Other Fixed Points
Uncertainty in sealed cell fixed point value (reference cell certification)	Weak Correlation
Uncertainty in fixed point value (non-ideal plateau)	Weak Correlation
Uncertainty in ice bath system	Strong Correlation
Uncertainty in hydrostatic head correction	Uncorrelated
Uncertainty due to non-ideal immersion profile	Uncorrelated
Uncertainty due to inhomogeneity (estimated)	Strong Correlation
Uncertainty due to low thermal switch thermal EMF	Strong Correlation
Uncertainty due to sensitive DVM long term stability	Strong Correlation
Uncertainty due to sensitive DVM calibration	Weak Correlation

It is easy to see that uncertainties in the ice bath would be correlated if the same ice bath was common to each point of the calibration and the same can be said for the low thermal switch. Uncertainties due to inhomogeneity are believed to be correlated between fixed points based on data reported in [3]. However it is difficult to directly observe the covariance in practice. Yet it is possible to make judgments about the degree of correlation qualitatively and a metrologist may be able to put upper and lower bounds on the percentage of variation at one temperature that is explainable by variation at another. The R-square statistic tells us the percentage of variation in the dependent variable that is attributable to variation in the independent variable. The square root of the R-square statistic is the correlation coefficient. If we could estimate for example that variation in the measured voltage at the Tin point due to the ice bath was 90% explainable by the variation in the measured voltage at the Zinc point due to the ice bath then we could estimate that the correlation coefficient would be the square root of 0.90, which is 0.95. A similar procedure could be used to put upper and lower bounds on the correlation coefficients. One way of synthesizing this information into correlation coefficients for the total combined uncertainties would be through a simulation exercise. A Monte Carlo simulation could be used to incorporate the physical insight of the metrologist regarding the individual uncertainty components into an estimate of the correlation coefficients of the total combined uncertainties. An example of a covariance matrix in symbolic form is:

$$\begin{bmatrix} \sigma_{Sn}^2 & \sigma_{Zn}\sigma_{Sn}r(x_{Zn},x_{Sn}) & \sigma_{Al}\sigma_{Sn}r(x_{Al},x_{Sn}) & \sigma_{Ag}\sigma_{Sn}r(x_{Ag},x_{Sn}) \\ \sigma_{Sn}\sigma_{Zn}r(x_{Sn},x_{Zn}) & \sigma_{Zn}^2 & \sigma_{Al}\sigma_{Zn}r(x_{Al},x_{Zn}) & \sigma_{Ag}\sigma_{Zn}r(x_{Ag},x_{Zn}) \\ \sigma_{Sn}\sigma_{Al}r(x_{Sn},x_{Al}) & \sigma_{Zn}\sigma_{Al}r(x_{Zn},x_{Al}) & \sigma_{Al}^2 & \sigma_{Ag}\sigma_{Al}r(x_{Ag},x_{Al}) \\ \sigma_{Sn}\sigma_{Ag}r(x_{Sn},x_{Ag}) & \sigma_{Zn}\sigma_{Ag}r(x_{Zn},u_{Ag}) & \sigma_{Al}\sigma_{Ag}r(x_{Al},x_{Ag}) & \sigma_{Ag}^2 \end{bmatrix} \quad (1)$$

Clearly, the metrologist providing the report of calibration has the best information regarding correlated uncertainties and is therefore in the best position to estimate propagated uncertainties for his client. A method for doing so is provided below.

3. MATHEMATICS OF UNCERTAINTY PROPAGATION

The equation referred to by [4] as the law of propagation of uncertainty is based on a first-order Taylor series expansion of the equation:

$$Y = f(X_1, X_2, ..., X_N) \quad (2)$$

Y is the observed output and the X_N are inputs that may or may not be observed. Solutions to the first-order Taylor series can be obtained directly, by numerical methods, or by a method recently described using Lagrange polynomials [5]. However it is also possible using matrix methods to solve for the propagation of uncertainty curves directly without the use of a first-order Taylor series approximation. This turns out to be computationally more efficient and demonstrably equivalent to the other methods. Furthermore the author believes that matrix methods provide more insight into the relationship between covariance and the propagation of uncertainty and therefore it is the preferred method for this paper. Since the author is unaware of references to this particular method in the literature a brief explanation is provided.

If the argument of $f(X_1, X_2, ..., X_N)$ is rewritten as the vector X then Equation (2) becomes:

$$Y = Xb \quad (3)$$

Now the vector b represents the calibration coefficients and the vector X represents the calibration data. If we want to predict what the interpolated mean response $\hat{Y}$ would be to some other set of inputs X_h then we can write the relationship as follows:

$$\hat{Y} = X_h b \quad (4)$$

If Y is a random vector with expected variance-covariance matrix $\sigma^2\{Y\} = E\{[Y - E\{Y\}][Y - E\{Y\}]^T\}$ and Equation (4) defines the interpolated response $\hat{Y}$ for any given set of inputs X_h, it can easily be shown that:

$$\sigma^2\{\hat{Y}\} = E\{X_h \sigma^2\{b\} X_h{}^T\} \tag{5}$$

where the solution to Equation (3) is $b = X^{-1}Y$ and leads to the equation $\sigma^2\{b] = E\{X^{-1}\sigma^2\{Y\}(X^{-1})^T\}$. By combining this result with Equation (5) we obtain:

$$\sigma^2\{\hat{Y}\} = E\{X_h X^{-1}\sigma^2\{Y\}(X_h X^{-1})^T\} \tag{6}$$

The propagated uncertainties of the response $\hat{Y}$ for a given input X_h are the diagonal elements of the variance-covariance matrix $\sigma^2\{\hat{Y}\}$. In contrast, the diagonal elements of the variance-covariance matrix $\sigma^2\{Y\}$ are values estimated by a metrologist through the usual process of uncertainty analysis. They are simply the squares of the standard uncertainties associated with the vector *Y*. The off-diagonal elements are the covariance and their estimation requires knowledge about the degree of correlation between the uncertainties along the diagonal of the matrix. The covariance is defined:

$$\sigma(x_i, x_j) = \sigma(x_i,)\sigma(x_j)r(x_i, x_j) \tag{7}$$

where $r(x_i, x_j)$ is the correlation coefficient.

The solution to the over-determined case is similarly derived by choosing the appropriate solution to Equation (3). Equation (7) is where this approach normally comes to a halt for the user of a calibration certificate because $r(x_i, x_j)$ usually is unknown. Sometimes it is estimated as having a value of one. At other times the metrologist uses his "best judgment" and ignores correlation. However, frequently the case is that the user of the report knows the true value is probably somewhere between the two extremes but does not know how to evaluate it.

4. MONTE CARLO ANALYSIS

Monte Carlo analysis is a statistical simulation method with a wide variety of applications. By representing a problem in terms of probability distribution functions (rather than differential equations) it is possible to draw out numeric solutions to very difficult problems that would have been near impossible to solve with traditional methods.

Recall that one suggested method of dealing with covariance is to treat propagated uncertainty as if covariance was zero. In the case of the Au/Pt thermocouple calibration described above this is unlikely to be the expected value of the covariance. The question arises then, "Is it likely that setting covariance to zero will result in the most useful description of propagated uncertainty?”

When no information is provided in the report of calibration about the values or likely distributions of the correlation coefficients then it seems reasonable to model the dispersion of possible values for the correlation coefficients with a rectangular distribution. In the first case considered, nothing is left off the table. The range of all possible values for correlation coefficients is by definition -1 to 1. However in the second case it is stated as an opinion that depending on the facts available about the calibration it might be possible to narrow the likely range of potential correlation coefficients to between 0 and 1. Graphical results of both cases are shown in the figures below.

Uncertainties appropriate for an Au/Pt thermocouple calibration by fixed point were assumed in this simulation. At Sn, Zn, Al and Ag the $k=2$ values were taken to be 16.8, 15.1, 17.0 and 19.6 mK respectively. By drawing combinations of correlation coefficients from a random set of data, 18,316 curves were generated in one case and 20,000 curves were generated in another representing potential propagated uncertainty curves for the assumed uncertainties. The first case assumed that correlation coefficients could vary between -1 and 1 and the second case assumed only positive correlation coefficients. The correlation coefficient matrices were symmetric with the diagonal set equal to one. As a normalization condition the matrices were required to be positive definite [7] by the following method. Each primary submatrix was tested for a positive determinant to ensure that all eigenvalues would also be positive. A deviation function of the form $f(t) = a \times t + b \times t^2$ was chosen and the over-determined form of equation (6) was used to generate the curves. The resulting output was divided into quartiles.

The environment used to conduct the analysis was a system for statistical computation and graphics called R [8]. The algorithm used for generating the uniformly distributed random numbers needed for the simulation was the Mersenne Twister [9] which has a period of 2^{19937}-1.

5. RESULTS

Figure 1 below displays the results of the Monte Carlo Simulation in graphical form. The dispersion of values generated was divided into quartiles as indicated by the solid lines in Figure 1. The median value is indicated by the solid line in the center of the curve and the maximum and minimum values obtained at each temperature are indicated by the outer solid lines. Additionally three other curves are shown. The solid circles represent the special case where all uncertainties approach 100% correlation between calibration points. The empty circles represent another special case where none of the uncertainties are correlated at any of the fixed points. Finally there is a third curve indicated by stars which was calculated as the average of the two curves above which had all correlation coefficients set effectively to one for the correlated case or to zero for the uncorrelated case.

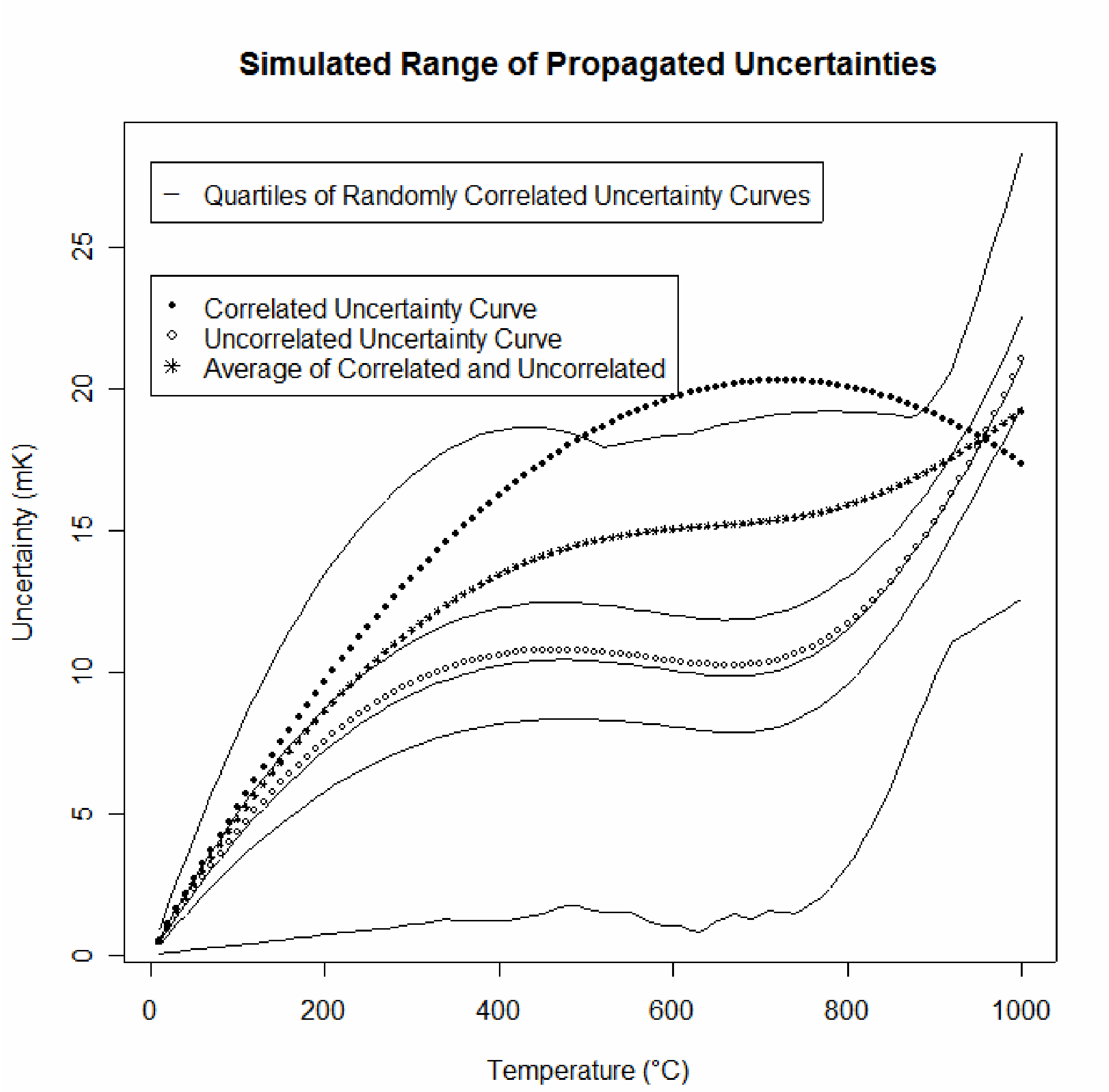

Figure1: The range of propagation of uncertainty curves was determined through a Monte Carlo investigation utilizing 18,316 simulations. The simulated curves were produced by choosing covariance matrices that represented random degrees of correlation between calibration points. Correlation coefficients were uniformly distributed between -1 and 1. Correlation coefficient matrices were symmetric, invertible and accepted if and only if they were positive definite matrices. For this simulation an over-determined quadratic deviation function with two degrees of freedom was chosen.

It is interesting to note that in Figure 1 where correlation coefficients were allowed to vary between -1 and 1 that the uncorrelated case ($r_{ij}=0$ when $i \neq j$ else $r_{ij}=1$) was a fairly useful predictor of the median of the distribution. On the other hand in Figure 2 the average of the correlated and uncorrelated curves was a better approximation to the curve representing the median of all the simulations and may present the easiest method of calculating a maximum likelihood estimate curve for the propagation of uncertainty when correlations are expected to be positive. If this turns out to be true in other scenarios then further research should try to determine whether an averaging technique would also be useful when the upper and lower bound on the correlation coefficients are other than 0 and 1.

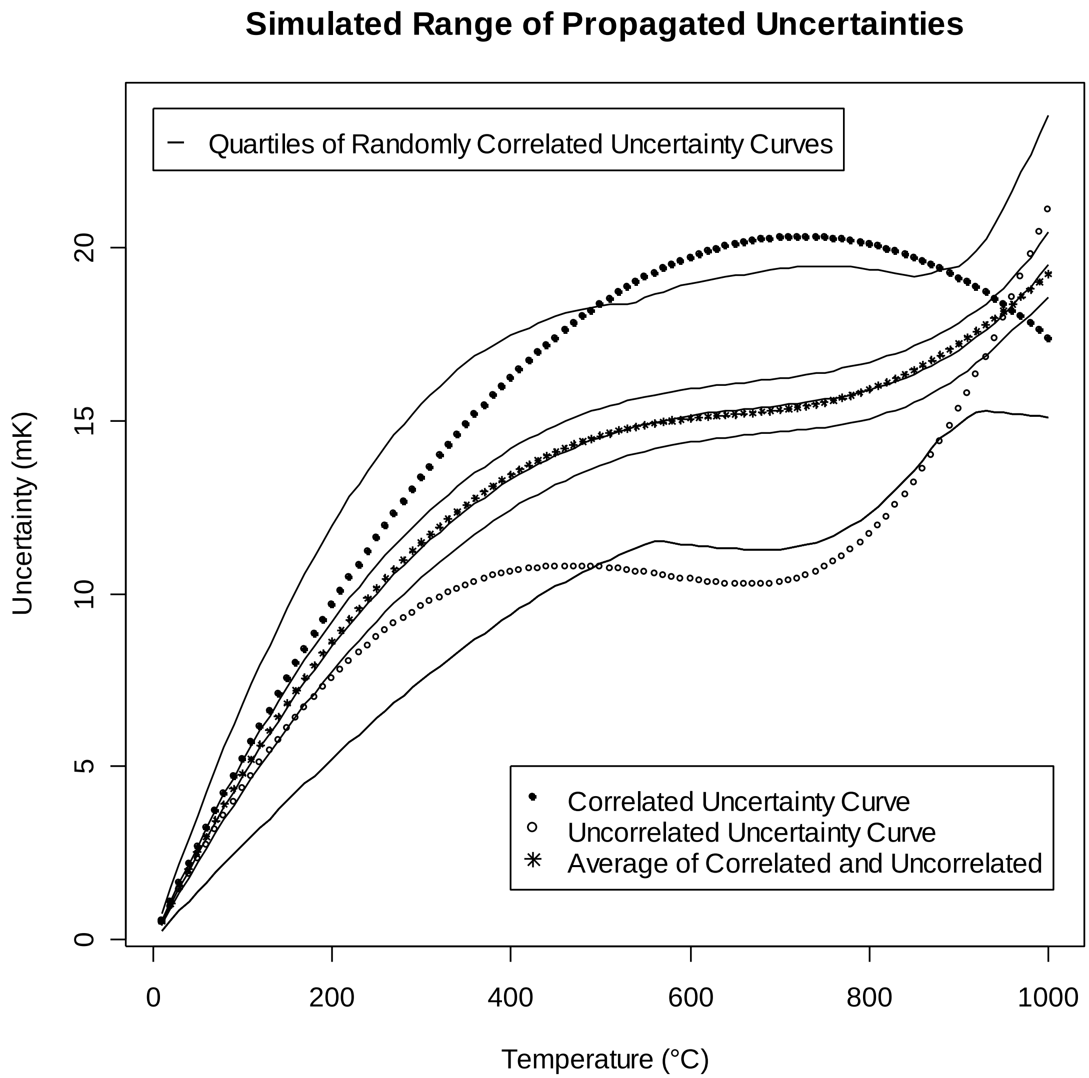

Figure2: The range of propagation of uncertainty curves was determined through a Monte Carlo investigation utilizing 20,000 simulations. The simulated curves were produced by choosing covariance matrices that represented random degrees of correlation between calibration points. Correlation coefficients were uniformly distributed between 0 and 1. Correlation coefficient matrices were symmetric, invertible and accepted if and only if they were positive definite matrices. For this simulation an over-determined quadratic deviation function with two degrees of freedom was chosen.

When negative correlations are believed to be unlikely it appears that the propagation of uncertainty curve will be misrepresented by an uncorrelated determination. However if no information is present regarding correlation or if it is believed to be equally likely to be positive as it is to be negative then no evidence has been presented which contradicts the validity of assuming covariance is equal to zero.

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Address of the Author:

Ainsworth Ronald, Hart Scientific, 799 East Utah Valley Drive, American Fork UT 84003, USA, tel. 801 763 1700, fax 801 763 1010, e-mail: Ron.Ainsworth@HartScientific.com