On the use of least-squares and redundant fixed-points with ITS-90 SPRT interpolations

D R White
Measurement Standards Laboratory of New Zealand
PO Box 31310, Lower Hutt, New Zealand
email: r.white@irl.cri.nz

Abstract

The preliminary results of an investigation into the benefits of using the method of least squares with the SPRT interpolations of ITS-90 are reported. The first section analyses the application of least squares to first and second order ITS-90 equations, and presents guidelines on the calculation of analytic expressions for the sensitivity coefficients for fixed-point measurements. This is followed by examples of least squares applied to three of the ITS-90 sub-ranges, namely the mercury-gallium, water-indium and water-zinc sub-ranges. It is found that for these cases, even a single additional fixed-point measurement in the determination of the SPRT calibration constants provides benefits in respect of reduced uncertainty in the interpolation. In some cases with extrapolation, the uncertainty increases, and this is believed to be an artefact of the ITS-90 constraint of forcing all of the interpolation equations through the point $(W, W_r) = (1,1)$. The paper concludes with suggestions for further work in order to develop a better understanding of the limitations of the method of least squares. This includes investigations of a greater variety of specific cases and weighted least squares. It is also noted that some uncertainty in the interpolation arises from interpolation error, which is manifest as non-uniqueness, and more work is required in this area but dependent on the collection of more W vs. W data above 0 °C.

1. Introduction

Most NMIs use redundant fixed points in SPRT calibrations. Extra points provide assurance that all measurements are consistent, confirm that the thermometer interpolates well, and provide users of the SPRT with greater flexibility in the choice of sub-range for any particular application. Over the years, there has been speculation on the utility of least-squares fits in such situations [e.g. 1,2]: the method of least squares being suited to the determination of calibration constants in over-determined systems. Anscin, in particular, noted the reduction in sensitivity coefficients in the water-zinc sub-range with the use of least squares [2], and argued that lower uncertainty interpolations would be obtained for any given sub-range if all available fixed point data are used.

There are two main obstacles to the acceptance of the application of least squares to ITS-90 interpolations. Firstly, the lore surrounding the use of least squares advises that one should have at least two or three measurements per fitted parameter in order to get sensible values for the parameters, and ITS-90 does not have a sufficient number of fixed points to satisfy this criterion. Secondly, until recently the sensitivity coefficients and total uncertainty for both least squares and direct interpolation have been computed only numerically, so there have been few and only empirical results for a comparison of least squares with direct interpolation.

Recent papers discussing the propagation of uncertainties with interpolation [3,4], provide the basis for an algebraic comparison of the two methods and give cause to raise the question of the utility of least-squares again. Two points can be noted. Firstly, as is well known, least squares with N measurements and N unknown parameters yields fitted parameters and uncertainties identical to those for 'direct' interpolation. Secondly, for points that are evenly spread the propagated uncertainty with polynomial least-squares interpolation is very similar to that for polynomial (Lagrange) interpolation except that the total uncertainty is reduced by a factor approximately equal to $\sqrt{\rho / N}$, where ρ is the number of fitted parameters and N is the number of measurements. Both observations suggest that any over-determination of the calibration constants results in a lower uncertainty, i.e. even one degree of freedom is better than none.

This paper further investigates the propagation of uncertainty with least-squares as applied to the two simplest interpolation equations of ITS-90. The paper begins with an algebraic analysis, including the general uncertainly formula for ITS-90 SPRT interpolations and the mathematical principles of the fits as applied to ITS-90 interpolations. The paper then presents expressions for the sensitivity coefficients for the first and second order ITS-90 interpolations when least squares is employed, and outlines a generalisation that allows determination of the sensitivity coefficients for any interpolation where the fitted parameters are linear coefficients. In Section 3 these

formulae are applied to examples for 3 different sub-ranges covering the range between the mercury and zinc points. The paper finally outlines aspects of interpolation warranting further investigation and draws some conclusions.

2. The mathematical foundations

2.1 Propagation of uncertainty

Although the ITS-90 interpolations, many of which are a form of Lagrange interpolation [3], and least-squares fits of the same equations involve quite different analysis, both can be written in the form of a linear expansion of interpolation functions $F_i(W)$ with the reference values as coefficients [4]:

$$W_{\mathrm{r}}(W) = \sum_{i=1}^{N} W_{\mathrm{r},i} F_i(W, W_1...W_N) , \qquad (1)$$

where $W_{\mathrm{r}}(W)$ is the interpolated value of reference resistance ratio, $W_{\mathrm{r},i}$ are the defined values of reference resistance ratio for the N fixed points used to determine the equation, W_i are the measurements of resistance ratio at the various fixed points, and $F_i(W)$ are functions of measured resistance ratio only. Following the line of argument presented in [5], and in the absence of correlations other than that due to the common value of $R(0.01 \ °C)$ used for all W values, the uncertainty in the ITS-90 interpolations is propagated as:

$$u_{T_{90}}^2 = \left(\frac{dT_{90}}{dW_{\mathrm{r}}} \right)^2 \left(\frac{1}{R(0.01 \ ^{\mathrm{o}}\mathrm{C})} \right)^2 \sum_{i=1}^{N} u_{Ri}^2 F_i^2(W, W_1...W_N) , \qquad (2)$$

where u_{Ri} are the combined uncertainties associated with each of the fixed point realisations and accompanying measurements, including one term for the uncertainties associated with realisation and measurement of the triple point of water. It is clear from (2) that the $F_i(W)$ are the sensitivity coefficients for uncertainties associated with the respective fixed points. The problem of propagating uncertainty then reduces to the determination of the $F_i(W)$ for any particular interpolation.

Note that the usual treatments of uncertainties in least-squares are different from that described here. The usual treatment adopts one of two approaches. Firstly, it may use measurements to make an estimate of the uncertainty based on two assumptions: that the uncertainties are associated with the dependent variable only, and that the uncertainty is the same for each point. Under these conditions, it follows that the standard deviation of an unweighted least squares fit is a Type A estimate of the standard uncertainty in the dependent variable. The second standard approach is to use a priori estimates of the uncertainties in the dependent variables to weight the least-squares fit, and obtain an experimental estimate of the number of degrees of freedom. This estimate can then be subject to statistical tests to evaluate the quality of the fit.

The treatment outlined in [4] and used here instead treats the least squares algorithm simply as a mathematical relationship between input and output variables. Thus, the propagation of uncertainty formula is used to propagate uncertainties in both the independent and dependent variables. This can be done with both weighted and unweighted least squares, and there are no constraints on the uncertainties or on correlations between them. The method does however require *a priori* estimates of the uncertainties.

2.2 First order ITS-90 interpolations

For the water-gallium and water-indium sub-ranges the ITS-90 interpolation equation is

$$W_{\mathrm{r}} = W - a(W - 1) . \qquad (3)$$

Although this equation has only one free parameter it is an interpolation through two points; (1,1) and $(W_X, W_{\mathrm{r},X})$, where $W_{\mathrm{r},X}$ is the reference resistance ratio at the one fixed point used to determine the parameter a, W_X is the measured resistance ratio at the same fixed point, and X indicates gallium or indium according to the sub-range chosen. In the case of the ITS-90 interpolation, once the value of a has been determined, (3) may be expanded in the form of (1), as

$$W_{\rm r} = W_{\rm r,H_2O}\left(\frac{W - W_X}{1 - W_X}\right) + W_{\rm r,X}\left(\frac{W - 1}{W_X - 1}\right) = W_{\rm r,H_2O}L_{\rm H_2O}(W) + W_{\rm r,X}L_X(W) \,. \tag{4}$$

Equation (4) clearly identifies the $F_i(W)$ functions in parentheses. In this case they are first order Lagrange polynomials, which are denoted as $L_{\rm H_2O}(W)$ and $L_X(W)$. Note that the reference resistance ratio for the triple point of water has been written as a variable rather than the number 1 to highlight the form of the equation.

When un-weighted least-squares is applied to the first order interpolation the value of the parameter a is determined by minimising

$$s^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(W_{\rm r,i} - W_i + a(W_i - 1)\right)^2 \,, \tag{5}$$

where the problem has been written so that s measures the standard deviation of the residual errors in the fit. The algebraic solution to this problem, is

$$W_{\rm r} = W + \frac{\sum (W_{\rm r,i} - W_i)(W_i - 1)}{\sum (W_i - 1)^2}(W - 1) \,, \tag{6}$$

which, after some manipulation, can be arranged in the form of equation (1) as

$$W_{\rm r} = W_{\rm r,H_2O}\frac{\sum (W_i - W)(W_i - 1)}{\sum (W_i - 1)^2} + \sum W_{\rm r,i}\frac{(W_i - 1)(W - 1)}{\sum (W_i - 1)^2} \,. \tag{7}$$

Where a single fixed point is used this simplifies to equation (4). For a first order least squares interpolation using two fixed points (mercury and gallium), the solution is

$$W_{\rm r} = W_{\rm r,H_2O}\left[\frac{(W_{\rm Hg} - W)(W_{\rm Hg} - 1) + (W_{\rm Ga} - W)(W_{\rm Ga} - 1)}{(W_{\rm Hg} - 1)^2 + (W_{\rm Ga} - 1)^2}\right]$$

$$+ W_{\rm r,Hg}\left[\frac{(W_{\rm Hg} - 1)(W - 1)}{(W_{\rm Hg} - 1)^2 + (W_{\rm Ga} - 1)^2}\right] + W_{\rm r,Ga}\left[\frac{(W_{\rm Ga} - 1)(W - 1)}{(W_{\rm Hg} - 1)^2 + (W_{\rm Ga} - 1)^2}\right] \tag{8}$$

$$= W_{\rm r,H_2O}F_{\rm H_2O}(W) + W_{\rm r,Hg}F_{\rm Hg}(W) + W_{\rm r,Ga}F_{\rm Ga}(W)$$

There are several interesting points that arise from this equation. Firstly, (8) clearly identifies (in square brackets) the sensitivity coefficients for uncertainties associated with the three fixed points (water, mercury and gallium). As with the Lagrange polynomials, these functions satisfy the relations

$$F_{\rm H_2O} + F_{\rm Ga} + F_{\rm Hg} = 1 \quad \text{and} \quad F_{\rm H_2O} + W_{\rm Ga}F_{\rm Ga} + W_{\rm Hg}F_{\rm Hg} = W \,, \tag{9}$$

and it is the second of these relationships, when applied to the propagation of uncertainty formula (see [5] for the derivation), that clearly identifies $F_{\rm H_2O}$ as the sensitivity coefficient for uncertainties associated with the triple point of water. Secondly, the sensitivity coefficient for uncertainties associated with the triple point of water (first square bracket in (8)) is not reduced at all by the least squares process. At $W = 1$ the sensitivity coefficient is still equal to 1.0 as with the Lagrange interpolation (see equation (4)). Further, in some cases the uncertainty may propagate further than in the Lagrange case. We can highlight this point by noting that the term is equal to zero when (from equation (7))

$$\sum (W_i - W)(W_i - 1) = 0, \tag{10}$$

which occurs when

$$W = W_{\text{ave}} = \frac{\sum W_i(W_i - 1)}{\sum (W_i - 1)}, \tag{11}$$

so that the zero occurs at a weighted average value of the W_i. Since in some cases $W_i - 1$ is negative, it is possible for either the denominator or the numerator of (11) to be zero. This very nearly occurs in the mercury-water-gallium case, where W_{ave} takes the physically unreasonable value of –0.006. Extreme values of W_{ave} show simply that the uncertainty in the triple point of water propagates almost constantly over the interpolation range. This case with indium and gallium is considered further in Example 1 below.

Thirdly, comparison of (8) with the equivalent Lagrange interpolation (4) shows that the sensitivity coefficient for the gallium point has been reduced by the factor

$$\frac{(W_{\text{Ga}} - 1)^2}{(W_{\text{Ga}} - 1)^2 + (W_{\text{Hg}} - 1)^2}, \tag{12}$$

and a similar factor attenuates the influence of the uncertainties associated with the mercury point. Recognition of these factors leads to the observation that (8) can be rewritten

$$W_{\text{r}} = \left\{ \frac{(W_{\text{Hg}} - 1)^2}{(W_{\text{Hg}} - 1)^2 + (W_{\text{Ga}} - 1)^2} \left[W_{\text{r,H}_2\text{O}} L_{\text{H}_2\text{O}}^{\text{Hg}}(W) + W_{\text{r,Hg}} L_{\text{Hg}}^{\text{Hg}}(W) \right] \right\}$$
$$+ \left\{ \frac{(W_{\text{Ga}} - 1)^2}{(W_{\text{Hg}} - 1)^2 + (W_{\text{Ga}} - 1)^2} \left[W_{\text{r,H}_2\text{O}} L_{\text{H}_2\text{O}}^{\text{Ga}}(W) + W_{\text{r,Ga}} L_{\text{Ga}}^{\text{Ga}}(W) \right] \right\}, \tag{13}$$

where the superscripts on the Lagrange polynomials refer to the fixed points (other than the triple point of water) used to determine the function. The two expressions within square brackets are first order Lagrange interpolations of the form of equation (4). It can be seen now that the least squares process develops an average of the two possible Lagrange interpolations available with the two fixed points (indium and gallium), with the weights in the average of the form of (12). Since both of the factors in (13) of the form of (12) are numbers less than one and summed in quadrature in the calculation of uncertainty, we can conclude that the total uncertainty propagated from these points is generally less than would be the case for a single pure Lagrange interpolation.

2.3 Second order interpolations

The second order Lagrange interpolation used by ITS-90 in the mercury-gallium, water-tin and water-zinc sub-ranges takes the form

$$W_{\text{r}} = W - a(W - 1) - b(W - 1)^2. \tag{14}$$

For direct ITS-90 interpolations this can be expressed in the form of equation (1) as:

$$W_{\text{r}} = W_{\text{r,H}_2\text{O}} \left[\frac{(W - W_X)(W - W_Y)}{(1 - W_X)(1 - W_Y)} \right] + W_{\text{r},X} \left[\frac{(W - 1)(W - W_Y)}{(W_X - 1)(W_X - W_Y)} \right] + W_{\text{r},Y} \left[\frac{(W - 1)(W - W_X)}{(W_Y - 1)(W_Y - W_X)} \right]$$
$$= W_{\text{r,H}_2\text{O}} L_{\text{H}_2\text{O}}(W) + W_{\text{r},X} L_X(W) + W_{\text{r},Y} L_Y(W) \tag{15}$$

where X and Y are the two fixed points used to determine a and b. The F_j functions are clearly identified in the square brackets and are second order Lagrange polynomials.

The least-squares solution to the problem is found by minimising

$$s^2 = \frac{1}{N-2}\sum_{i=1}^{N}\left(W_{r,i} - W_i + a(W-1) + b(W-1)^2\right)^2 \tag{16}$$

which leads to the formula

$$W_r = W + \frac{(W-1)}{\Delta}\left[\left(\sum_i (W-1)^4\right)\left(\sum_j (W_{r,j}-W_j)(W_j-1)\right)-\left(\sum_i (W-1)^3\right)\left(\sum_j (W_{r,j}-W_j)(W_j-1)^2\right)\right]$$
$$+ \frac{(W-1)^2}{\Delta}\left[\left(\sum_i (W-1)^2\right)\left(\sum_j (W_{r,j}-W_j)(W_j-1)^2\right)-\left(\sum_i (W-1)^3\right)\left(\sum_j (W_{r,j}-W_j)(W_j-1)\right)\right] \tag{17}$$

where

$$\Delta = \left(\sum_i (W_i-1)^2\right)\left(\sum_i (W_i-1)^4\right)-\left(\sum_i (W_i-1)^3\right)^2 .$$

By expanding this equation in the form of (1) we can identify the sensitivity F_j functions for the fixed points (other than the triple point of water) as

$$F_j(W) = \frac{(W_j-1)(W-1)}{\Delta}\sum (W_i-1)^2(W_i-W_j)(W_i-W) . \tag{18}$$

The $F_{H_2O}(W)$ function is then most simply determined using the first of the identities

$$\sum F_j = 1, \quad \sum W_j F_j = W, \quad \sum W_i^2 F_j = W^2 . \tag{19a-c}$$

As with the F_j for the first order case the weights for the F_j decrease as the number of fixed points increases, again indicating an averaging process for the determination of the constants. Also, as with the first order case, the water function does not decrease with N. This can be seen by noting that all of the F_j for the other fixed points have a zero at $W=1$, and therefore to satisfy (19a), the water function must always be equal to 1.0 at $W=1$.

For the specific case of a least squares fit using the tin, cadmium and zinc points the solution can be written in the form of (1) to highlight the sensitivity coefficients, but a far more compact form is

$$W_r = \left\{\frac{(W_{Sn}-1)^2(W_{Zn}-1)^2(W_{Sn}-W_{Zn})^2}{\Delta}\left[W_{r,H_2O}L_{H_2O}^{Sn,Zn}(W)+W_{r,Sn}L_{Sn}^{Sn,Zn}(W)+W_{r,Zn}L_{Zn}^{Sn,Zn}(W)\right]\right\}$$
$$+\left\{\frac{(W_{Cd}-1)^2(W_{Zn}-1)^2(W_{Cd}-W_{Zn})^2}{\Delta}\left[W_{r,H_2O}L_{H_2O}^{Cd,Zn}(W)+W_{r,Cd}L_{Cd}^{Cd,Zn}(W)+W_{r,Zn}L_{Zn}^{Cd,Zn}(W)\right]\right\} \tag{20}$$
$$+\left\{\frac{(W_{Sn}-1)^2(W_{Cd}-1)^2(W_{Sn}-W_{Cd})^2}{\Delta}\left[W_{r,H_2O}L_{H_2O}^{Sn,Cd}(W)+W_{r,Sn}L_{Sn}^{Sn,Cd}(W)+W_{r,Cd}L_{Cd}^{Cd,Sn}(W)\right]\right\}$$

where

$$\Delta = (W_{Sn}-1)^2(W_{Zn}-1)^2(W_{Zn}-W_{Sn})^2 + (W_{Cd}-1)^2(W_{Zn}-1)^2(W_{Zn}-W_{Cd})^2 + (W_{Sn}-1)^2(W_{Cd}-1)^2(W_{Sn}-W_{Cd})^2 .$$

In this form we can see again that the least squares process has formed an average of all possible Lagrange interpolations of the form of (15) (identified in square brackets). As with any average we can expect the uncertainty in the average to be less than that of any of the contributing terms. We must be careful however; because the three interpolations identified in (20) share fixed point measurements some of the terms in (20) are not independent. To identify the sensitivity coefficients for each fixed point measurement simply gather all of the coefficients of the respective reference resistance ratio. The corresponding Lagrange polynomials are also identified by subscript. Accordingly, the sensitivity coefficient for uncertainties in the tin point is the linear sum of the terms that include $L_{\text{Sn}}^{\text{Sn,Zn}}(W)$ and $L_{\text{Sn}}^{\text{Sn,Cd}}(W)$, and the sensitivity coefficient for uncertainties in the triple point of water is the linear sum of the first term in each of the three Lagrange interpolations.

Example 3 below considers the use of several redundant points for the water-zinc sub-range.

2.4 Higher order interpolations

The algebra for the second order interpolations is quite onerous, suggesting that the algebra for third order interpolations or higher would be next to impossible to manage. However, some simple observations lead to a simple method for determining the sensitivity coefficients. (The same generalisation applies to weighted least squares.)

In the matrix formulation of least squares the solution to the second order problem is

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \sum (W_i - 1)^2 & \sum (W_i - 1)^3 \\ \sum (W_i - 1)^3 & \sum (W_i - 1)^4 \end{pmatrix}^{-1} \begin{pmatrix} -\sum (W_{\text{r},i} - W_i)(W_i - 1) \\ -\sum (W_{\text{r},i} - W_i)(W_i - 1)^2 \end{pmatrix}. \tag{21}$$

To identify the $F_j(W)$ sensitivity coefficient we could (as we did above) carry out the matrix inversion and multiplications and then identify and separate the term for which the coefficient is $W_{\text{r},j}$. However, we can do this more efficiently by recognising that the term we want is given by one element in the summation of the vector on the RHS of the equations. Hence, the sensitivity coefficients for all the fixed points except the water triple point are given by

$$F_j(W) = -a_j(W - 1) - b_j(W - 1)^2 \tag{22}$$

where

$$\begin{pmatrix} a_j \\ b_j \end{pmatrix} = \begin{pmatrix} \sum (W_i - 1)^2 & \sum (W_i - 1)^3 \\ \sum (W_i - 1)^3 & \sum (W_i - 1)^4 \end{pmatrix}^{-1} \begin{pmatrix} -(W_j - 1) \\ -(W_j - 1)^2 \end{pmatrix}. \tag{23}$$

This is a simple operation since the inverted matrix is purely numerical and is used to calculate not only the sensitivity coefficients for all values of j, but also the solution to the least-squares problem itself. The sensitivity coefficient for the water triple point can be found from the first identity (19a) or as

$$F_{H_2O}(W) = W - a_{H_2O}(W - 1) - b_{H_2O}(W - 1)^2 \tag{24}$$

where

$$\begin{pmatrix} a_{H_2O} \\ b_{H_2O} \end{pmatrix} = \begin{pmatrix} \sum (W_i - 1)^2 & \sum (W_i - 1)^3 \\ \sum (W_i - 1)^3 & \sum (W_i - 1)^4 \end{pmatrix}^{-1} \begin{pmatrix} \sum W_i(W_i - 1) \\ \sum W_i(W_i - 1)^2 \end{pmatrix} \tag{25}$$

Note that the second option follows from the identification of the terms in (21) that do not depend on the $W_{\text{r},i}$ values. In addition, it can also be seen to be the application of the second identity (19b).

The procedure is readily generalised to all linear interpolations of any order, including weighted least-squares.

3. Examples

Example 1: Mercury-Water-Gallium sub-range

Figure 1 shows the total propagated uncertainty for the mercury-water-gallium range for three different styles of interpolation. Firstly, with second order Lagrange interpolation (according to ITS-90 definition), secondly with two first order Lagrange interpolations (according to ITS-90 definition only for the water-gallium sub-range), and thirdly with a first order least squares fit. Note that the resistance ratio is the natural variable for propagating uncertainties so the horizontal and vertical axes in the graph has been scaled according to $T_{90}(W)$ of dT/dW respectively so that the results can be presented in terms of temperature.

Figure 1 illustrates that the least-squares approach does indeed offer a reduced propagated uncertainty despite the low number of degrees of freedom. In this example, there is one parameter fitted using two fixed-point measurements, so there is only one degree of freedom. A second benefit is the improved uncertainty with extrapolation, which in this case arises primarily due to the use of a first order interpolation rather than second order. Although the uncertainty in water triple point value propagates almost constantly in the least squares case, the low value of the uncertainty means that this is not a major factor in the propagated uncertainty.
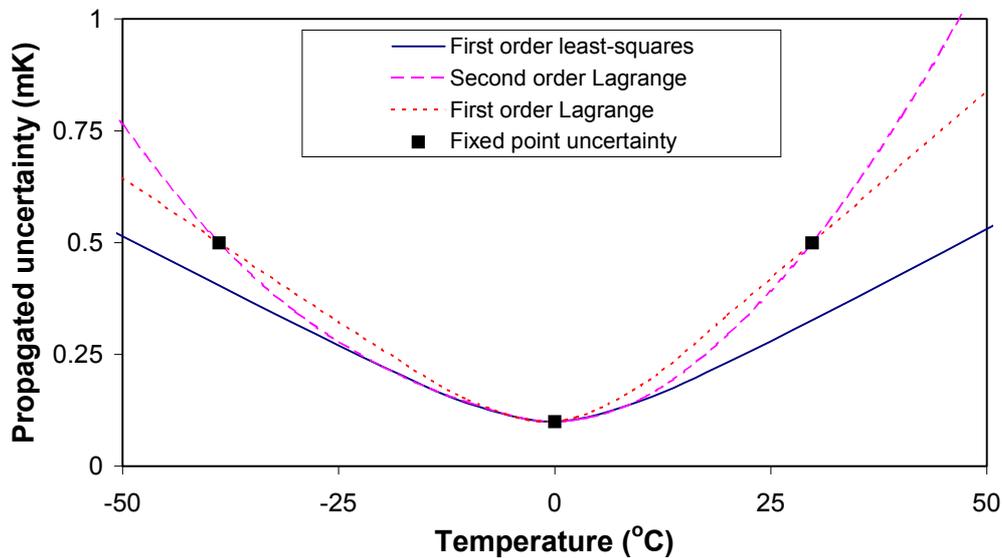

Figure 1: Comparison of the total propagated uncertainty for ITS-90 (Lagrange) and least-squares interpolation over the range between the mercury and gallium points. It is assumed that the uncertainty in the water triple point is 0.1 mK and the uncertainties in the other fixed points is 0.5 mK. In this case the benefits of the least squares approach are apparent at the ends of the interpolation range and when extrapolating. Note that the Lagrange interpolations pass through the marked points representing the uncertainties in each of the fixed points while the least squares uncertainties are less.

Example 2: Water-indium sub-range

Figure 2 shows the total propagated uncertainty for the water-indium sub-range firstly with a first order Lagrange interpolation (according to ITS-90 definition) and secondly with the least squares applied to the first order interpolation using gallium as the redundant fixed point.

This particular interpolation is an example where little is gained from the unweighted least squares approach. At first sight, the small difference between the two curves in Figure 3 may be surprising. The explanation lies in the weighting given to each of the two possible Lagrange interpolations used in the least squares solution (as suggested by equation (13)),

$$\frac{(W_{Ga}-1)^2}{(W_{Ga}-1)^2+(W_{In}-1)^2} \quad \text{and} \quad \frac{(W_{In}-1)^2}{(W_{Ga}-1)^2+(W_{In}-1)^2}$$

respectively. The ratio of the weights is more than 26. The impact of the gallium point is further reduced in the total uncertainty because the weights are added in quadrature, yielding a reduction in uncertainty of only a few percent near the indium point. The heavier weight given to the indium point tells us that the addition of the gallium point to the least-squares sum contributes very little new information to the value of the calibration constant a. With weighted least-squares and a more realistic value for the gallium point uncertainty (the lower curve in Figure 2) the disparity between the indium point and the gallium point weighting is not so great. Note that if the two fixed points are given equal weighting at the indium point, the total uncertainty should be reduced to 70.71% of the Lagrange value. With a low uncertainty assigned to the gallium point and weighted least squares, the improvement in uncertainty approaches this value.

A curious feature of the weighted least squares, is that the uncertainty in the extrapolated values is increased for temperatures below the triple point of water. This seems to be an artefact of the ITS-90 definition of the interpolation equation, i.e. forcing the interpolation through (1,1) so that the sensitivity coefficient for the gallium point must pass through zero at W=1. With a general first order polynomial least squares the uncertainty is less everywhere.
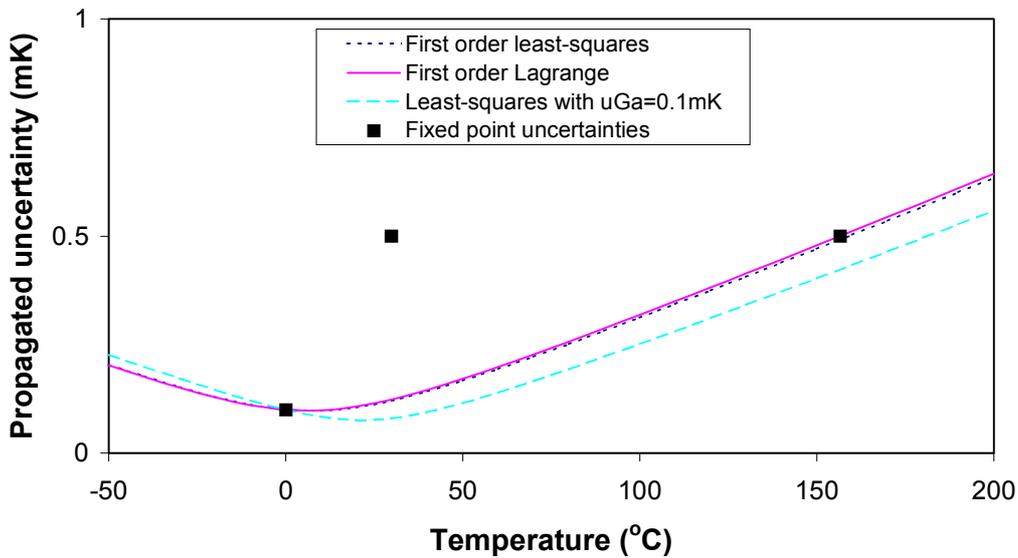

Figure 2: The total propagated uncertainty for the ITS-90 interpolation and the least-squares interpolation over the water-indium sub-range. Two least squares curves are shown, one for un-weighted least squares, one with weighted least squares. For all curves, the uncertainty associated with the triple point of water is 0.1 mK. The two least squares curves correspond to uncertainties in the gallium point of 0.5 mK and 0.1 mK respectively.

Example 3: water-zinc sub-range

Figure 3 shows the total propagated uncertainty for a second order ITS-90 interpolation and a number of least squares interpolations over the water-zinc sub-range. The upper curve shows the uncertainty for the Lagrange interpolation (according to ITS-90 definition), the lower curve a least squares interpolation with additional fixed point data from the gallium, indium and cadmium points. The three curves in between show the total uncertainty for the cases with least squares interpolation and a single additional fixed point. These three curves correspond to solutions of the form of Equation (20). Note that for all three of the cases with a single redundant fixed point the uncertainty is everywhere less than for the pure Lagrange case. In addition, the least squares interpolation with the three redundant fixed points is everywhere less than all of the other curves.
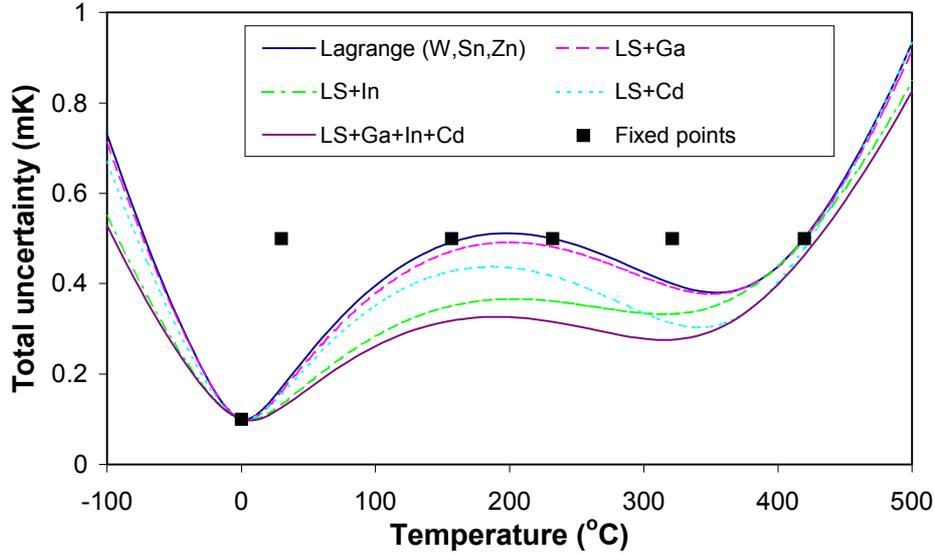
Figure 3: The total propagated uncertainty over the water-zinc sub-range with Lagrange interpolation and a variety of least squares interpolations. The uncertainty assigned to the triple point of water is 0.1 mK with 0.5 mK assigned to all of the other fixed points. The uncertainty in each fixed point is also indicated.

4. Discussion and Conclusions

4.1 Observations

The paper has described a method for calculating the total uncertainty and sensitivity coefficients for least squares interpolations using the ITS-90 SPRT interpolating equations, and provided examples for un-weighted least squares for first and second order SPRT interpolations of ITS-90. The procedure is readily extended to include weighted least squares fits.

It is found for the interpolations investigated, (un-weighted least squares in first and second order ITS-90 equations) the addition of redundant fixed points and the use of least squares reduces the total propagated uncertainty within the interpolation range of an interpolation. The algebraic expansions of the least squares interpolation for the cases with one extra point suggest that the least squares method provides an average of all possible interpolations of the same order based on all possible combinations of the fixed points measured. Because the least squares solution is an average, the total uncertainty will be less. It is concluded that in general for interpolation (as opposed to extrapolation) any over-determination of the calibration constants is beneficial. While this may be in contradiction with least squares lore, it perhaps reflects on the relatively poor quality of Lagrange interpolations rather than highlight a misunderstanding of least squares. Indeed one could classify a Lagrange interpolation as the least squares solution to a problem distinguished from other least squares solutions by the fact that it has zero degrees of freedom.

The ITS-90 definitions of the interpolations introduce a single mathematical artefact into the interpolations that distinguishes them from general least squares fits. The forcing of the interpolations through the point (1,1) causes the sensitivity coefficients for uncertainties associated with fixed points (other that the triple point of water) to pass through zero at $W =1$. The consequences appear to be that uncertainties associated with fixed points relatively close to the triple point of water can be amplified as compared with a general polynomial least squares. The practical consequence is that least squares may not always yield lower uncertainties with extrapolation.

One of the limitations in the construction of ITS-90 was the need to choose sub-ranges for which available fixed points are evenly distributed. This is necessary to prevent the undesirable amplification of uncertainties that occurs when the fixed points are not evenly distributed. The least squares approach allows such points to be included in the measurements. Note that the leading multiplying factors in equations (13) and (20) appear to derate

interpolations that result in highly amplified uncertainties. (The use of a logarithmic variable for low temperature interpolations may have the same benefits).

4.2 The benefits of Least squares

The use of redundant fixed points has a number of benefits to the calibration process:

- The extra data provide a consistency check of the quality of other fixed point measurements.
- It enables an assessment of the interpolating quality of the thermometer under test.
- It provides users with flexibility in the choice of interpolation equations.

Additionally, if least squares analysis is used to determine the calibration constants for an SPRT:

- The total uncertainty propagated from uncertainties in the fixed point measurements calibration is reduced.
- The standard deviation of the residuals to the fit (Equations (5) and (16)) provides a measure of the non-uniqueness of the scale realised on the SPRT (see discussion below).

4.3 Non-uniqueness arising from interpolation error

It must be noted that evaluating the uncertainties at each fixed point and propagating them according to the formulae derived does not complete the calculation of the standard uncertainty. In addition, one must also consider the non-uniqueness arising from interpolation error, i.e. the equation for the thermometer not reflecting the true behaviour of the thermometer. Interpolation error depends on the fixed points chosen, and the form of the interpolating equation chosen. Thus, in addition to the uncertainties associated with the fixed points, it makes a significant contribution to the various types of non-uniqueness identified in [6].

In principle, the method of least squares provides the means to assess the interpolation error arising in the thermometer under test (i.e. Type 1 non-uniqueness), since the standard deviation of the fit will include such errors. However, the utility of this approach is perhaps questionable. Firstly, the standard deviation may have only one degree of freedom so that any estimate of expanded uncertainty based on the Type A assessment will have a coverage factor of $k = 14$, which is probably too large for practical estimates of uncertainty. Secondly, the uncertainty calculation would include only effects due to the thermometer under test, whereas the accuracy with respect to all other realisations of ITS-90 requires an additional estimate of the other types of non-uniqueness. Although the standard deviation may be useful in the identification of thermometers that are good interpolators, the best assessment of uncertainty is a Type B assessment based on non-uniqueness studies such as that presented in the BIPM supplementary information [7]. This study of course only covers the range below 273.16 K, and as yet there is no corresponding data of comparable detail for the temperature range above 273.16 K.

One of the possible concerns with the use of least squares it that it might somehow give rise to non-uniqueness that is fundamentally different from that obtained with the direct ITS-90 interpolations. Equations (13) and (20) show that the any interpolation error arising from the use of least squares is simply a weighted sum of the errors arising from individual interpolations. Therefore, the interpolation error is certainly no worse than that for the direct interpolations and probably a little reduced because of the averaging process. A major difference in the interpolation errors arises because the fitted equation does not necessarily pass through any of the measured points. Consequently, whereas there is almost zero interpolation error for temperatures near fixed points with the direct interpolation, with least squares the interpolation errors will be distributed over all temperatures.

4.4 Further work

Further work is required in at least two areas to develop a clearer understanding of the possible limitations in the use of least squares. Firstly, there must be more algebraic or numeric experiments of the kind given here, for other ITS-90 interpolations, with both weighted and un-weighted least squares, and more than one redundant fixed point. In principle, this is not difficult since the process can be largely automated using the general formulae given in Section 2.3. Perhaps also this is not essential since it is possible for a user to evaluate the uncertainty for any equation and any combination of fixed points, and choose only those interpolations for which the uncertainty is satisfactory.

Secondly, there must be work done on the non-uniqueness associated with both direct ITS-90 interpolations and least squares interpolations at temperatures above 0 °C. This is currently severely limited by the paucity of published papers giving W versus W data, i.e. measured resistance ratios for different thermometers at the same

temperatures. The Ward and Compton data [8] and the data emerging from the CCT-KC2 comparison [9] both cover the low temperature regime well, but as yet there is no comparable data for temperatures above 0 °C.

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