Application of Data Fusion techniques to Thermometry Data

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ABSTRACT

The ITS-90 scale is an internationally-agreed protocol for relating thermodynamic temperature to its practical implementation by means of Platinum Resistance Thermometers (PRTs). The key step is the calibration of PRTs at given Fixed Points of thermodynamic temperature. Thermal metrologists are continually refining the precision of these fixed points, with consequent effects on the temperature scale. The functions which are used to calibrate the PRTs are also under review, and comparison exercises are regularly undertaken to support these activities. If a revision to the scale is proposed, it needs to be supported by reliable evidence and data fusion can help in this regard. In particular, it may determine consistency between sources of data and motivate improvements to the functional approximation of the data. This report describes some numerical experiments which were performed to determine the consistency of the data sources and to develop a good overall approximation to the data, which was then compared with the ITS-90 approach.

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1 Introduction

The aims of the project for which this report constitutes the final deliverable are to

(1) Determine the consistency of a set of PRT (platinum resistance thermometer) measurements of (electrical) resistance and temperature (Figure 1), where the measurements were provided by a number of sources (Figure 2)[1];

(2) Derive a method for aggregating the data in a way which takes account of its error behaviour;

(3) Determine a faithful representation of the data, with estimates of uncertainty according to the ISO *Guide to the Expression of Uncertainty in Measurement* (GUM) [10].

This document meets two requirements, viz., a prototype representation of the NZMSL (New Zealand Measurement Standards Laboratory) data *and* a report describing the approach used.

More generally, the problem addressed is but one example of *data fusion* problems in metrology, where the metrologist combines data from several sources, evaluates the evidence in favour of each source, and develops an understanding of the combined data which is greater than the understanding which might be derived from each data source individually. It is supported in this sense by the presence of a model (the ITS-90 temperature scale [9]).

The design aims are discussed in greater detail in reference [4]. This report provides the following

- A description of the raw data, in Section 2;
- A discussion of data fitting over the entire temperature range, looking for inconsistencies source by source, in Section 3;
- A discussion of comparison with ITS-90 [9] to motivate a more "physically informed" data analysis, in Section 4;
- A representation of the temperature data set, analogous to that of ITS-90, in Section 5.
- Concluding remarks and scope for further work in Section 6.

More information on ITS-90 is provided in Appendix A and in references [9,14].

2 The raw data

The following observations were made concerning the data.

1. There are 687 data points distributed among 39 sources.
2. The distribution of the points is far from uniform (see Figure 1), either in terms of number of data points per source, or the spacing of the data points in each source. Furthermore, the data is relatively sparse at high temperatures.
3. No single source extends over the entire range of the data (Figure 2).
4. Some data points appear to be replicated across a number of sources (Figure 2), particularly those relating to fixed points in the ITS-90 scale, but most are not.

The plot of the data (Figure 1) indicated an apparent functional relationship between resistance and temperature. Statistical inferences would be possible once this relationship had been

[1]The data was assembled by Dr J V Nicholas, of New Zealand's Measurement Standards Laboratory.

established.

It was clear even from this preliminary analysis that a simple analysis of variance based on replications between sources, or even between individual points, would be insufficient and that fitting would be needed both to determine the data inconsistencies (if any) and to provide a representation of the data.

3 Preliminary analysis of the aggregate data

The entire data set was aggregated, viz., fused in a way which initially regards all data sources as having comparable credibility. It was then submitted for analysis, fitting temperature, T, as a function of resistance, R. From the nature of the data, a polynomial in R was chosen, with a log-transformation of both dependent and independent variables, such that the observation equations are

$$\log(T_i) = P_n(\log(R_i)) + f_i, \quad (1)$$

where (T_i, R_i) is the i^{th} data point, P_n is a polynomial of degree n and f_i is the transformed data error e_i in T_i. It can be shown that $f_i \approx \hat{f}_i = T_i e_i$, an approximation which is very good for small-residual problems, which is the case here; see Appendix M. Polynomial fits of degrees $n = 0, 1, .., 50$ were computed. The Table in Appendix C summarises the behaviour of polynomial fits to such data, using the approximate f_i above, for different polynomial degrees; see also [1,2] for more information on regression model selection. The chosen degree (= 19) is associated with

(a) a root-mean-square (RMS) residual error which is near-minimal; the RMS has settled to an approximately constant value (Figure 3) which is consistent with the error in the data,
(b) residuals which appear random, in the sense that no obvious systematic behaviour remains, and
(c) no apparent oscillation (of the polynomial fit) between the data points.

In respect of (c), oscillation first appears at the high temperature end as the degree of the fit is successively increased, since the data is more sparse in this region.

No account is taken in the above analysis of the possibility that each source (and possibly each data point) might have its own unique data error structure. This is because the data is unweighted[2] and hence the whole data set is considered to be consistent; in statistical terms, the following assumptions are made

(a) the f_i are members of the same population distribution, and
(b) the error distribution is symmetric (zero mean) (since least-squares fitting is used). Indeed, if the error distribution is Gaussian, the least-squares estimate will be both unbiased and statistically efficient.

With regard to assumption (a) above, the following cross-validation algorithm was used to check the consistency of the data:

(a) Determine the "best" least-squares fit using all data, fused as above, recording the polynomial degree n and the RMS residual, RMS. The RMS value is represented by the

[2] "Weights" T_i are introduced to recover from a gross bias in the residuals which would result from minimising the sum of squares of the e_i instead of the f_i, but these take no account of the (unknown) variance profile of the original e_i.

continuous horizontal line in Figure 4.

(b) For each source k

(c) Determine the least-squares fit, with the same polynomial degree n, to all the data *excluding* source k. This is equivalent to fusing all the data with equal weight, except that the data in source k is accorded zero weight. Record the RMS residual, RMS(k) and plot the residuals (individual points in Figure 4).

(d) Compute the *influence* of source k on the overall fit, which is defined to be the difference RMS-RMS(k).

(e) Identify, for further analysis, any source whose (unsigned) *influence* is considered "large" and/or for which a relatively large residual disappears when that source is excluded.

The null hypothesis is that each source is consistent with the others, such that exclusion of that source alone does not materially affect the overall fit. The method is intuitively attractive, but there are several issues which need careful consideration

- The null hypothesis will be rejected only if there is sufficient evidence to the contrary. Therefore, evidence is needed (e.g., changes in the shape of the fit, the RMS residual, the disappearance of a single relatively large residual) and a method of judging its significance.
- Some sources will, by their nature, have an enormous effect on the fit. For example, source 37 contains just two points, one of which is the isolated point at the end of the range. In such a case, cross-validation will merely serve to confirm what is already known, which is that source 37 is critical to the fit, without saying much about how consistent it is.
- If a source does appear inconsistent with its peers, this could be caused by
  - (a) the presence of one or more discordant values in that set;
  - (b) a systematic error affecting all values from that source;
  - (c) the influence of factors such as the span of the data from that source, the number of points, etc.

Therefore the source *influence* is difficult to interpret, since the least-squares fit when different sources have been excluded, even for fixed degree, will be different in general. The situation is similar to that of univariate outlier detection where the population statistics are unknown: the tests are based solely on the sample values. However, the larger the *influence*, the more likely it is that it is caused by an anomalous source. The sign of the *influence* is a guide to whether the source is "better" or "worse" than average, being negative or positive, respectively. Therefore, for the purposes of this analysis, a large, positive *influence value* is significant.

The above cross-validation algorithm was implemented and executed for $n = 19$, the selected degree. From the table and plots in Appendix D, it can be seen that

(a) There is a generally high degree of agreement between the RMS residuals (Figure 4), apart from a limited number of sources, where it appears that removal of the source materially changes the RMS of the remaining data.

(b) There are instances in which the removal of a source, particularly sources 38 and 39, causes an appreciable decrease in the RMS residual calculated for the remaining points (Figure 4 again).

(c) More generally, sources 32, 33, 35, 38 and 39 each have a large *influence* since they relate to higher temperatures, where the residuals are usually larger.

It also appears that source 3 contains a rogue point, with $R = 1.6418$ and $T = 47.1618$ K, at

aggregate position 32 in the overall data set (Figures 5-8). When this point is removed from the source and treated as a separate source (source 40), the following occurs. The reduced source 41 (see the table and the plot in Appendix D) no longer contains a wild point (note the loss of an isolated relatively large residual near the middle of the range of log(R)), the *influence* of the reduced source is less than that of the full source, and it is clear that exclusion of source 40 has almost the same effect as exclusion of source 3, implying that much of the contribution from source 3 to the RMS residual is due to a single point.

Therefore, this analysis has indicated that

(a) a single point in source 3 is suspect,

(b) generally, the dependence of the error upon source membership is less than its dependence on temperature, and

(c) the resulting variance profile of the residuals appears not to be constant.

The evidence in favour of (a) is not conclusive, largely because it is confounded by the effect of (c). Hence a new, more informed method of analysis is needed to prove or disprove (a) and to support and, if appropriate, make use of (b) and (c).

4 Use of ITS-90 as a reference function

ITS-90 [9] provides

- A reference function for the calibrated response of a reference thermometer. The calibration curve is *fully specified* and the curve passes through certain fixed points defined by the standard;
- The functional form of deviation functions which are used by the metrologist to relate a particular thermometer to the reference thermometer. The parameters of the *deviation functions* are to be determined by fitting.

Strictly, two reference functions are defined, one for low temperature (from the triple point of equilibrium hydrogen (13.8033 K) to the triple point of water (273.16 K)) and the other for high temperature (from the triple point of water (0.01 °C) to the freezing point of silver (961.78 °C)). The functions are continuous in value at 273.16 K. In Appendix A reference functions both for the low and the high temperature ranges are illustrated.

Another feature is that *resistance ratio*, W, rather than resistance, R, is used. The resistance ratio is the ratio of the measured PRT resistance to its resistance at 273.16 K (equivalently, 0.01 °C).

The ITS-90 low temperature reference function for temperature takes the form of a polynomial in the sixth root of resistance ratio, W. The high temperature reference function is a polynomial in W. The independent variable in each case is approximately normalised and the polynomial is written in its monomial (power series) form.

These considerations motivated the following strategy:

(1) Comparison between the measured data and the ITS-90 reference in order to estimate the variance profile of the data;

(2) Use of a fitting strategy analogous to ITS-90, viz.
   (a) Using W instead of R;
   (b) Splitting the data into low temperature and high temperature ranges;
   (c) Use of $W^{1/6}$ and W as the independent variable in the low temperature and high temperature ranges, respectively;
   (d) Separate fitting to data in each range;

(3) Improving and validating the representation [9], viz.

(a) Use of a Chebyshev representation [6], instead of the monomial representation, of the polynomials;
(b) Use of weights based on (1) above;
(c) Removal of clearly invalid points;
(d) Use of *within-family* model validation by comparing fits for different polynomial degrees;
(e) Further model validation based on statistical tests on the residuals.

(4) Providing estimates of uncertainty of the fit at the ITS-90 fixed points and the Chebyshev coefficients for both temperature ranges as follows:

In the low temperature range (that for which $0.00119007 \le W \le 1$), the transformed independent variable satisfies $0.32553392 \le W^{1/6} \le 1$ and the Chebyshev series has the form

$$T_l(u) = \frac{1}{2}a_0 + \sum_{j=1}^{n} a_j \theta_j(u), \qquad (2)$$

where a_j are the Chebyshev coefficients, u is the normalised $W^{1/6}$ and θ_i is the Chebyshev polynomial basis function[3] of degree j in the normalised variable u. In the high temperature range (that for which $1 \le W \le 3.3760086$), the Chebyshev series has the analogous form

$$T_h(u) = \frac{1}{2}b_0 + \sum_{j=1}^{n} b_j \theta_j(u), \qquad (3)$$

where u is the normalised W. In the case of (1) above, temperature deviations $d_i^{(90)}$ were calculated as follows:

$$d_i^{(90)} = T_i - f^{(90)}(W_i), \qquad (4)$$

where $f^{(90)}(W_i)$ is the appropriate ITS-90 reference function evaluated at W_i. The (piecewise linear) variance profile is obtained by

(i) grouping those points whose W_i lie in each interval delimited by successive pairs of fixed points defined by ITS-90, and
(ii) calculating the variance of the $d_i^{(90)}$ in each group.

The weights used for fitting are the inverse of the square roots of these variances, which again have a piecewise linear dependence on W.

Because of Formulae (2) and (3), it is clear from comparisons of Figures 9 and 10 how the transformation of W, for $W \le 1$, makes the data more suitable for approximation by a polynomial. In Figure 11 it is clear that, for $W \ge 1$, no such transformation appears necessary, since the underlying function already appears "polynomial-like".

It is also clear that some points lie outside the range of resistance ratios and temperatures covered by ITS-90. These points were excluded from the analysis, not because of any inherent faults, but because no ITS-90-inspired reference point is available for comparison. Coincidentally, one of these points is the isolated point at the high temperature end, which was recommended for exclusion (see Appendix A). One of the points at the low end just fails to be included, being approximately 0.01 K below the relevant fixed point; however, temperature measurements in this region have a typical uncertainty of about 0.1 mK (see Appendix A) which means that the point can be regarded as lying outside the range of resistance ratios and temperatures covered by ITS-90. A total of six points were excluded using this criterion. See the

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[3]Since T is reserved for *temperature*, $\theta_j(u)$ is used to denote the Chebyshev polynomial of the first kind of degree j in u.

table in Appendix F for details.

Inspection of Figures 12 and 13 suggests that the variance of the residuals generally increases with temperature, and this fact can be seen more clearly in Figures 14 and 15.

In Appendix H, it is clear in Figure 16 that the RMS residual, fitting T as a polynomial in $W^{1/6}$, has stabilised at about degree 12. It is clear from comparison of Figures 17 and 18 that there is little to be gained from using degree 16 (the degree specified by ITS-90 in the low temperature range) compared with the chosen degree 12.

Inspection of both residual plots shows a generally satisfactory pattern except for one point, which is precisely the point which was flagged as suspect during the preliminary analysis of the aggregate data. Removal of this point provides an altogether better fit (see Figures 19-21), without changing the choice of best degree.

Further model validation was performed by calculating various statistical measures for the fits. These included the skewness of the set of weighted residuals, which was consistent with the set being a sample from a Normally-distributed population. This is further evidence of the quality of the fit.

The situation in respect of the high temperature range is similar. It is clear from Figure 22 that the RMS residual saturates earlier; a degree of 6 was chosen which satisfies the validation criteria and is as good as (indeed the 95% uncertainty bands are better than) the fit at the ITS-90 recommended degree (which is 10); compare Figures 23 and 24.

An additional form of validation is possible by looking at the behaviour of the residuals and seeing how they compare with the confidence limits. In particular, if the statistical assumptions are correct, approximately 5% of weighted residuals (hence points) should lie outside the 95% confidence limits, and 1% of points lie outside the 99% confidence limits. As reported in Appendix K, there is good agreement with theory in this regard.

A further form of validation is obtained by comparison of the best representation of the data with the ITS-90 reference fixed points (see Appendix L). There is no guarantee that the ITS-90 reference function is the best representation, but it should be reasonably close. This is the case, as inspection of the table in Appendix L will reveal. One interesting factor is that there is a discontinuity in temperature which is less than the predicted uncertainty of temperature, so the discontinuity is not significant. Figures 25 and 26 illustrate the calculated differences.

5 Results

The following tables list the Chebyshev coefficients in both temperature ranges for the selected polynomial fits (Tables I and II), together with their standard uncertainties and 95% confidence limits. The standard uncertainties and 95% confidence limits on the representation of T computed from these coefficients at reference values of resistance ratios are provided in Table III. Note that the uncertainty is insignificant with respect to the likely measurement error in T.

Table I - Chebyshev coefficients for the low temperature range [$0.32553392 \leq W^{1/6} \leq 1$]			
Coefficients		Standard uncertainties on the coefficients	Confidence limits - 95 %
$\frac{1}{2}A_0$	94.2731040	0.0000860	± 0.0001686
A_1	113.2086448	0.0001246	± 0.0002442
A_2	45.5908091	0.0000845	± 0.0001656
A_3	16.0238163	0.0001235	± 0.0002421
A_4	3.7310064	0.0001317	± 0.0002581
A_5	0.4455417	0.0001272	± 0.0002493
A_6	-0.1284914	0.0001342	± 0.0002630
A_7	-0.0148637	0.0001167	± 0.0002287
A_8	0.0167316	0.0000885	± 0.0001735
A_9	0.0173996	0.0000981	± 0.0001923
A_{10}	-0.0000540	0.0001050	± 0.0002058
A_{11}	-0.0020377	0.0000962	± 0.0001886
A_{12}	-0.0015435	0.0000701	± 0.0001374
- Coefficients for equation (2)			

Table II - Chebyshev coefficients for the high temperature range [1 ≤ W ≤ 3.3760086]			
Coefficients		Standard uncertainties on the coefficients	Confidence limits - 95 %
½B_0	594.3995746	0.0011997	±0.0023514
B_1	329.6642377	0.0018849	±0.0036944
B_2	8.8666663	0.0008393	±0.0016450
B_3	0.4950442	0.0009154	±0.0017942
B_4	0.0608356	0.0014057	±0.0027552
B_5	0.0062821	0.0011825	±0.0023177
B_6	-0.0020281	0.0005713	±0.0011197
- Coefficients for the equation (3)			

Table III - Standard uncertainties of the resulting Chebyshev polynomial representations evaluated at reference values of resistance ratios according to ITS-90		
Wr(T90)	Standard Uncertainties [K]	Confidence limits - 95 % [K]
Low Temperature Range : T ≤ 273.16 K		
0.00119007	0.00017690	± 0.00034672
0.00229646	0.00008324	± 0.00016315
0.00423536	0.00004940	± 0.00009683
0.00844974	0.00007642	± 0.00014978
0.09171804	0.00011325	± 0.00022196
0.21585975	0.00015569	± 0.00030514
0.84414211	0.00030749	± 0.00060268
1.00000000	0.00032215	± 0.00063142
High Temperature Range : T ≥ 273.16 K		
1.00000000	0.00041679	± 0.00081690
1.11813890	0.00027669	± 0.00054231
1.60980190	0.00041966	± 0.00082254
1.89279770	0.00051483	± 0.00100907
2.56891730	0.00152567	± 0.00299031
3.37600860	0.00129880	± 0.00254564

6 Conclusions and scope for further work

The following objectives were achieved using concepts from data fusion, model validation and statistics:

- to deduce the underlying accuracies of the various contributions to the overall data set;
- to identify any inaccuracies present, and hence provide information regarding their resolution;
- to provide weights for the various contributions, thus permitting their unbiased aggregation;
- to compute families of possible data representations;
- to select a representation from the family that best achieves (practical) limiting accuracy;
- to provide a mechanism for estimating uncertainties (according to the ISO Guide [10]) associated with the curve.

In general, it was found that the most important determinant of the accuracy of any single measurement was not the source from which it came, but its position in the temperature scale.

With regard to future work, the following would be beneficial

- Addition of value (and possible higher-order) continuity constraints at 273.16 K (= 0.01 °C) (see Appendix N).
- Use of the validated representation as data to test alternative, more physically-based representations, such as Debye functions [13].

Acknowledgements

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Appendix A: Temperature measurement background

Dr Richard Rusby (RLR), Head of NPL's Temperature and Humidity Standards Section within the Centre for Basic and Thermal Metrology (CBTM), reported that much international work on temperature measurement is dedicated to providing thermodynamic calibration of platinum resistance thermometers (PRTs) such that there would be a more direct link between PRTs and the definition of temperature. However, thermodynamic temperature measurement is difficult, with incompletely characterised and controlled Types A and B evaluation of uncertainty[4].

Traditionally, independent, internationally-agreed temperature scales were used as a "bridge" between thermodynamic and more practical measurements of temperature. For example, IPTS-68 defined an interpolation scheme based on a number of fixed points of temperature, the pivotal one being the triple point of water at 273.16 K [9]. Above this temperature, a second degree polynomial is used; below it, a 20th degree polynomial is used. The data above that point is used to define the end conditions for the reference function below that point, such that the scale is C^1 continuous, i.e., continuous in value and first derivative (slope).

Temperature measurement is often based on trade-offs between measurement systems. For example, at high temperatures, e.g., above 600 K, vacancy formation in the crystal lattice of platinum limits the accuracy of PRTs. Conversely, direct thermodynamic measurement of temperature improves: the thermal radiation emitted from a blackbody in a closed cavity follows Planck's Law, in which temperature is inversely proportional to the wavelength of the emitted radiation; from 700 K upwards, that radiation is intense enough to be measured with some precision.

Another important aspect of temperature measurement is the fact that the measuring device used for one range of temperature frequently differs from that used at another range. For example, 0.25 Ω resistors are often used in PRTs used in high-temperature measurement; at low temperatures, 25 Ω resistors are used, and the PRTs are physically quite different.

RLR suggested that Temperature (T) should be fitted to resistance ratios (W, $R_T/R_{273.16}$) rather than vice-versa. The motivation is as follows. The uncertainty in R is largely constant, with a relative precision of approximately 2×10^{-7}. Conversely, T is generally known[5] to much lower precision. He suggested that the uncertainty in T be treated as constant, at 0.1 mK, below 273.16 K, and suggested a linear rise above this temperature, such that at the freezing point of zinc, at about 693 K, it was theoretically 1 mK; more practically, it would probably be about 3 mK. At 273.16 K, the resistance ratio is unity, by definition, and the uncertainty is correspondingly zero. Moreover, since the uncertainty in *W* is several orders of magnitude less than that in *T*, orthogonal distance regression (ODR), the appropriate technique if errors are present in both variables, probably presents few practical advantages over simple, weighted least-squares fitting of *T* to *W*.

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[4]This classification of uncertainty can be found in the ISO Guide to the Expression of Uncertainty in Measurement.

[5]Exceptions occur at the fixed points in the scale, e.g., the triple point of water, which, by international agreement, has a temperature of exactly 273.16K.

RLR suggested that the ITS-90 reference functions [9] be used as a basis for determining the quality of the data and the consistency of the sources. ITS-90 has superseded IPTS-68. In particular, between the triple point of equilibrium hydrogen (13.8033 K) and the freezing point of silver (961.78 °C) , the following reference functions are defined. In the range 13.8033 K to 273.16 K, the reference function is

$$\ln[W_r(T_{90})] = A_0 + \sum_{i=1}^{12} A_i \left[\frac{\ln(T_{90}/273.16K)+1.5}{1.5} \right]^i \quad (5)$$

with an inverse, correct to 0.1 mK, of

$$T_{90}/273.16K = B_0 + \sum_{i=1}^{15} B_i \left[\frac{W_r(T_{90})^{1/6}-0.65}{0.35} \right]^i \quad (6)$$

For the range 0 °C to 961.78 °C, the reference function and its inverse (correct to 0.13 mK) are

$$W_r(t_{90}) = C_0 + \sum_{i=1}^{9} C_i \left[\frac{t_{90}/^oC-481}{481} \right]^i \quad (7)$$

and

$$t_{90}/^oC = D_0 + \sum_{i=1}^{9} D_i \left[\frac{W_r(t_{90})-2.64}{1.64} \right]^i, \quad (8)$$

with prescribed polynomial coefficients in each case.

RLR suggested that the high temperature point in Source 37[6] be eliminated from the analysis, and that the range would then be reduced to one in which the data is reasonably well distributed. He assumed that the NZMSL-supplied data had already been adjusted to relate to a *common thermometer*.

Given that an actual PRT will have *W* (resistance ratios) which differ from the ITS-90 values at the fixed points, deviation functions are defined to relate the characteristic curve of a given PRT to the ITS-90 reference, which serves as the common thermometer. Deviation functions apply to specific subranges of the data and are typically in (transformed) polynomial form as defined in [9]. The parameters of the deviation function are obtained by calibrating the PRT at certain fixed-points.

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[6]Source 37 contains just two points, both relating to high temperature. Indeed, there is a large gap between the second of these points and the remaining data.

Appendix B: Plots of the data set supplied by NZMSL

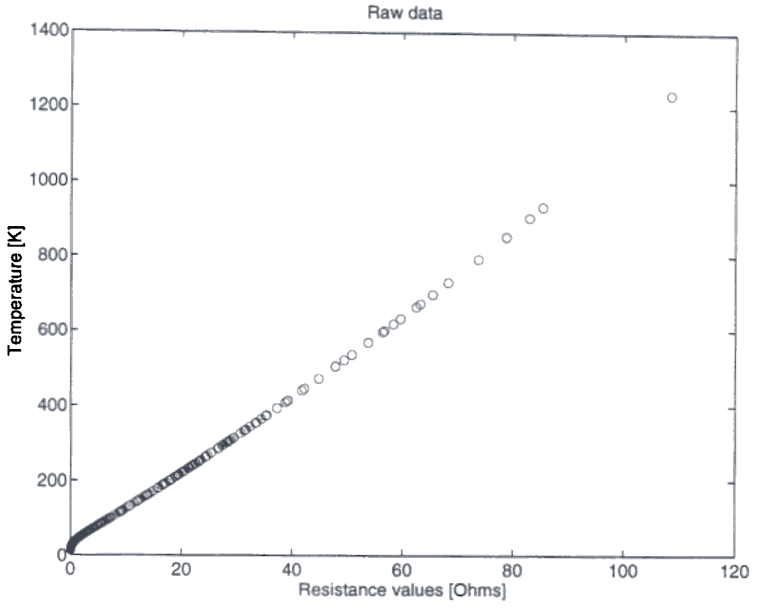

Figure 1 - The data set supplied by Dr Nicholas, New Zealand Measurement Standards Laboratory.

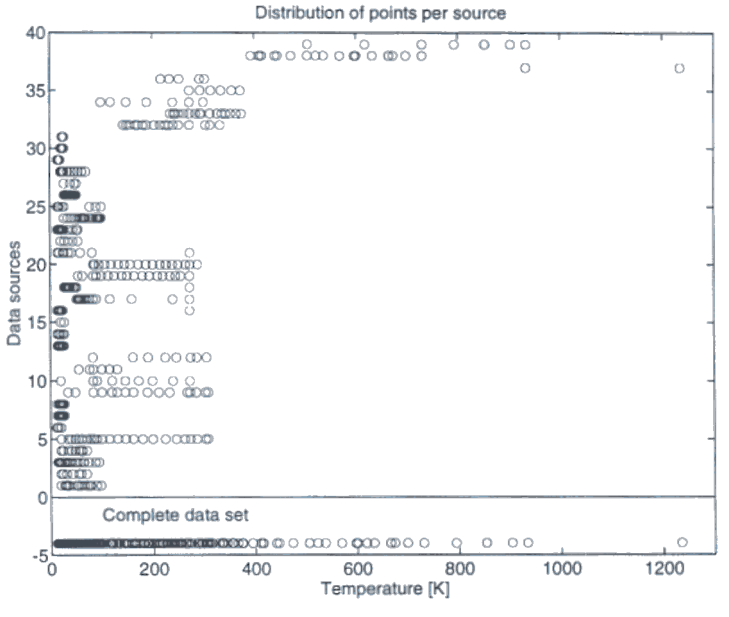

Figure 2 - Data, indexed by source (laboratory) number. Note the preponderance of low temperature measurements. The aggregate data is also shown at the bottom of the graph, for information.

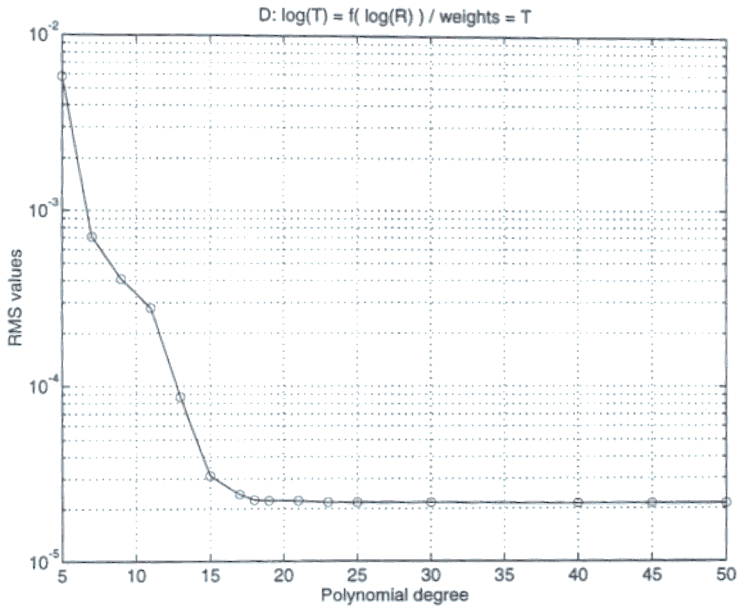

Figure 3 - RMS residuals for fitting data over the whole range: log(T) = P_n(log(R)).

Appendix C: Results of fitting the complete data set

Table IV: Polynomial fit of log(T) = Pn(log(R)).			
Tested Degrees	RMS residuals	Remarks	
		Oscillations	Residuals
5	0.005803	No	Systematic *
7	0.0007103	"	Systematic **
9	0.0004081	"	Systematic
11	0.000279	"	"
13	0.00008672	"	"
15	0.00003122	"	"
17	0.00002429	"	"
18	0.00002242	"	Becoming Random
19	0.00002228	"	Random *
21	0.00002223	"	"
23	0.00002178	"	"
25	0.00002176	"	"
30	0.0000217	"	"
40	0.00002143	"	"
45	0.0000214	Small oscillations ***	"
50	0.0000214	Yes	"

General observations :
* trend to large residuals in the right-most points (large values of R)
** trend to large residuals in the left-most points (small values of R)
*** oscillations beginning in both ends

Processed file : data_llw.dat

Appendix D: The consistency of the data across sources

Table V: Polynomial fit of log(T) = Pn(Log(R)), removing each individual data source.					
Removed data Source	RMS degree 19	Remarks			
		Residuals	Rogue points	Data points per source	Used Points
1	0.0000213	Random	One	21	666
2	0.0000222	"	"	7	680
3*	0.0000219	"	None	27	660
4	0.00002218	"	One	11	676
5	0.00002256	"	"	51	636
6	0.00002205	"	"	17	670
7	0.00002199	"	"	23	664
8	0.00002195	"	"	27	660
9	0.00002276	"	"	33	654
10	0.00002236	"	"	14	673
11	0.00002227	"	"	6	681
12	0.00002245	"	"	10	677
13	0.00002215	"	"	10	677
14	0.00002218	"	"	8	679
15	0.00002224	"	"	3	684
16	0.0000222	"	"	10	677
17	0.00002229	"	"	15	672
18	0.00002219	"	"	14	673
19	0.0000224	"	"	19	668
20	0.00002241	"	"	25	662
21	0.00002224	"	"	9	678
22	0.00002213	"	"	13	674
23	0.00002197	"	"	28	661
24	0.00002214	"	"	35	652
25	0.00002219	"	"	13	674
26	0.00002199	"	"	30	657

Table V: Polynomial fit of log(T) = Pn(Log(R)), removing each individual data source.

Removed data Source	RMS degree 19	Remarks			
		Residuals	Rogue points	Data points per source	Used Points
27	0.00002223	"	"	5	682
28	0.00002212	"	"	17	670
29	0.00002212	"	"	12	675
30	0.0000222	"	"	7	680
31	0.00002222	"	"	5	682
32	0.00002162	"	"	17	670
33	0.00002291	"	"	17	670
34	0.00002228	"	"	7	680
35	0.00002302	"	"	17	670
36	0.00002256	"	"	12	675
37	0.00002248	"	"	2	685
38	0.00001699	"	Some	71	616
39	0.00001594	"	"	20	667
40**	0.00002216	"	None	1	686
41***	0.00002201	"	One	26	661

General observations :
- no oscillations observed
- best polynomial degree based on Appendix C. RMS value = 0.00002228

* - Source 3 before creating source 40. (Includes suspected point!)
** - Includes only the suspected point removed from source 3.
*** - Source 3 after creating source 40. (Does not include suspected point!)

Processed file : dtllw_K.dat, where K stands for the removed data source

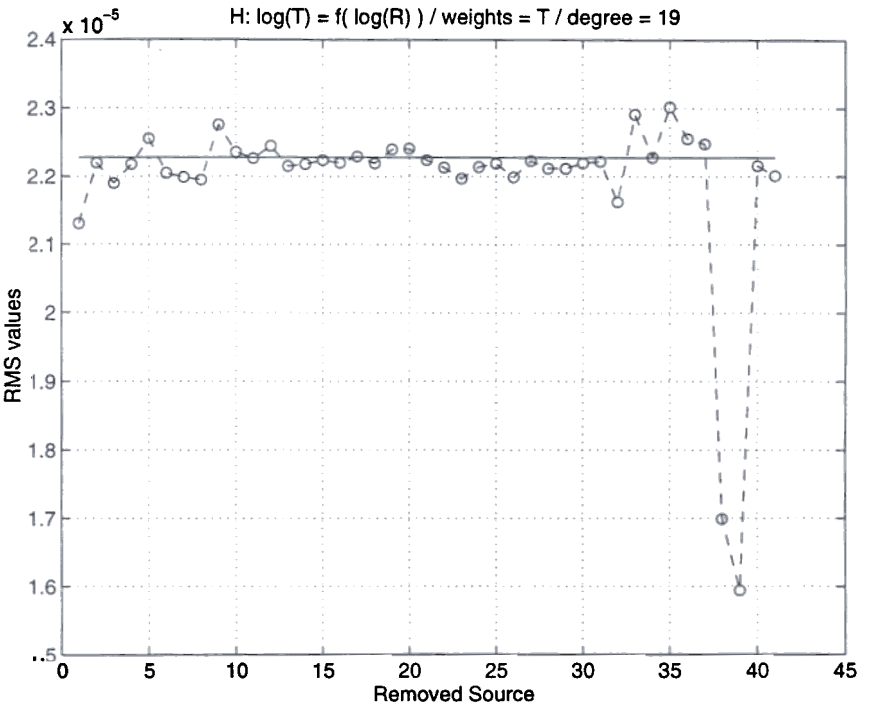

Figure 4 - Influence of individual sources when fitting over the whole range.

Appendix E: Individual analysis for rogue point in source number 3

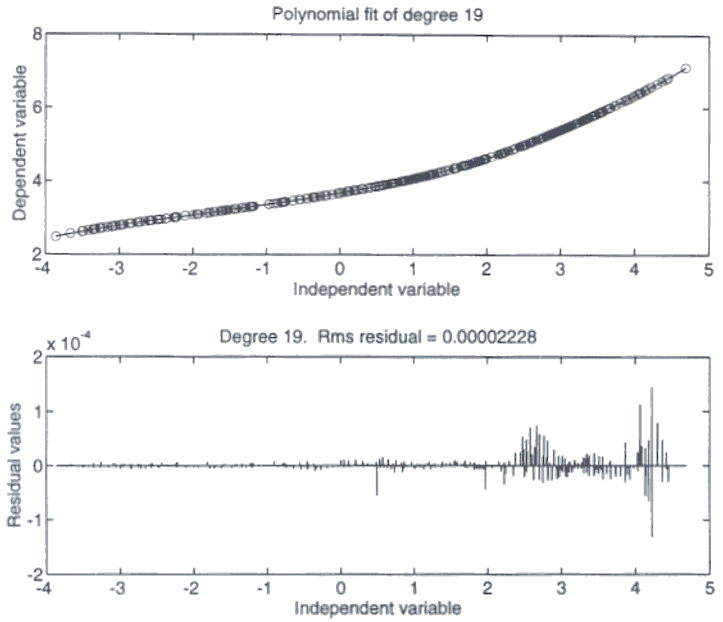

Figure 5 - Residuals for polynomial fitting with degree 19 using all data.

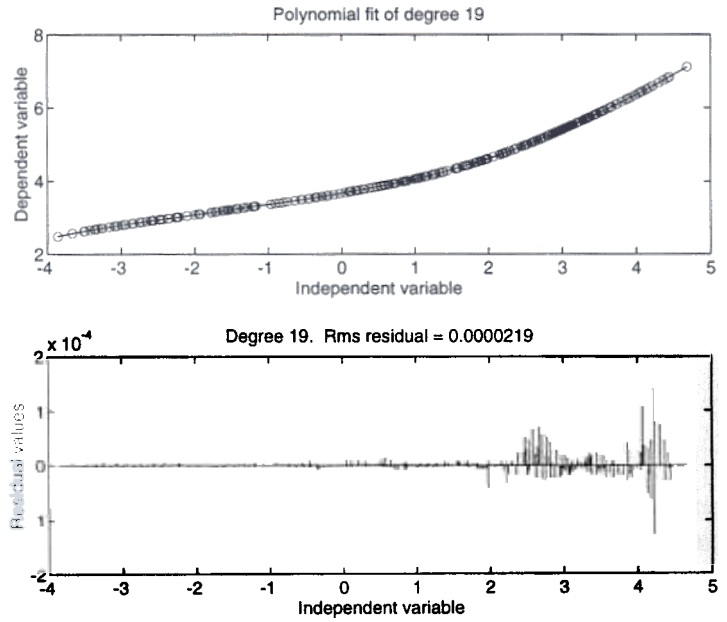

Figure 6 - Residuals for polynomial fitting over the full range, using degree 19, after removing source number 3, and before creating sources 40 and 41.

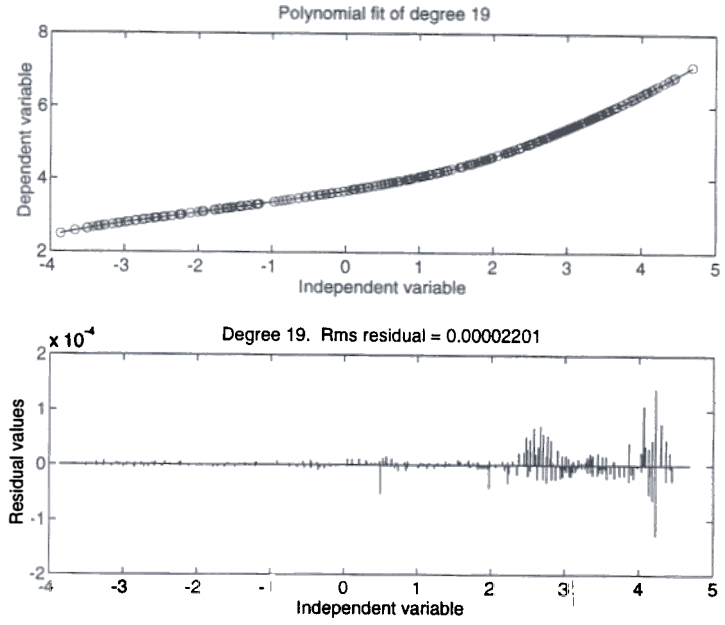

Figure 7 - Residuals for polynomial fitting over the whole range, using degree 19, removing sources 3 and 41 but keeping source 40 (the possible rogue point).

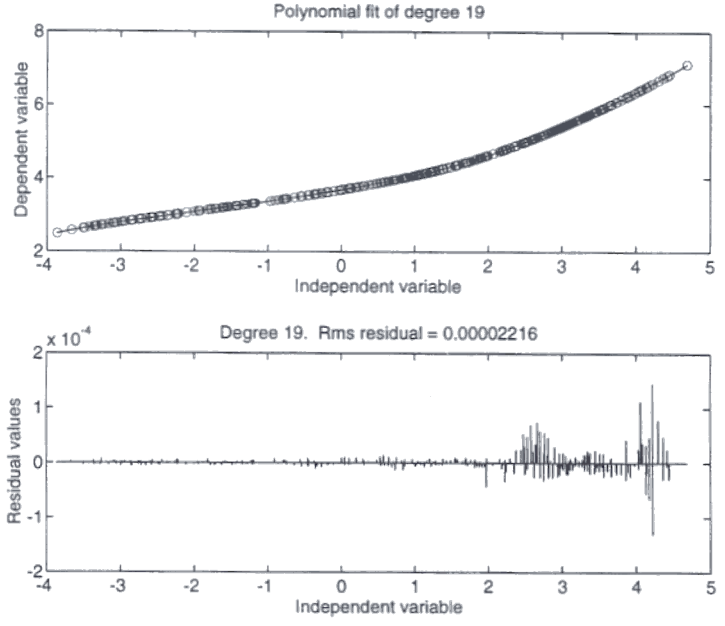

Figure 8 - Residuals for polynomial fitting using degree 19, removing sources 3 and 40 (the possible rogue point) but keeping source 41.

Appendix F: Analysis according to ITS-90

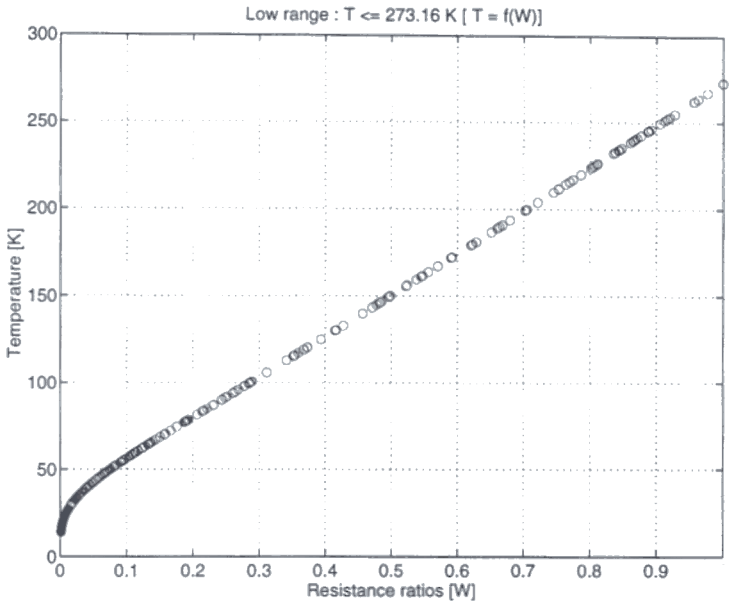

Figure 9 - Data set for W(T90) ≤ 1.

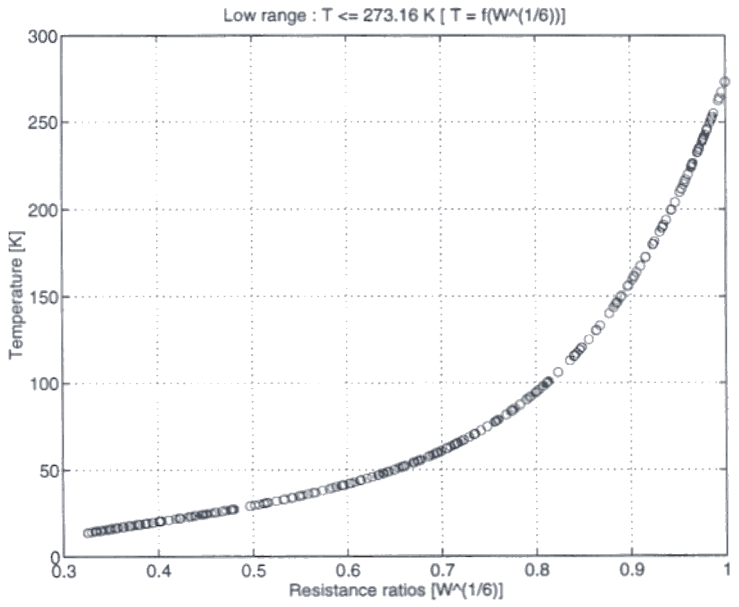

Figure 10 - Data set for $W(T90)^{(1/6)} \leq 1$.

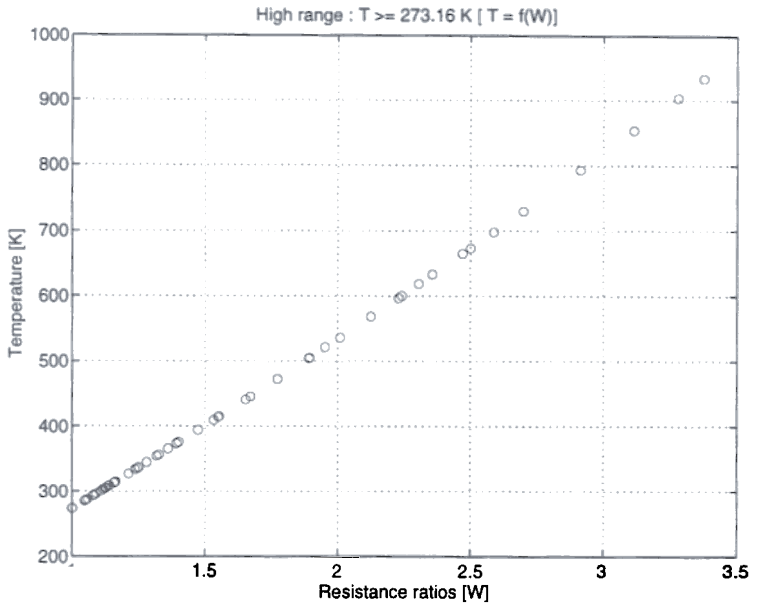

Figure 11 - Data set for W(T90) ≥ 1

Table VI: Data exclusion according to ITS-90 limits			
Low temperature range : W(T90) ≤ 1.0			
Source	**Resistance**	**Resistance ratio**	**Temperature**
6	0.0210	0.0008	11.9937
6	0.0210	0.0008	11.9941
6	0.0256	0.0010	12.9953
6	0.0256	0.0010	12.9977
7	0.0300	0.0012	13.7917
High temperature range : W(T90) ≥ 1.0			
37	108.4	4.2864	1235.00
Total of points removed: 6 data points			

Appendix G: Comparison between ITS-90 and the data set to define the variance profile

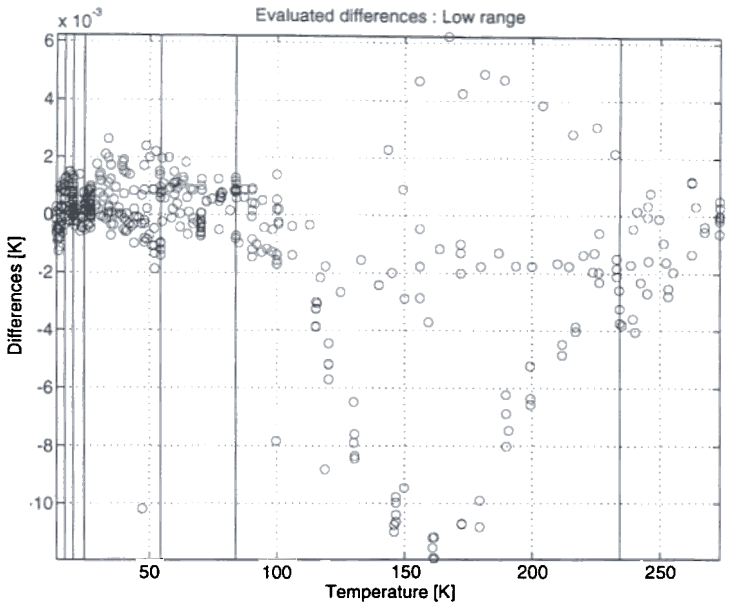

Figure 12 - Comparison of data with ITS-90: low range.

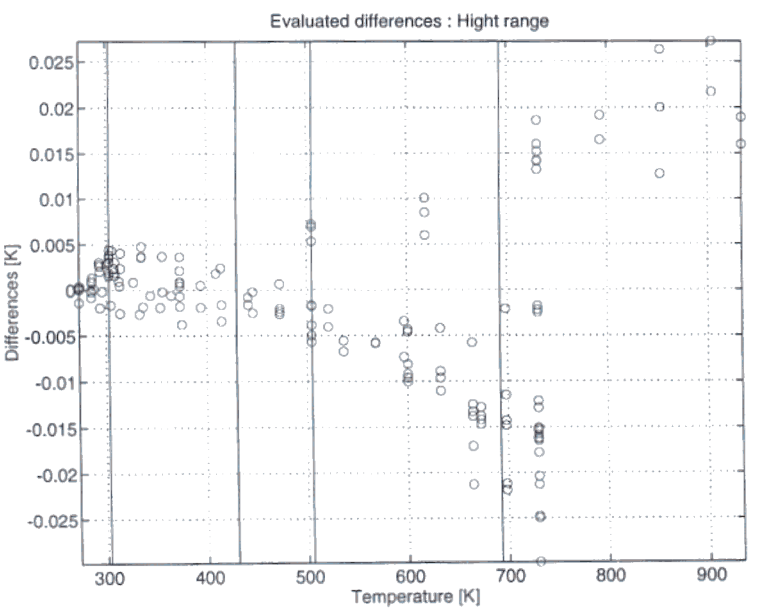

Figure 13 - Comparison of data with ITS-90: high range.

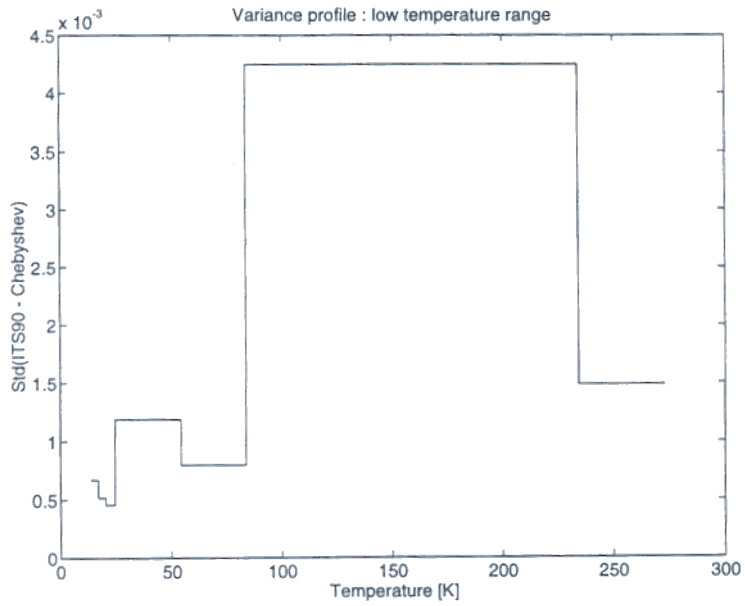

Figure 14 - Variance profile: low range.

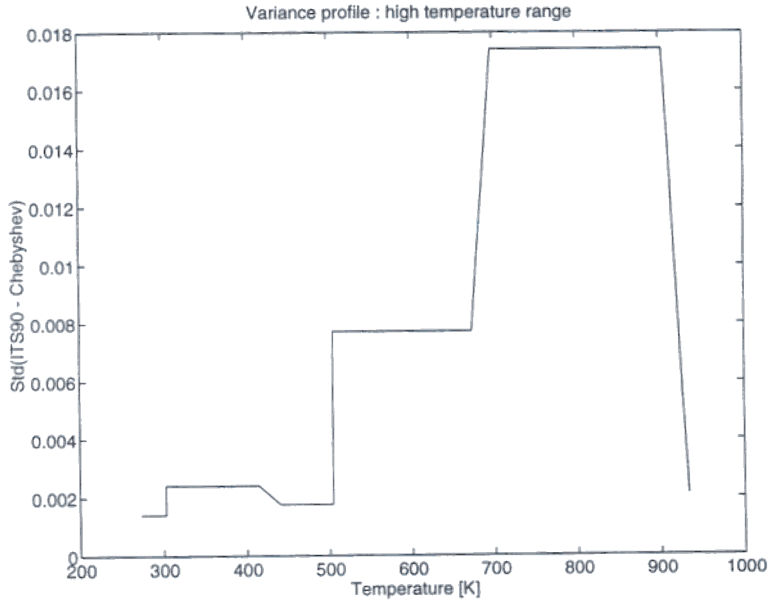

Figure 15 - Variance profile: high range.

Appendix H: Data analysis for the low range using the estimated variance profile

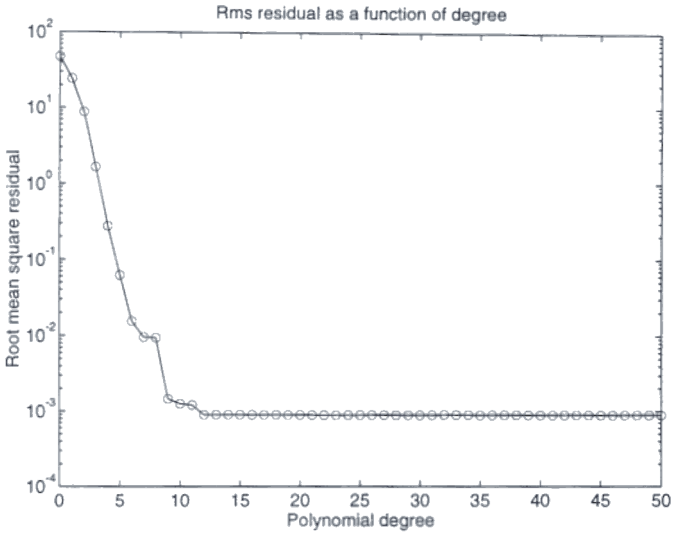

Figure 16 - RMS residual plot for fits of T as polynomials in $W^{1/6}$: low range.

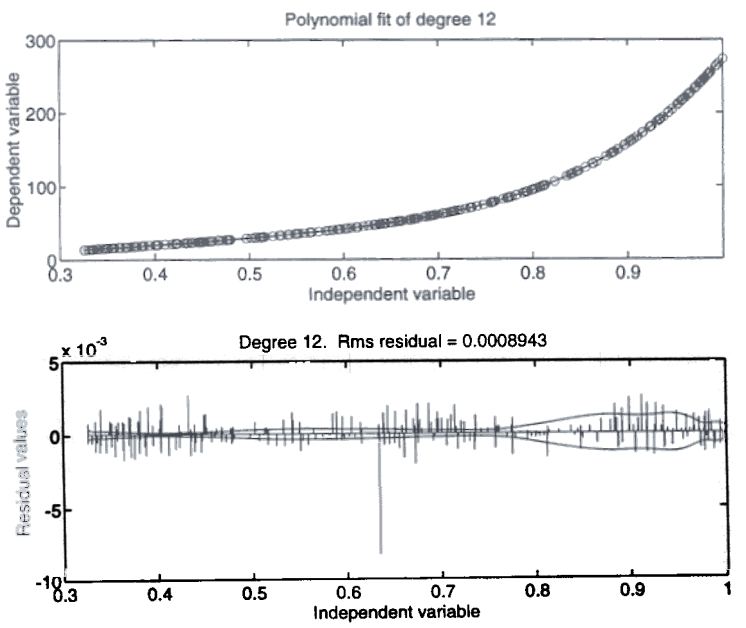

Figure 17 - The fit of T as a polynomial of degree 12 in $W^{1/6}$: low range.

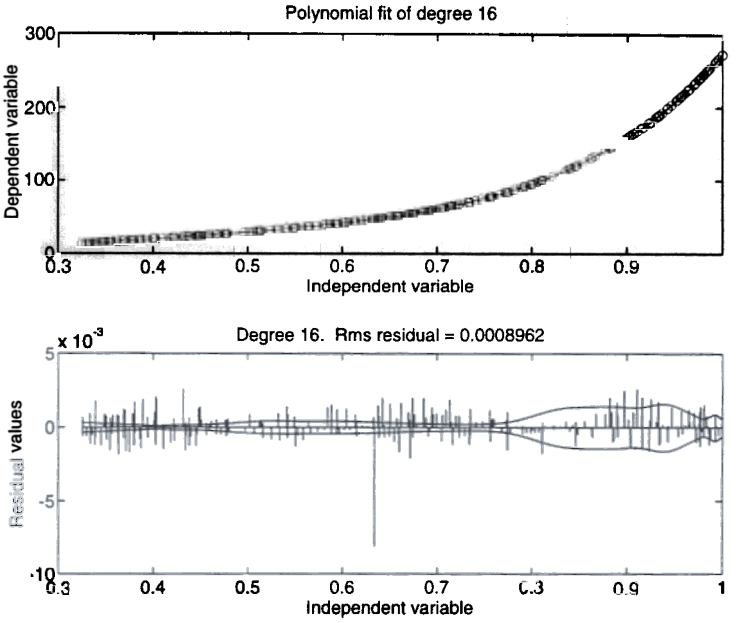

Figure 18 - As Figure 17 but for the ITS-90 recommended degree: low range.

Appendix I: Eliminating the rogue point in the low range

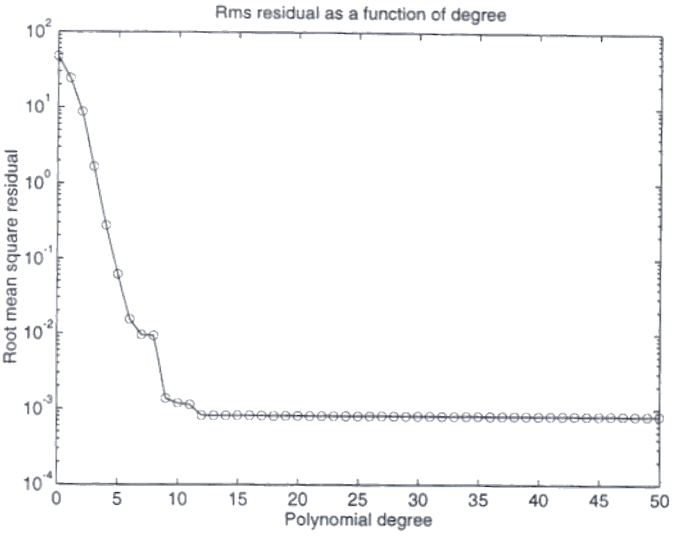

Figure 19 - RMS residual plot for fits of T as polynomials in $W^{1/6}$, after removing rogue point: low range.

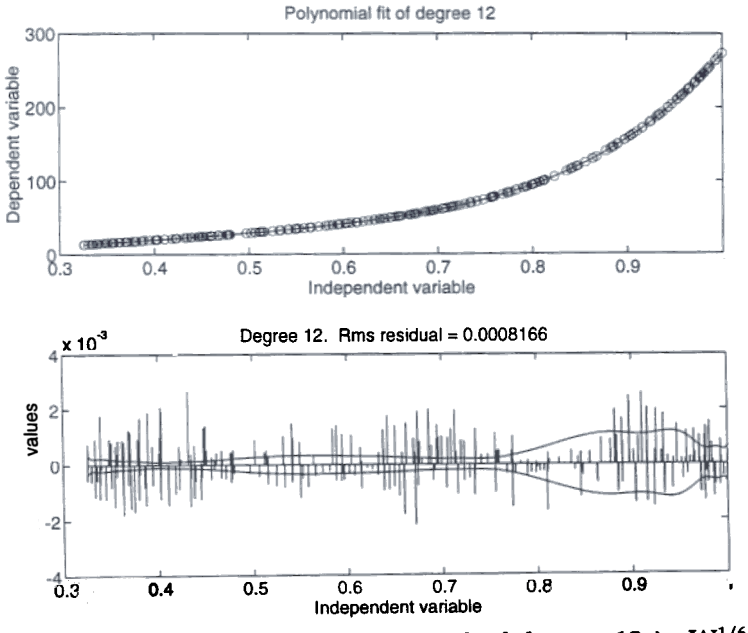

Figure 20 - The fit of T as a polynomial of degree 12 in $W^{1/6}$: low range.

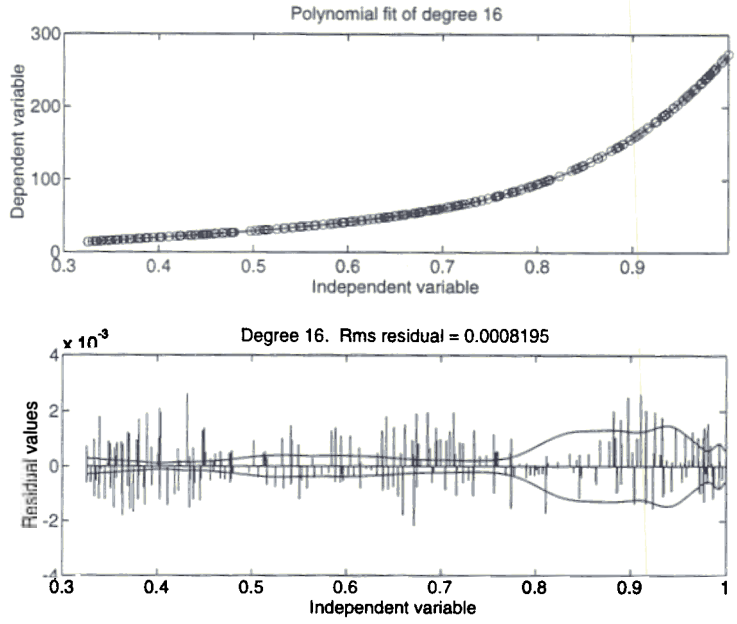

Figure 21 - As Figure 20 but for the ITS-90 recommended degree, after removing rogue point: low range.

Appendix J: Data analysis for the high range using variance profile

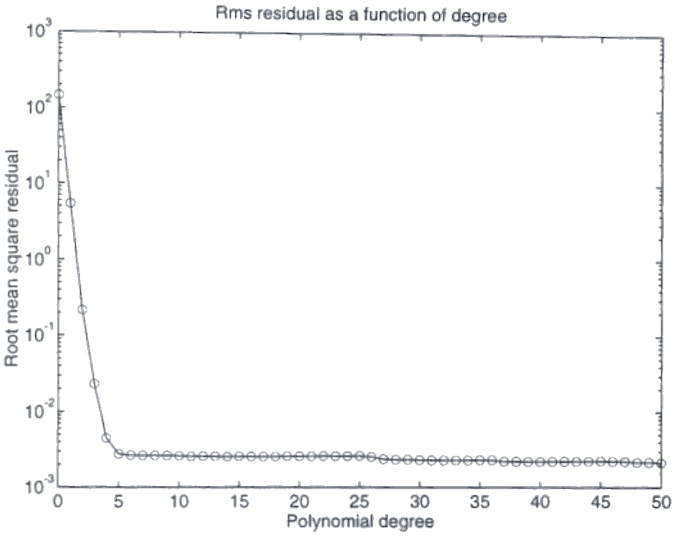

Figure 22 - RMS residuals plot for fits of T as polynomials in W: high range.

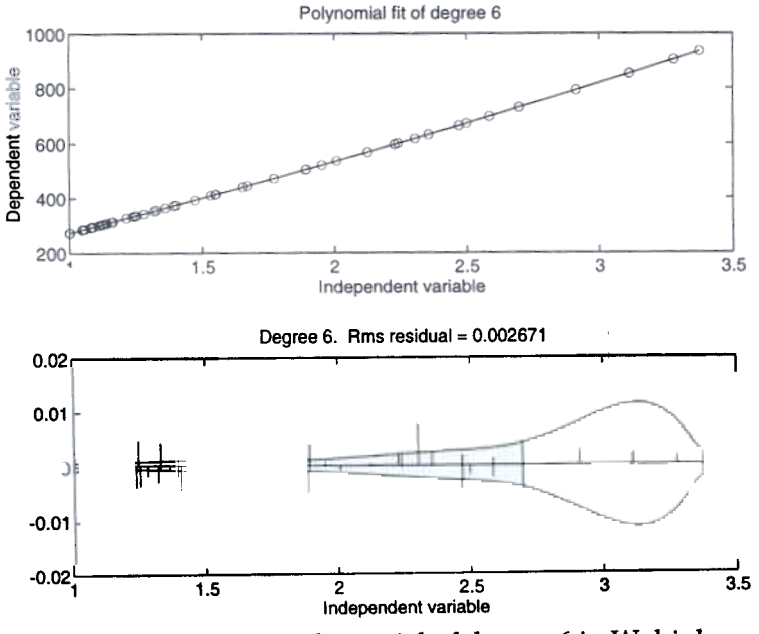

Figure 23 - The fit of T as a polynomial of degree 6 in W: high range.

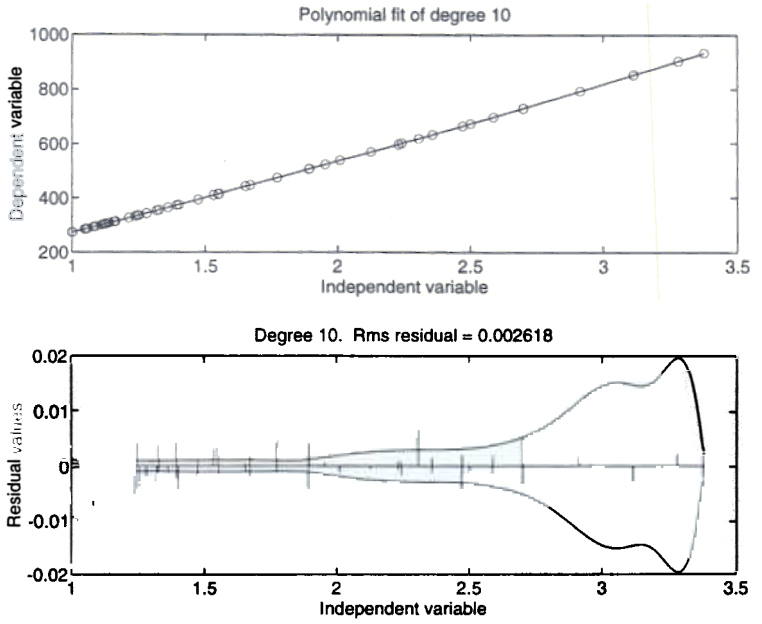

Figure 24 - As Figure 23 but for the ITS-90 recommended degree: high range. Note the wider confidence intervals at high temperatures, owing to the use of a moderately high polynomial degree and sparseness of the data.

Appendix K : Testing confidence limits for the residuals: Low and High ranges

In the low range, the limiting value for the 95% confidence limits on the weighted residuals is 1.582 mK; 27 of the 529 points in the low range lie outside this limit, compared with an expected number of 26. The limit value for the 99% confidence limit is 2.087 mK; 4 of the 529 points lie outside this limit (where the expected number is 5).

In the high range, the limiting value for the 95% confidence limits on the weighted residuals is 5.165 mK; 5 of the 152 points in the high range lie outside this limit (where the expected number is 8). The limit value for the 99% confidence limit is 6.799 mK; 3 of the 152 points lie outside this limit (where the expected number is 2).

Appendix L: Comparison between ITS-90 reference values and fitted values

Table VII: Absolute and relative deviations between ITS-90 Reference values and fitted values			
Resistance ratios Wr(T90)	**Temperature [K]**	**Deviation [K]**	**Deviation [%]**
Low Temperature range : T ≤ 273.16 K			
0.0012	13.8030	-0.0003	-0.0021
0.0023	17.0356	0.0006	0.0034
0.0042	20.2704	0.0004	0.0018
0.0084	24.5562	0.0001	0.0004
0.0917	54.3587	0.0003	0.0006
0.2159	83.8063	0.0005	0.0005
0.8441	234.3134	-0.0022	-0.0009
1.0000	273.1601	0.0001	0.0000
High Temperature range : T ≥ 273.16 K			
1.0000	273.1595	-0.0005	-0.0002
1.1181	302.9165	0.0019	0.0006
1.6098	429.7476	-0.0009	-0.0002
1.8928	505.0752	-0.0028	-0.0005
2.5689	692.6677	-0.0093	-0.0013
3.3760	933.4906	0.0176	0.0019

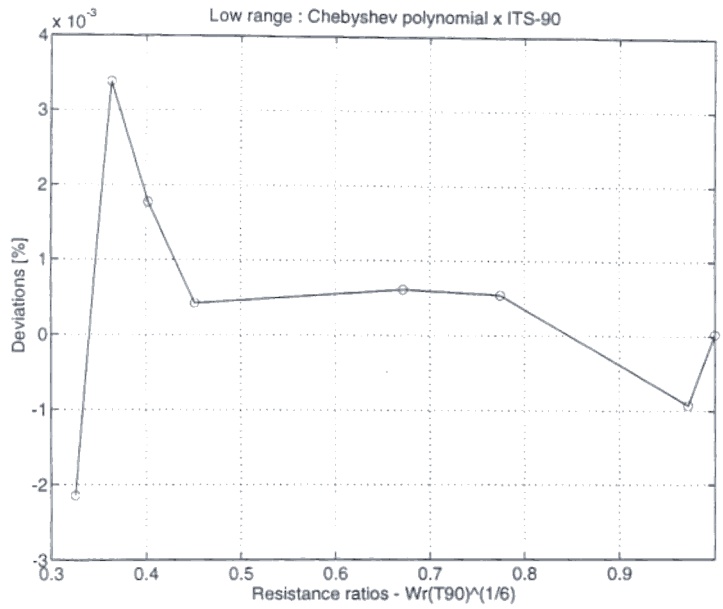

Figure 25 - Differences between ITS-90 and Chebyshev polynomial of degree 12: low range.

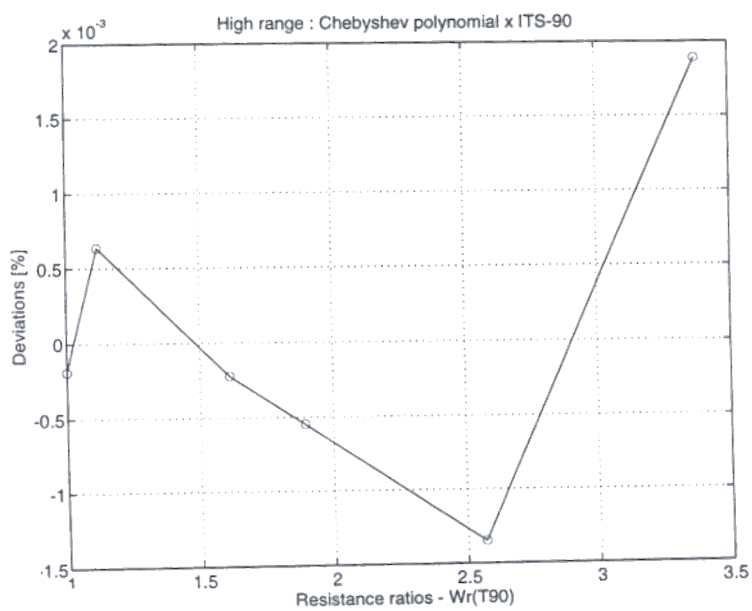

Figure 26 - Differences between ITS-90 and Chebyshev polynomial of degree 6: high range.

Appendix M: Fitting data with transformations: Generalised Additive Models

In data approximation, it is often the case that transformations of the data make it easier to fit using simple model families such as polynomials and splines.

Let

$$y = F(x, \boldsymbol{a}, \boldsymbol{a}^{(p)}, \boldsymbol{a}^{(q)}) \doteq q^{-1}(f(p(x, \boldsymbol{a}^{(p)}), \boldsymbol{a}), \boldsymbol{a}^{(q)}) \tag{9}$$

be an explicit function relating the dependent variable (response) y to the independent (control) variable x, with parameters $\boldsymbol{a}$ to be determined in the course of the approximation procedure. Note that

1) $f(x; \boldsymbol{a})$ is typically a simple linear function (e.g., polynomial, spline or trigonometric series) of parameters $\boldsymbol{a}$
2) the transformation functions $p(\square,\boldsymbol{a}^{(p)})$ and $q(\square,\boldsymbol{a}^{(q)})$ are prescribed *before* fitting, with known parameters $\boldsymbol{a}^{(p)}$ and $\boldsymbol{a}^{(q)}$, respectively. Note that $\square$ is a placeholder for a data abscissa value;
3) the transformation functions are formally invertible and define new variables u and v as follows:

$$\begin{aligned} u &= p(x, \boldsymbol{a}^{(p)}); \quad x = p^{-1}(u, \boldsymbol{a}^{(p)}); \\ v &= q(y, \boldsymbol{a}^{(q)}); \quad y = q^{-1}(v, \boldsymbol{a}^{(q)}). \end{aligned} \tag{10}$$

An *independent variable transformation* is defined by means of the function $u = p(x; \boldsymbol{a}^{(p)})$ and a *dependent variable transformation* by means of the function $v = q(y; \boldsymbol{a}^{(q)})$. By incorporating appropriate variable transformations, the richness of the model family defined by f is increased. The choice of which transformations to choose, if any, is motivated by examining the data. Indeed, a simple method of determining the suitability of a dependent variable transformation is to apply the transformation q to the dependent variable y and to plot the transformed variable v in order to test whether v is more simple to fit than y. That is, it is often more instructive to consider the transformation q as a means of simplifying the data y than the inverse transformation q^{-1} as a means of extending the simple model function f.

Independent variable transformations are not as easy to determine, though they have their uses, particularly in making the "speed" of the independent variable more uniform, which may be necessary if the function being fitted has a *chirp*-like behaviour[7]. Alternatively, independent variable transformations may be suggested by the presence of non-uniform sampling of the independent variable. The goal in the latter case is to choose a transformation p such that the corresponding sampled values u_i are sampled more uniformly than the original values x_i.

[7] A *chirp* is a data series which has oscillatory behaviour and the period of the oscillations is not a constant function of the independent variable. The name is descriptive: bird song includes snippets where the frequency of the sound varies while other factors stay mainly constant.

M.1 Dependent variable transformations

Given an invertible dependent variable transformation $v = q(y; a^{(q)})$, the problem of determining a from the model $y = q^{-1}(f(x; a, a^{(q)})) + e^{(q)}(x)$ is equivalent to determining a from $v = q(y; a^{(q)}) \doteq f(x; a) + e(x)$.

Therefore, when using regression to determine the a parameters, we solve the following problem:

$$\min_{a} E,$$

where

$$E \doteq \sum_{i=1}^{n} e_i^2, \quad e_i \doteq e^{(q)}(x_i) = y_i - q^{-1}(f(x_i; a, a^{(q)})) \doteq \sum_{i=1}^{n} (w_i d_i)^2, \quad d_i \doteq e(x_i) = q(y_i) - f(x_i; a). \tag{11}$$

Note that the transformation weights w_i have been introduced to ensure that the two expressions are statistically consistent. Furthermore, comparing terms, we have $e_i = w_i d_i$ and hence

$$w_i \doteq \frac{e_i}{d_i} = \frac{y_i - q^{-1}(f(x_i; a, a^{(q)}))}{q(y_i) - f(x_i; a)} \tag{12}$$

In practice, w_i cannot be computed *a priori* since a is not known. It can be *estimated*, either by assuming values for a, or by assuming that the residuals e_i and d_i are small. For such small-residual problems, the limiting value, which estimates w_i, can be obtained from de l'Hôpital's rule as

$$w_i = \frac{\partial}{\partial x} q^{-1}(f(x, a), a^{(q)}) \bigg|_{x=x_i} \tag{13}$$

assuming

$$\frac{\partial f}{\partial x}(x, a) \bigg|_{x=x_i} \neq 0. \tag{14}$$

If the latter does not hold, further application of de l'Hôpital's rule would be required.

The standard uncertainty in the parameters a, denoted $u(a)$, is obtained from the square root of the diagonal of the covariance matrix $C = C(a)$ of the parameters, which is estimated from

$$C \approx \frac{E^2}{m-n} (A^T A)^{-1} \quad A_{ij} = \frac{\partial f(x_i, a)}{\partial a_j} \tag{15}$$

where E is as defined previously, m-n is the number of degrees of freedom of the fit and A is the $m \times n$ Jacobian (matrix of partial derivatives of the m observations and n parameters); see [11].

The standard uncertainty of the fitted function $u(y_{(k)})$ associated with a general point ($x_{(k)}$, $v(f(x(k), \boldsymbol{a}))$) can be estimated (to first-order) by computing the n-vector of partial derivatives of the transformed model function as follows:

$$\boldsymbol{D}_{(k)j} \quad \frac{\partial}{} q^{-1}(f(x_{(k)},\boldsymbol{a})) = \left(\frac{\partial}{\partial f(x_{(k)},\boldsymbol{a})} q^{-1}(f(x_{(k)},\boldsymbol{a})) \right) \frac{\partial f(x_{(k)},\boldsymbol{a})}{\partial a_j} \quad \left(\frac{\partial}{\partial f(x_{(k)},\boldsymbol{a})} q^{-1}(f(x_{(k)},\boldsymbol{a})) \right) A_{(k)j} \quad \textbf{(16)}$$

and by using this to estimate the variance (to first order) from

$$V_{(k)} \approx D_{(k)}^T C(\boldsymbol{a}) D_{(k)}$$

and the corresponding standard uncertainty $u(y_{(k)}) = (V_{(k)})^{-½}$, see [11].

Therefore, given thermometry data (R_i, T_i), the parameters in model **(1)** are determined by considering

a) $v = q(\square) = \exp(\square)$, hence $y = q^{-1}(v) = \log(\square)$ and no $\boldsymbol{a}^{(q)}$ parameters are required

b) $u = p(\square) = \exp(\square)$, hence $x = p^{-1}(u) = \log(\square)$ and no $\boldsymbol{a}^{(p)}$ parameters are required

c) The weights w_i are determined as follows:

$$w_i \approx \frac{\partial q}{\partial x}(f(x, \boldsymbol{a}), \boldsymbol{a}^{(q)})\Big|_{x=x_i} = \frac{\partial}{\partial x}(\exp(p_n(R, \boldsymbol{a}))\Big|_{R=R_i} = \exp(p_n(R, \boldsymbol{a}))\Big|_{R=R_i} \approx T_i$$

d) Given the parameters $\boldsymbol{a}$, the fitting function can be computed by evaluating the polynomial $p_n(R, \boldsymbol{a})$ and hence $\exp(p_n(R, \boldsymbol{a}))$.

e) The uncertainty is computed as described above, with

$$D_{(k)j} = \frac{\partial \exp(p_n(R_{(k)},\boldsymbol{a}))}{\partial p_n(R_{(k)},\boldsymbol{a})} \frac{\partial p_n(R_{(k)},\boldsymbol{a})}{\partial a_j} = \exp(p_n(R_{(k)},\boldsymbol{a}))A_{(k)j} = f(R_{(k)},\boldsymbol{a})A_{(k)j} = T_{(k)}A_{(k)j}.$$

Hence $u(R_{(k)})$ is computed as above.

M.2 Independent variable transformations

Independent variable transformations can be seen as modifying the basis functions directly. For simplicity, but without loss of generality, it is assumed that there are no dependent variable transformations (the latter can be included by following the treatment described above). Let A be the $m \times n$ Jacobian (matrix of partial derivatives of the m observations and n parameters) used in estimating $\boldsymbol{a}$ and $C = C(\boldsymbol{a})$ is the variance matrix of the parameters. Then

$$C \approx \frac{E^2}{m-n}(A^T A)^{-1} \quad A_{ij} = \frac{\partial}{\partial a_j} f(u_i, \boldsymbol{a}) \quad u_i = p(x_i, \boldsymbol{a}^{(p)}) \qquad \textbf{(20)}$$

and the uncertainties are estimated as in the untransformed case.

In the case of the temperature model **(1)**, the inclusion of the independent variable transformation $u_i = \log(R_i)$ introduces a nonlinear transformation of the variable which is implemented before a linear transformation of the variable so that it (u_i) is mapped into the interval [-1, 1]. The ITS-90 low temperature range transformation $u_i = W_i^{1/6}$ is similar in these respects.

Appendix N: Fitting a composite ITS-90 function which preserves continuity

The m thermometry data points are denoted $\{(W_i, T_i)\}$ for consistency with ITS-90, where W_i is the ith value of the resistance ratio and T_i is the corresponding thermodynamic temperature. Let $T_0 = 273.16$ K be the temperature at which the ITS-90 representation changes from the low- to the high-temperature representation, and let W_0 be the corresponding resistance ratio.

A *composite* fitting function of the form

$$T = \begin{cases} f_{\mathrm{Lo}}(W), & W < W_0, \\ f_{\mathrm{Hi}}(W), & W \geq W_0 \end{cases}$$

is required, subject to the continuity condition

$$f_{\mathrm{Lo}}(W_0) = f_{\mathrm{Hi}}(W_0)$$

To maintain compatibility with ITS-90, we require f_{Lo} to be a polynomial in the transformed variable $W^{1/6}$ and f_{Hi} to be a polynomial in W.

The continuity condition applied to f_{Lo} and f_{Hi} represented as Chebyshev polynomials implies that

$$\sum_{j=0}^{n_{\mathrm{Lo}}} a_j \theta_j(1) = \sum_{j=0}^{n_{\mathrm{Hi}}} b_j \theta_j(-1) \qquad \textbf{(23)}$$

and hence

$$\sum_{j=0}^{n_{\mathrm{Lo}}} a_j = \sum_{j=0}^{n_{\mathrm{Hi}}} b_j (-1)^j \qquad \textbf{(24)}$$

As before, we use the non-standard notation of $\theta_j(x)$ representing Chebyshev polynomial of the first kind, since T is reserved for temperature. Therefore, from **(24)**, the b_0 term can be eliminated as follows:

$$b_0 = \sum_{j=0}^{n_{\mathrm{Lo}}} a_j - \sum_{j=1}^{n_{\mathrm{Hi}}} b_j (-1)^j \qquad \textbf{(25)}$$

and hence

$$f_{\mathrm{Hi}}(W) \doteq p_{\mathrm{Hi}}(x) = b_0 + \sum_{j=1}^{n_{\mathrm{Hi}}} b_j \doteq \sum_{j=0}^{n_{\mathrm{Lo}}} a_j T_j(x) + \sum_{j=1}^{n_{\mathrm{Hi}}} b_j \left(T_j(x) - (-1)^j\right), \qquad \textbf{(26)}$$

where b_0 is as given above and x is that value of W normalised over the interval $[W_0, W_{\max}]$

If the observation equations are numbered (or renumbered if necessary) so that the m_{Lo} temperatures below T_0 precede the m_{Hi} temperatures at or above T_0, the observation equations may be written in matrix form as $Ac \approx t$, where t is the vector $\{T_i\}$, $c^{\mathrm{T}} = [a^{\mathrm{T}}, b^{\mathrm{T}}]$, $a^{\mathrm{T}} = [a_0, \ldots, a_{n\mathrm{Lo}}]$, $b^{\mathrm{T}} = [b_0, \ldots, b_{n\mathrm{Hi}}]$ and A has the form

$$A = \begin{bmatrix} A_{\mathrm{Lo}} & \mathbf{0} \\ \mathbf{1} & \tilde{A}_{\mathrm{Hi}} \end{bmatrix}, \tag{27}$$

where $\mathbf{0}$ is the $m_{\mathrm{Lo}} \times n_{\mathrm{Hi}}$ matrix of zeros, $\mathbf{1}$ is the $m_{\mathrm{Hi}} \times n_{\mathrm{Lo}}$ matrix of ones and A_{Lo} and $\hat{A}_{\mathrm{Hi}}$ are the matrices whose (i, j) elements are

$$\begin{aligned} A_{\mathrm{Lo}}(i,j) &= \theta_j(x_i), \\ \hat{A}_{\mathrm{Hi}}(i,j) &= \theta_j(x_i) - (-1)^j, \end{aligned} \tag{28}$$

respectively