Calibration Intervals from Variables Data[1]

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Abstract

Historically, calibration results have typically been recorded and stored in the form of attributes data. In the past few years, however, an apparent trend has begun to emerge for recording and storing calibration results in the form of variables data. This is partly due to ISO/IEC 17025 requirements for uncertainty analysis and partly due to the growing implementation of six-sigma or other SPC quality control systems. The growing availability of variables data has positive implications for calibration interval analysis.

This paper describes a methodology for determining calibration intervals from variables data. A regression analysis analytical approach is developed and algorithms are given for setting parameter calibration intervals from the results of variables data analysis.

1 Introduction

Cases where the value of a calibrated parameter drifts with time are often encountered in practice. In many instances, while the parameter value changes with time, the statistical variance remains essentially constant.

In this paper, a method is developed for determining calibration intervals for parameters whose values change with time elapsed since calibration. The method employs as-left and as-found variables data taken during calibration. Parameter values are assumed to be normally distributed with mean $y(t)$ and variance σ^2, where t is the time elapsed since calibration, i.e., we assume that parameter values are $N[y(t), \sigma^2]$.

Regression analysis with polynomial models of arbitrary degree is applied to estimate both $y(t)$ and σ^2.[2] Based on the results of regression analysis, calibration intervals are determined that satisfy end of period (EOP) in-tolerance criteria or maximum allowable uncertainties.

1.1 The Parameter Value Model

The basic model for $y(t)$ is

$$y(t) = y_0 + \delta(t)\,,$$

where t is the time elapsed since calibration, y_0 is the value of y measured at time $t = 0$, and $\delta(t)$ is the deviation in parameter value as a function of t. We model the function $\delta(t)$ with a polynomial function $\hat{\delta}(t)$, yielding a predicted value

$$\hat{y}(t) = y_0 + \hat{\delta}(t)\,.$$

1.2 Uncertainty in the Projected Value

The uncertainty in the predicted value for y is estimated as the square root of the variance of $\hat{y}(t)$

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[1] Presented at the NCSLI 2005 Workshop & Symposium in Wasington, D.C. Revised January 18, 2006 for publication in Measure Magazine.

[2] A first degree polynomial regression approach for $N[y(t), \sigma^2(t)]$ cases has been developed by Jackson [16].

$$u_y \cong \sqrt{\text{var}[\hat{y}(t)]}\,,$$

where

$$\text{var}[\hat{y}(t)] = u_0^2 + \text{var}[\hat{\delta}(t)]\,.$$

In this expression, the quantity u_0 is the uncertainty in the measurement y_0. The quantity $\text{var}[\hat{y}(t)]$ is estimated in Section 5.4.

2 Background

The analysis of calibration intervals has a legacy of working with as-found attributes data. As-found and as-left variables data have not been available until recently. Since there exists some inertia in moving from collecting and analyzing attributes data to collecting and analyzing variables data, some justification for making this move is given in this section.

2.1 The Early Years

Calibration interval analysis has its infancy in the late '50s through the '60s. Several algorithmic schemes were implemented in which intervals were lengthened or shortened if found in- or out-of-tolerance during calibration. During this period, many if not most measuring or test equipment (MTE) were single-parameter items. Data entry was manual and interval adjustments were typically performed by technicians.

In the late '60s and early '70s, interval analysis came under the scrutiny of statisticians and engineers with backgrounds in probability and statistics. At this point, it became apparent that (1) the percentage of items received for calibration in an in-tolerance condition was frequently a function of time elapsed since calibration and (2) algorithmic methods were not viable for controlling this percentage.[3]

From reviews of calibration service history, it was decided that calibration intervals needed to be adjusted to meet an end of period (EOP) percent in-tolerance criterion and interval adjustments needed to be based on historical service data. The term "reliability target" was coined to represent the percent in-tolerance criterion and the available service history data indicated an item's as-found condition as in-tolerance, out-of-tolerance, damaged, etc. Data of this sort came to be referred to as "attributes data."

During the late '60s and '70s methods began to appear that determined calibration intervals from such data. These methods employed maximum likelihood estimation (MLE) and reliability modeling tools [2 - 4]. They were later refined and expanded [5, 8, 17], have been documented in the public domain [10, 14] and have been implemented in commercially available software [12].

2.2 Today

Much of the MTE in today's inventories are multiparameter items or consist of individual single-parameter items, such as gage blocks, treated in the aggregate as a "set." Ordinarily, an item is pronounced out-of-tolerance if any single instrument parameter or item in a set is found out-of-tolerance. This practice is costly and seriously compromises risk management.

That the practice is costly stems from the fact that the calibration intervals of multiparameter MTE are often driven by a small subset of calibrated parameters. Since the identity of the offending parameters is obscured, intervals are shortened by the performance of the subsets, and the bulk of parameters are calibrated needlessly. This is a particularly undesirable outcome if the out-of-tolerance parameters are scarcely or never used.

The risk management compromise is due to the fact that risks are present at the parameter level, while data needed to do risk analysis are supplied at the item level. Since the whole purpose of periodic calibration is to control false accept and false reject risks, [9, 11, 13] this is a major disconnect that should not be taken lightly.

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[3] The non-viability of algorithmic methods was subsequently supported by studies performed later. [6, 18]

So, what are the obstacles to implementing data collection by parameter? In the early years, they were the following

- Manual data entry.
- Lack of availability of computing power.
- Expense of data storage in mainframe-based systems.
- Slow data processing speeds.
- Lack of analysis methodology.

Today, most of the above obstacles are essentially nonexistent. Only the first is a possible snag. However, since on-line cal procedures and automated calibrations are becoming increasingly prevalent, manual data entry becomes less of a cost driver than previously. Moreover, in cases where data are entered manually, the benefit of recording the results of parameter calibrations can be easily shown to outweigh the cost. This is especially true if parameter as-found attributes data are replaced by as-found and as-left variables data.

With regard to analysis methodology, the same MLE methods used to analyze attributes data at the item level can be used to analyze attributes data at the parameter level.

Another factor in interval analysis in today's environment is that we are beginning to see the emergence of commercially available calibration data management systems that feature both attributes and variables data collection [22 - 26]. While such systems are not "mom and pop" level cheap, in large or even moderately sized operations, they can offer a significant return on investment.

3 Parametric Interval Analysis

As the above indicates, either attributes or variables calibration history data can be maintained and analyzed. The virtues and drawbacks of working with each type of data are discussed below.

3.1 Attributes Data Analysis

The feasibility of interval analysis of parametric attributes data is based on the following points:

- Methods are well established [5, 8, 10, 14, 17].
  - MLE methods
  - Reliability modeling tools
- Algorithms are available for adjusting item recall cycles using parameter calibration intervals [7, 12].
  - Adjustment using parameter reliability targets
  - Adjustment using item level reliability targets
  - Adjustment for stratified calibration[4]
  - Application of reliability targets to individual parameters or parameter subsets
- Identification of problem parameters is expedited.
- Data are taken that allow risk analysis and management at the parameter level.
- The utility of history data is less sensitive to calibration procedure changes, except in cases where tolerance limits are altered.

3.2 Variables Data Analysis

Interval analysis of parametric variables data yields all the benefits of the analysis of parametric attributes data listed above. Additional benefits are listed below.

- Parameter values and bias uncertainties can be projected as functions of time elapsed since calibration.

[4] Stratified calibration is a practice in which only parameters that need calibration are calibrated at a given recall cycle. Individual parameter intervals are set at multiples of the parameter with the shortest interval.

- Either EOP reliability targets or EOP uncertainty targets can be met.
- The utility of history data is rarely affected by calibration procedure changes.
- Meaningful feedback control can be established for parameters found out-of-tolerance at calibration [20].
- The "shelf-life" problem, in which delays exist between calibration and receipt for service or return to service, can be more readily dealt with than with attributes data.
- Less data are needed to produce viable intervals than with attributes data analysis.[5]
- Parameter bias drift trends can be displayed using SPC-style charts.
- As-found data as well as drift information can be provided to MTE users, if desired.

The only potential drawbacks of variables data analysis as compared to attributes data analysis are (1) that, while articles have been written providing analysis methodologies [15, 16], a widely accepted analytical methodology has not yet been established within the metrology community and (2) variables data entry seems at first to be more time consuming than attributes data entry. This paper is intended as a step toward overcoming the first drawback. As for the second, it can be argued that the time and effort required to assess whether a measured value is out-of-tolerance may be more costly than the time required to simply enter the measurement result and let data processing do the rest.

4 Analysis of Variables Data

The application of variables data to calibration interval analysis involves establishing a functional relationship or "drift model" between resubmission time t and parameter bias drift $\delta(t)$

$$\delta(t) \cong \hat{\delta}(t, \boldsymbol{\theta}), \tag{1}$$

where $\boldsymbol{\theta}$ is a vector of drift model coefficients.

A resubmission time is defined as the time elapsed between a parameter's calibration date and its previous calibration date.[6] Bias drift is defined as the difference between the parameter's as-found value at one calibration and its as-left value at its previous calibration.

4.1 Assumptions

As Eq. (1) shows, a bias drift model is determined by its functional form and by the values of its coefficients. In this paper the functional form will be assumed to be a polynomial of arbitrary degree whose coefficient values can be estimated using regression analysis. The treatment in the paper also assumes that an unweighted fit is appropriate. Weighted fits will be treated in future publications and in an upcoming release of NCSLI's RP-1.[7] As mentioned earlier, the variable δ is assumed to be normally distributed with mean $y(t)$ and variance σ^2.

The minimum data elements needed for unweighted fits are exemplified in Table 1.

Table 1. Example raw data sample showing the minimum fields required for estimating calibration intervals using unweighted fits.

Service Date	As-Found Value	As-Left Value	Calibration Uncertainty
29-Mar-03	5.173	5.073	0.2700
11-Jul-03	5.123	5.048	0.2825
31-Dec-03	4.633	4.993	0.2771
15-May-04	4.915	5.126	0.2700
29-Oct-04	5.086	5.024	0.2825

[5] See Method S2 in RP-1 [14].

[6] Some adjustment for shelf life may be made, if needed.

[7] A methodology for weighted fits for the first degree polynomial model was reported by Castrup [15].

23-Jan-05	4.913	5.208	0.2771
03-Apr-05	5.108	5.451	0.2759

5 Regression Analysis

Imagine that we observe n pairs of as-found and prior as-left values with corresponding resubmission times. Let Y_i represent the as-found parameter value at time X_i whose prior as-left value is y_i taken at time x_i. We form the variables

$$\delta_i = Y_i - y \tag{2}$$

and

$$t_i = X_i - x_i\,, \tag{3}$$

note that $\delta(0) = 0$, and write the bias drift model as

$$\hat{\delta}_i = b_1 t_i + b_2 t_i^2 + \cdots + b_m t_i^m\,. \tag{4}$$

We use regression analysis on the sample of observed bias drifts and resubmission times to solve for the coefficients $b_j, j = 1, 2, \cdots, m$. In Section 6, the degree of the polynomial m will be treated as a variable to be determined based on goodness of fit. Figure 1 shows a first degree ($m = 1$) polynomial regression fit for the data of Table 1.

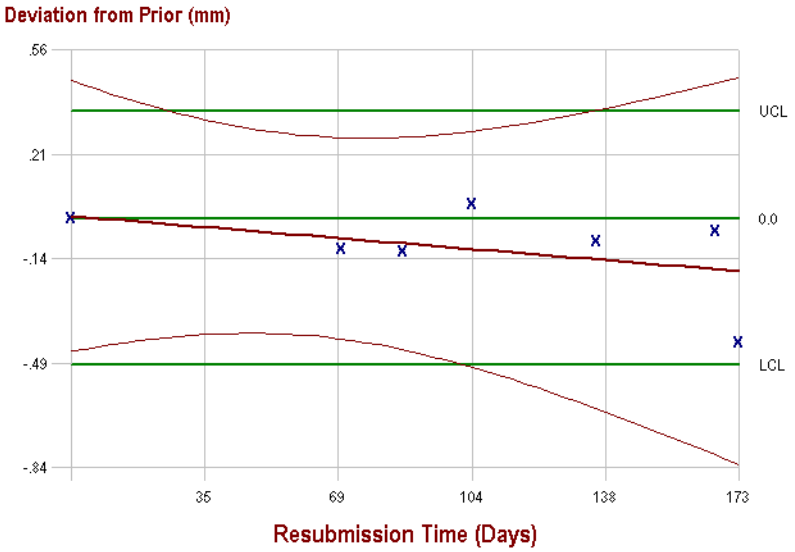

Figure 1. First degree regression fit to the data of Table 1. The variable δ is shown as "Deviation from Prior."

5.1 Residual Sum of Squares

The regression analysis consists of finding an unweighted fit to the variables δ. For an unweighted fit, each drift value or sampled "deviation" is treated equally, and the residual sum of squares is given by

$$\mathrm{RSS} = \sum_{i=1}^{k} \left(\delta_i - \hat{\delta}_i\right)^2\,, \tag{5}$$

where δ_i is the ith observed deviation and $\hat{\delta}_i$ is computed from the value t_i using Eq. (4). The coefficients of the model are solved for by minimizing RSS.

5.2 Regression Model Coefficients

The solutions for the coefficients are most readily obtained using matrices. These solutions are given by

$$\mathbf{b} = \left(\mathbf{T}'\mathbf{T}\right)^{-1}\mathbf{T}'\mathbf{D}\,, \tag{6}$$

where

$$\mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix} \quad \mathbf{T} = \begin{pmatrix} t_1 & t_1^2 & t_1^3 & \cdots & t_1^m \\ t_2 & t_2^2 & t_2^3 & \cdots & t_2^m \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ t_n & t_n^2 & t_n^3 & \cdots & t_n^m \end{pmatrix} \quad \mathbf{D} = \begin{pmatrix} \delta_1 \\ \delta_2 \\ \vdots \\ \delta_n \end{pmatrix}, \tag{7}$$

and **T**' is the transpose of **T**.

5.3 Variance-Covariance Matrix

The variance-covariance is used to estimate uncertainties in values of δ projected using Eq. (4). The matrix is given by

$$\mathbf{V} = (\mathbf{T}'\mathbf{T})^{-1}\mathbf{S}, \tag{8}$$

where the *m* x *m* diagonal matrix **S** is

$$\mathbf{S} = \begin{pmatrix} s^2 & & 0 \\ & \ddots & \\ 0 & & s^2 \end{pmatrix}. \tag{9}$$

The quantity s^2 , is an estimate of σ^2, the variance in the deviations. It is computed according to

$$s^2 = \frac{\text{RSS}}{n-m}. \tag{10}$$

The square root *s* is called the *standard error of estimate*. It represents the typical amount by which actual values of δ differ from the estimated values $\hat{\delta}$.

With the above equation for **V**, the variances of the estimated coefficients and the covariances between coefficients are solved for, since

$$\mathbf{V} = \begin{bmatrix} \text{var}(b_1) & \text{cov}(b_1,b_2) & \text{cov}(b_1,b_3) & \cdots & \text{cov}(b_1,b_m) \\ \text{cov}(b_2,b_1) & \text{var}(b_2) & \text{cov}(b_2,b_3) & \cdots & \text{cov}(b_2,b_m) \\ \text{cov}(b_3,b_1) & \text{cov}(b_3,b_2) & \text{var}(b_3) & \cdots & \vdots \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ \text{cov}(b_m,b_1) & \cdots & \cdots & \cdots & \text{var}(b_m) \end{bmatrix}, \tag{11}$$

where

$$\text{var}(b_i) = \text{variance of } b_i, \quad i = 1,2,\cdots,m,$$

and

$$\text{cov}(b_i,b_j) = \text{covariance between } b_i \text{ and } b_j, \; i = 1,2,\cdots,m \quad j = 1,2,\cdots,m \quad i \neq j.$$

Note that

$$\text{cov}(b_i,b_j) = \text{cov}(b_j,b_i) \quad i \neq j.$$

5.4 Predicted Values and Uncertainties

Using the above matrices, a value $\hat{\delta}$ is computed for a given value of *t* according to

$$\hat{\delta}(t) = \mathbf{t}'\mathbf{b}, \tag{12}$$

where

$$\mathbf{t}' = \begin{pmatrix} t & t^2 & t^3 & \cdots & t^m \end{pmatrix}. \tag{13}$$

The variance in $\hat{\delta}$ is estimated using

$$\text{var}[\hat{\delta}(t)] = \mathbf{t}'\mathbf{V}\mathbf{t}, \tag{14}$$

where **t** is the transpose of **t'**. The quantity $\sqrt{\text{var}[\hat{\delta}(t)]}$ is the standard error in a predicted mean value of δ for a given value of t. Since the actual value of δ varies about the true mean value with a variance estimated by s^2, the variance of an *individual* predicted value is given by

$$s_{\delta|t}^2 = s^2 + \mathbf{t}'\mathbf{V}\mathbf{t}\, s^2 .$$

The quantity

$$s_{\delta|t} = s\sqrt{1 + \mathbf{t}'\mathbf{V}\mathbf{t}} \tag{19}$$

is called the *standard error of the forecast*. It represents the uncertainty in a projected individual value of δ, given a value of t.

6 Bias Drift Model Selection

Selecting the best model is equivalent to selecting the polynomial degree m that best represents the relationship between drift and time. While it is often the case that a larger value of m will produce a fit that seems to follow the observed data better than a smaller value of m, it may be that the larger value of m does not represent the drift-time relationship as well as the smaller value.

Accordingly, the best model is selected as the model with the lowest standard error of estimate s. The following algorithm applies to an analysis in which it has been determined that the largest realistic value for m is some integer q.[8]

$s_{min} = 10^{307}$
$m = 1$
For $k = 1$ to q
    Fit the model $\hat{\delta}_k = b_1 t + \cdots + b_k t^k$
    Compute the variance $s_k^2 = \dfrac{1}{n-k}\sum_{i=1}^{n}(\delta_i - \hat{\delta}_{k,i})^2$
    If $s_k < s_{min}$ then
        $s_{min} = s_k$
        $m = k$
    End If
Next

7 Determining Calibration Intervals

Having established a regression fit for $\delta(t)$, we can project parameter values. Letting t represent time elapsed since calibration and letting $\hat{y}(t)$ represent projected value, we have

$$\hat{y}(t) = y_0 + \hat{\delta}(t)\,, \tag{20}$$

where y_0 is the estimated (measured) parameter value at the beginning of the calibration interval ($t = 0$) and $\hat{\delta}(t)$ is computed using Eq. (12).

Imagine that the nominal value of the parameter of interest is bounded by lower and upper tolerance limits $-L_1$ and L_2. If we knew the initial value, then we might suppose at first sight, that the approach to take in estimating a calibration interval would be to enter the initial value y_0 in Eq. (20) and solve for the time t required for $\hat{y}(t)$ to cross either $-L_1$ or $+L_2$.[9]

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[8] This number is usually ≤ 3. Larger values tend to produce unstable predictions for values of t larger than the largest observed value.

[9] We assume that $-L_1 \le y_0 \le L_2$.

This method, while conceptually palatable, is not recommended. Instead, we use two alternative approaches. In the first approach, labeled the *Reliability Target Method*, the calibration interval is established as the time corresponding to the point where the confidence that the parameter is in-tolerance drops to some minimum acceptable level, given by $1 - \alpha$. The variable α is usually something like 0.05, 0.01, etc. In the second approach, labeled the *Uncertainty Target Method*, the calibration interval is established as the time required for the uncertainty in $\hat{y}(t)$ to reach a maximum acceptable value.

7.1 Reliability Target Method

The probability or confidence that a parameter is in-tolerance is commonly referred to as *measurement reliability*. Accordingly, the approach for adjusting intervals to meet a given level of probability or confidence is labeled the *reliability target method*. We will now examine this method as applied to several alternative tolerancing options.

7.1.1 Two-Sided General Case: Asymmetric Tolerances

We consider a situation in which the upper and lower tolerance limits may not be equal. Suppose that the desired confidence for $\hat{y}(t)$ being confined to values less than L_2 is 1 - α and the desired confidence for $y(t)$ being restricted to values greater than $-L_1$ is 1 - β.

We seek a solution T as the lesser of T_1 and T_2 in the expressions

$$-L_1 = \hat{y}(T_1) - t_{\beta,\nu}\sqrt{u_0^2 + s_{\delta|T_1}^2} \; . \tag{21}$$

and

$$L_2 = \hat{y}(T_2) + t_{\alpha,\nu}\sqrt{u_0^2 + s_{\delta|T_2}^2} \; , \tag{22}$$

In these expressions, the variables $t_{\alpha,\nu}$ and $t_{\beta,\nu}$ are the t-statistics for confidence levels of $1 - \beta$ and $1 - \alpha$, respectively, with $\nu = n - m - 1$ degrees of freedom. The quantities $s_{\delta T}$ are computed using Eq. (19). The variable u_0 is the standard uncertainty in the value of y_0. For the present discussion, this uncertainty is equated to the uncertainty due to calibration process error.

Solutions for T_1 and T_2 are obtained by iteration. A good method to use is the bisection method [21]. This method starts by finding values of a variable t that yield positive and negative bracketing values for the functions

$$H_1 = \hat{y}(t) + t_{\alpha,\nu}\sqrt{u_0^2 + s_{\delta|t}^2} + L_1$$

and

$$H_2 = \hat{y}(t) + t_{\alpha,\nu}\sqrt{u_0^2 + s_{\delta|t}^2} - L_2 \; .$$

Values of t are iterated until $|H_1|$ or $|H_2|$ reaches some predetermined level of precision ε.[10] The minimum value of t that yields this result becomes the calibration interval T.

[10] The value 0.0001 has been found to be sufficient [19].

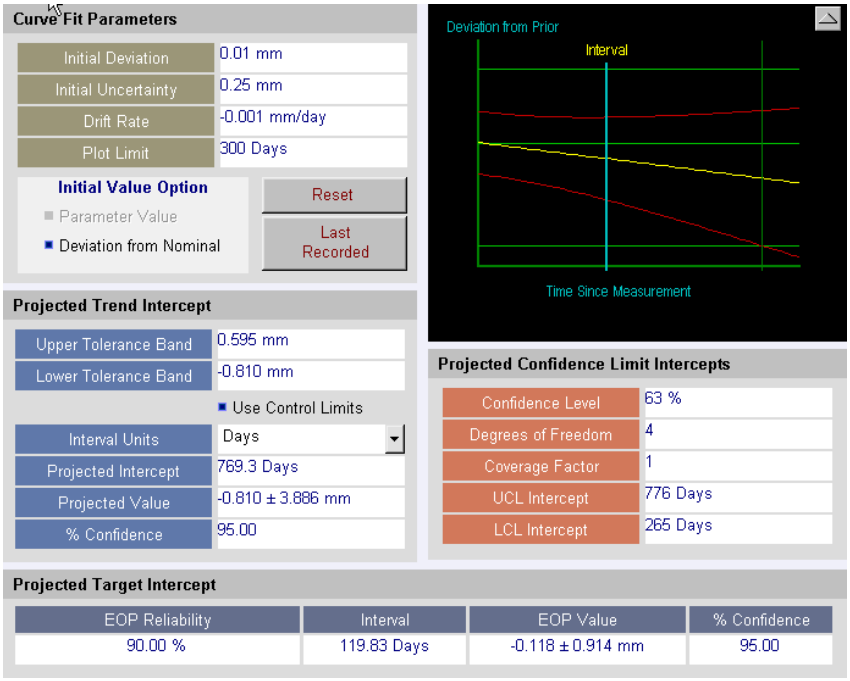

Figure 2. Interval adjustment to a minimum allowed in-tolerance probability. The projected interval of approximately 120 days reflects an initial value of 0.01 mm, an initial uncertainty u_0 of 0.25 mm, and corresponds to a confidence level of 90%. The projected bias at the end of the interval is -0.118 mm ±0.914 mm with 95% confidence. Note that the upper and lower control limits are asymmetric.[11]

Figure 2 shows a case where the interval is adjusted for an in-tolerance confidence level of 80%. The adjustment uses the regression analysis results of Figure 1.

7.1.2 General Single-Sided Upper Limit Case

For cases where the parameter of interest has only a single "not to exceed" tolerance limit L, we attempt to set a calibration interval that corresponds to a minimum acceptable confidence level 1 - α that the parameter's value will be less than or equal to L. The relevant expression is

$$L = \hat{y}(T) + t_{\alpha,\nu}\sqrt{u_0^2 + s_{\delta|T}^2} \ ,$$

The solution for the interval T employs the bisection method, iterating the variable t in the function

$$H = \hat{y}(t) + t_{\alpha,\nu}\sqrt{\text{var}[\hat{y}(t)]} - L$$

until $|H| \leq \varepsilon$.

7.1.3 General Single-Sided Lower Limit Case

In this case, we attempt to determine a calibration interval that corresponds to a minimum acceptable confidence level 1 - α that the parameter's value will be greater than or equal to L. The relevant expression is

$$L = \hat{y}(T) - t_{\alpha,\nu}\sqrt{u_0^2 + s_{\delta|T}^2} \ ,$$

The solution for the interval T employs the bisection method, iterating the variable t in the function

$$H = \hat{y}(t) - t_{\alpha,\nu}\sqrt{u_0^2 + s_{\delta|T}^2} - L$$

until $|H| \leq \varepsilon$.

[11] Computed with SPCView [19].

7.2 Uncertainty Target Method

We return to the assertion that the uncertainty in a projected parameter value increases with time elapsed since measurement. The approach for controlling this uncertainty to a maximum allowable value is labeled the *uncertainty target method*.

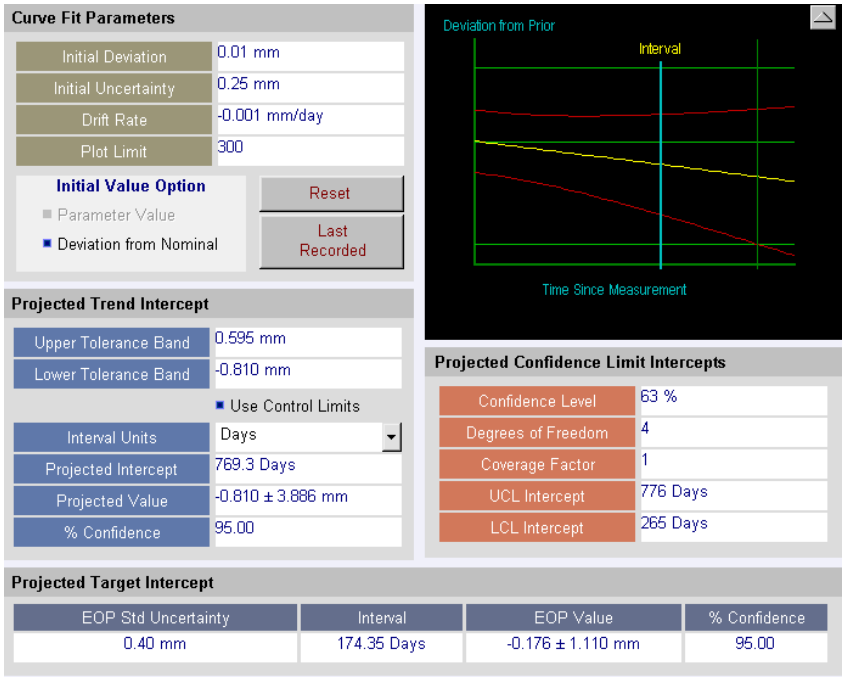

Figure 3. Interval adjustment to a maximum allowed bias uncertainty. The example shown reflects an initial uncertainty u_0 of 0.25 mm and a drift rate of –0.001 mm/day. The time required for the bias uncertainty to reach the maximum allowable value of 0.40 mm is approximately 174 days. The projected bias at the end of that interval is -0.176 mm ±1.110 mm with 95% confidence.[12]

With this method, the tolerance of the parameter of interest is not a factor. Instead, we solve for the time T that it takes the uncertainty in the parameter bias to grow from an initial value u_0 to some maximum allowable target value u_{targ}.

The relevant expression is

$$u_{targ}^2 = u_0^2 + s_{\delta|T}^2 \,.$$

Solving for the T employs the bisection method on the function

$$H = u_0^2 + s_{\delta|T}^2 - u_{targ}^2$$

until $|H| \leq \varepsilon$. Figure 3 shows the application of the uncertainty target method to the analysis results of Figure 1.

8 Conclusion

A method has been presented for determining calibration intervals for parameters whose value drifts with time with constant statistical variance. The method utilizes variables data in the analysis of the time-dependence of deviations between as-left and as-found values taken during calibration. The deviations consisted of the difference between a parameter's as-found value at a given calibration and its as-left value at a prior calibration. Each deviation had a

[12] Computed with SPCView [19].

corresponding resubmission time equal to the time elapsed between calibrations. All deviations were assigned equal weight.

As has been shown, the analysis of variables data offers advantages over attributes data analysis. For instance, variables data analysis can yield calibration intervals that meet either EOP reliability targets or satisfy maximum allowable uncertainty criteria. Another advantage is that, with variables data, the uncertainty in the value or bias of a parameter can be easily projected as a function of time elapsed since calibration. Other advantages are listed in Section 3.2.

These advantages suggest that, given the growing emergence of calibration data management systems that collect as-found and as-left measured values, the computing power of today's PC's and the availability of cheap data storage, variables data analysis is the future for the establishment and adjustment of calibration intervals.

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