

## On Exact Multiple-Use Linear Calibration Confidence Intervals

<sup>1</sup>V. Witkovský

<sup>1</sup>Institute of Measurement Science, Slovak Academy of Sciences, Bratislava, Slovakia  
Email: witkovsky@savba.sk

**Abstract.** *The multiple-use calibration problem is a problem of constructing appropriate simultaneous interval estimators (calibration confidence intervals) for values of the variable of primary interest, say  $x$ , based on possibly unlimited sequence of future observations of the response variable, say  $y$ , and on the results of the given calibration experiment, which was modeled/fitted by a linear regression model. Such calibration intervals can be obtained by inverting the simultaneous tolerance intervals constructed for the regression (calibration) function.*

*Keywords: Multiple-Use Calibration, Linear Regression Model, Simultaneous Tolerance Intervals, Calibration Confidence Intervals*

### 1. Introduction

In many experimental sciences, acquisition of the measurement results frequently requires measurement procedures involving instrument calibration which can be modeled as linear (polynomial) regression problem. Then, the required measurement result, say  $x$ , is obtained through measuring the observable response variable, say  $y$ , and by inverting the fitted regression (calibration) function. Here we consider a problem of constructing and computing the appropriate (exact according to the definition given below) confidence intervals for the unobservable values of the explanatory variable  $x$ , based on given fitted calibration function (a result of the calibration experiment), for possibly unlimited sequence of future observations of the response variable  $y$  (which are assumed to be independent of the calibration experiment and based on the assumption that the considered regression model was correctly specified).

As proposed by Scheffé (1973), such calibration intervals for  $x$  values can be obtained from simultaneous tolerance intervals for the considered regression (calibration) function, with warranted minimum  $(1 - \gamma)$ -content for all such intervals simultaneously, and with confidence at least  $(1 - \alpha)$ , for selected small probabilities  $\gamma$  and  $\alpha$ . The interpretation of this requirement is that such simultaneous tolerance intervals will cover at minimum  $(1 - \gamma) \times 100\%$  content of all values  $y$  from the same (unknown) population and this will be true in more than  $(1 - \alpha) \times 100\%$  of hypothetical calibration experiments.

However, the known simultaneous tolerance intervals in regression are typically conservative in that the actual confidence level exceeds the required nominal level  $(1 - \alpha)$ , and as such are generally broader than they necessarily should be. For a brief overview of the methods for simultaneous tolerance intervals in linear regression and suggested improvements see e.g. Chvosteková (2013). For more details on tolerance intervals see Mathew and Krishnamoorthy (2009).

The exceptions leading to narrower intervals are the simultaneous tolerance intervals as proposed by Mee et al. (1991) and Mathew and Zha (1997), however, they are based on slightly changed requirements. That is, the warranted properties of such simultaneous tolerance intervals are either valid on restricted range only, i.e. on a given and fixed interval  $x \in (x_{min}, x_{max})$ , and/or the requirement of warranted minimum content  $(1 - \gamma)$  for all

intervals is changed by the requirement that the average content is warranted to be  $(1 - \gamma)$ , for more detailed discussion see e.g. Mee and Eberhardt (1996). Moreover, the suggested methods and algorithms for computing such tolerance intervals seem to be too complicated for practical purposes.

## 2. Subject and Methods

We shall assume that the calibration experiment, say  $\mathcal{E}$ , is modeled by the linear regression model  $y = X\beta + \varepsilon$ , where  $y$  is  $n$ -dimensional vector of responses measured for  $n$  values  $x_i$ ,  $i = 1, \dots, n$ , of the explanatory variable  $x \in \mathcal{X} \subseteq \mathbb{R}^q$ . However, here we shall assume that the explanatory variable is one-dimensional, i.e. that  $x \in (x_{min}, x_{max}) \subseteq \mathbb{R}$ . Further, the matrix  $X$  represents the  $n \times (p + 1)$ -dimensional calibration experiment design matrix with rows  $f(x_i)'$  for  $i = 1, \dots, n$ , i.e.  $(p + 1)$ -dimensional functions of  $x_i$ .  $\beta$  is the  $(p + 1)$ -dimensional vector of regression coefficients and  $\varepsilon$  is  $n$ -dimensional vector of (homoscedastic) measurement errors with its assumed distribution  $\varepsilon \sim N(0, \sigma^2 I_n)$ .

For example, in simple  $p$ -order polynomial linear regression model we get  $f(x_i) = (1, x_i, x_i^2, \dots, x_i^p)'$  for  $x_i \in \mathcal{X} = (x_{min}, x_{max})$ . Based on the calibration experiment  $\mathcal{E}$  we get the best linear unbiased estimator (the least squares estimator) of the calibration function  $X\hat{\beta} = X(X'X)^{-1}X'y$  and the estimator of the measurement error variance  $S^2 = \frac{1}{\nu}(y - X\hat{\beta})'(y - X\hat{\beta})$ , with mutually independent distributions of the variables  $\frac{\hat{\beta} - \beta}{\sigma^2} \sim N(0, (X'X)^{-1})$  and  $\frac{S^2}{\sigma^2} \sim \frac{1}{\nu}\chi_{\nu}^2$ , where  $\nu = n - (p + 1)$ .

In the first step, given the results of the calibration experiment  $\mathcal{E}$ , we shall construct the simultaneous tolerance intervals for all possible future realizations of the response variable  $Y(x) = f(x)'\beta + \sigma Z$  (where  $x \in \mathcal{X}$  and  $Z \sim N(0, 1)$  is independent of the calibration experiment  $\mathcal{E}$ ), say  $(L_{x,\mathcal{E}}, U_{x,\mathcal{E}})$ , and such that

$$\Pr_{\{\mathcal{E}\}} \left( \Pr_{\{Y(x)\}} \left( L_{x,\mathcal{E}} \leq Y(x) \leq U_{x,\mathcal{E}} \mid \mathcal{E} \right) \geq 1 - \gamma, \text{ for all } x \in \mathcal{X} \right) = 1 - \alpha. \quad (1)$$

The two-sided simultaneous tolerance intervals,  $(L_{x,\mathcal{E}}, U_{x,\mathcal{E}})$ , are typically given in the form

$$L_{x,\mathcal{E}} = f(x)'\hat{\beta} - k(x)\sqrt{S^2}, \quad U_{x,\mathcal{E}} = f(x)'\hat{\beta} + k(x)\sqrt{S^2}, \quad (2)$$

where by  $k(x)$  we denote the required tolerance factors evaluated at  $x \in \mathcal{X}$ .

In the second step, for given observation  $Y_* = Y(x_*)$ , we shall construct the calibration confidence interval for the unobservable value of the explanatory variable, say  $x^* \in \mathcal{X}$ , by inverting the simultaneous tolerance intervals. So, the calibration confidence interval is given by the random set

$$\mathcal{S}(Y_*, \mathcal{E}) = \{x \in \mathcal{X} : Y_* \in (L_{x,\mathcal{E}}, U_{x,\mathcal{E}})\}. \quad (3)$$

Notice, that the set (3) is not necessarily an interval. However, for most practical situations where the calibration function is (significantly) strictly monotonic, the confidence set (3) typically results in an interval. Based on (1) and (3) we directly get basic probability property of the calibration confidence intervals:

$$\Pr_{\{\mathcal{E}\}} \left( \Pr_{\{Y(x_*)\}} \left( x^* \in \mathcal{S}(Y(x_*), \mathcal{E}) \mid \mathcal{E} \right) \geq 1 - \gamma \right) = 1 - \alpha. \quad (4)$$

### 3. Results

Here, we propose to consider a new method for computing the tolerance factors of the simultaneous tolerance intervals in linear regression by a straightforward generalization of the method for computing the tolerance factors for simultaneous tolerance intervals for  $m$  independent normal populations.

For given parameters  $d_x$ ,  $\nu$  and  $m$ , let  $k_x = k(d_x, \nu, m)$  be a solution to the following integral equation

$$2m \int_0^\infty \Pr_{\{Q_\nu\}} \left( Q_\nu \geq \frac{\nu \chi_{1,1-\gamma}^2(d_x z^2)}{k_x^2} \right) (2\Phi(z) - 1)^{m-1} \phi(z) dz = 1 - \alpha, \quad (5)$$

where  $d_x = f(x)'(X'X)^{-1}f(x)$  is the scale parameter at location  $x \in \mathcal{X}$ ,  $\nu$  represents the degrees of freedom used in estimation of the measurement error variance, and  $m \geq 1$  represents the parameter of simultaneosity, i.e. the number of independent normal populations for which the simultaneous tolerance intervals are to be constructed. Notice that for  $m = 1$  the tolerance factors given by (5) define the non-simultaneous tolerance intervals.

Further,  $\Phi(\cdot)$  denotes the CDF and  $\phi(\cdot)$  the PDF of the standard normal distribution, and  $Q_\nu \sim \frac{1}{\nu}\chi_\nu^2$  is a chi-square distributed random variable with  $\nu = n - q$  degrees of freedom ( $n$  denotes the sample size of the calibration experiment and  $q$  denotes the rank of the linear regression model design matrix  $X$  used for calibration). The probability  $1 - \alpha$  is the required nominal confidence level and  $\chi_{1,1-\gamma}^2(\delta^2)$  denotes the  $(1 - \gamma)$ -quantile of the non-central chi-squared distribution with 1 degree of freedom and the non-centrality parameter  $\delta$  ( $1 - \gamma$  is the required coverage/content of the tolerance interval).

For more details on derivation of the equation (5) see Mathew and Krishnamoorthy (2009), and their equations (1.2.3), (1.2.4), (2.5.7) and (2.5.8).

The suggested form of the proposed tolerance factors is  $\tilde{k}_x = k(d_x, \nu, \tilde{m})$ , where  $\tilde{m}$  denotes the appropriate value of the simultaneosity parameter, i.e. such value of  $\tilde{m} \geq 1$  (minimal possible) that the following criterion is fulfilled

$$\Pr_{\{B, Q_\nu\}} \left( \min_{x \in \mathcal{X}} \left\{ \Phi \left( f(x)'B + \tilde{k}_x \sqrt{Q_\nu} \right) - \Phi \left( f(x)'B - \tilde{k}_x \sqrt{Q_\nu} \right) \right\} \geq 1 - \gamma \right) = 1 - \alpha. \quad (6)$$

Here  $B \sim N(0, (X'X)^{-1})$  and  $Q_\nu \sim \frac{1}{\nu}\chi_\nu^2$  are independent random variables (which represent/model the variability of estimated parameters resulted from all hypothetical calibration experiments), and  $\mathcal{X}$  denotes the set of all potential values of the explanatory variable  $x$  in a possibly infinite sequence of future independent observations  $Y(x) = f(x)'\beta + \sigma Z$ ,  $Z \sim N(0, 1)$ , with  $d_x = f(x)'(X'X)^{-1}f(x)$ .

In linear regression model with  $p = 1$  we get  $f(x)'\beta = (1, x)(\beta_1, \beta_2)' = \beta_1 + \beta_2 x$ , with order  $p = 3$  we get  $f(x)'\beta = (1, x, x^2, x^3)(\beta_1, \beta_2, \beta_3, \beta_4)' = \beta_1 + \beta_2 x + \beta_3 x^2 + \beta_4 x^3$ .

Notice that here  $\tilde{m}$  can be any real number such that  $\tilde{m} \geq 1$ . The parameter  $\tilde{m}$  represents the complexity of the regression function  $f(x)'\beta$  over the considered range  $x \in \mathcal{X}$ .  $\tilde{m}$  depends on the on the design of the calibration experiment  $\mathcal{E}$ : the polynomial order  $p$ , the considered set  $\mathcal{X}$ , the design matrix  $X$ , and the degrees of freedom  $\nu$ . For example, in simple linear regression (polynomial of the order  $p = 1$ ) the value  $\tilde{m} = 2$  is a good starting point for

numerical (iterative) search procedure (i.e. the complexity of the simple linear regression function for all  $x \in \mathcal{X}$  is similar to the complexity of two independent normal populations). We have developed the MATLAB algorithm for efficient computation of the tolerance factors as defined by the integral equation (5).

An earlier version of the algorithm is available at the web page <http://www.mathworks.com/matlabcentral/fileexchange/24135-tolerancefactor>. The implementation of the algorithm suitable also for computing the tolerance factors as defined by the equations (5) and (6) and the related calibration confidence intervals (3) is currently under development and will be available on request from the author.

#### 4. Discussion

The new method for simultaneous tolerance intervals in linear regression was compared for several special situations with the methods for constructing simultaneous tolerance intervals as proposed by Mee et al (1991) and by Chvosteková (2013). Based on such preliminary studies, the new intervals lead to narrower simultaneous tolerance intervals with guaranteed minimum coverage  $(1 - \gamma)$  and the exact confidence level  $(1 - \alpha)$ .

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#### References

- [1] Scheffé H. A Statistical Theory of Calibration. *Annals of Statistics*, 1(1): 1-37, 1973.
- [2] Krishnamoorthy K, Mathew T. Statistical Tolerance Regions: Theory, Applications, and Computation. John Wiley & Sons, Inc., Hoboken, New Jersey, 2009.
- [3] Chvosteková M. Simultaneous Two-Sided Tolerance Intervals for a Univariate Linear Regression Model. *Communications in Statistics - Theory and Methods*, 42(7): 1145-1152, 2013.
- [4] Mee RW, Eberhardt KR, Reeve CP. Calibration and Simultaneous Tolerance Intervals for Regression. *Technometrics*, 33(2): 211-219, 1991.
- [5] Mee RW, Eberhardt KR. A Comparison of Uncertainty Criteria for Calibration. *Technometrics*, 38(3): 221-229, 1996.
- [6] Mathew T, Zha W. Multiple Use Confidence Regions in Multivariate Calibration. *Journal of the American Statistical Association*, 92(439) 1141-1150, 1997.