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Multiple Use Confidence Intervals for a Univariate Statistical Calibration

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The statistical calibration problem treated here consists of constructing the interval estimates for future unobserved values of a univariate explanatory variable corresponding to an unlimited number of future observations of a univariate response variable. An interval estimate is to be computed for a value x of an explanatory variable after observing a response Y_x by using the same calibration data from a single calibration experiment, and it is called the multiple use confidence interval. It is assumed that the normally distributed response variable Y_x is related to the explanatory variable x through a linear regression model, a polynomial regression is probably the most frequently used model in industrial applications. Construction of multiple use confidence intervals (MUCI's) by inverting the tolerance band for a linear regression has been considered by many authors, but the resultant MUCI's are conservative. A new method for determining MUCI's is suggested straightforward from their marginal property assuming a distribution of the explanatory variable. Using simulations, we show that the suggested MUCI's satisfy the coverage probability requirements of MUCI's quite well and they are narrower than previously published. The practical implementation of the proposed MUCI's is illustrated in detail on an example.

Keywords: Statistical calibration, linear regression model, tolerance interval, multiple use confidence interval.

1. Introduction

Univariate linear regression model $Y_x = f^T(x)\beta + \varepsilon, \varepsilon \sim N(0,\sigma^2)$, where ε is an error, Y_x is an observation corresponding to a value x, $f^T(x)$ is a q-dimensional known function of value x, vector $\beta = (\beta_0, \beta_1, \ldots, \beta_{q-1})^T$ and $\sigma^2 > 0$ are the unknown parameters of the model, is used in many applications. For example, the 2-order polynomial regression (i.e., $q = 3$, $f^T(x) = (1,\ x,\ x^2)$) was used to model the relationship between a one-dimensional response variable Y_x and a one-dimensional explanatory variable x in the example at the end of Section 3. The statistical calibration is typically motivated by the problem of estimating x for a subject in the case when measuring corresponding Y_x is relatively easier and it does not require so much effort or expenses, etc. It means that we want to make a statistical inference about x, but it is possible to measure only the dependent variable Y_x. A relation between the variables is fitted based on calibration data from a calibration experiment. In this article we suppose a univariate controlled calibration, i.e. in a calibration experiment $\mathscr{E}_n = \{(x_i, Y_{x_i}), i = 1,2,\ldots,n\}$ the value x_i, $i = 1,\ldots,n$ is treated as a known scalar and a response Y_{x_i}, $i = 1,\ldots,n$ is assumed to be a random variable. The calibration experiment is often designed so that the chosen values $x_1,\ldots,x_n$ span the range of the possible values, $\mathscr{X} = [x_{min}, x_{max}] \subset R$, and it is worth emphasizing that $f^T(x)\beta$ is a monotonic function on $\mathscr{X}$. An overview of statistical calibration tasks is provided in Osborne [15].

The statistical calibration problem treated here is to construct the interval estimates for the unknown independent values $x_{n+1}, x_{n+2}, \ldots$, corresponding to an unlimited sequence of additional observations $Y_{x_{n+1}}, Y_{x_{n+2}}, \ldots$ using the same calibration data, i.e. using the same estimates of the unknown parameters β, σ^2. Two sources of error must be taken into account in the problem, the uncertainty of the estimates of unknown parameters of the model from the calibration data, and the uncertainty of all future responses. Eisenhart [3] demonstrated that a $(1-\alpha)$-confidence set for a single future x can be obtained by inverting a $(1-\alpha)$-prediction interval in a linear regression. It means that the limits for the true x-value after observing the response Y_x are determined as the intersections of the $(1-\alpha)$-prediction band with the straight line $y = Y_x$, see Fig.1. If the fitted regression line was not strictly monotone on $\mathscr{X}$, we would get an ambiguous solution (i.e., we would find more than two intersections of the horizontal line $y = Y_x$ with a band around such a fitted calibration curve). Since the interval estimates for $x_{n+1}, x_{n+2}, \ldots$ are constructed by using repeatedly the same estimates of unknown parameters β, σ^2, we would like to make a simultaneous confidence statement about them. It must be pointed out that it is an incorrect interpretation that $100(1-\alpha)$ % of the interval estimates for $x_{n+1}, x_{n+2}, \ldots$ determined by inverting the $(1-\alpha)$-prediction band contain the true x-value. Indeed, the coverage is much less than $100(1-\alpha)$ % and it decreases as the num-

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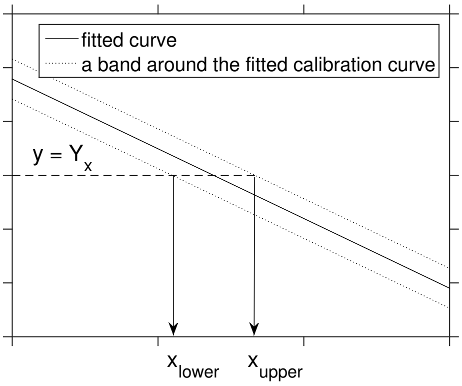

Fig. 1. Illustration of the construction of an interval estimate $[x_{lower}, x_{upper}]$ for the x-value corresponding to an observation Y_x by inverting a band around the fitted regression line.

ber of x_{n+i}'s increases. Mandel [11] considered the problem of constructing confidence sets for a prechosen number m of future responses, he suggested to invert the simultaneous prediction intervals. In literature proposed simultaneous predictions intervals (see e.g., Lieberman [9], Carlstein [2]) become extremely wide when m is large. We can conclude that the simultaneous prediction intervals cannot be used in the case of an unknown number of future observations and they are impractical for use in the case when m is large. If a prechosen number m of MUCI's is constructed by inverting the simultaneous prediction intervals, then the MUCI's contain the corresponding true values with a prescribed confidence $1-\alpha$. This strong condition, that all m constructed MUCI's contain the true x-value, was replaced with the condition that at least γ proportion of them contains the corresponding true value with a confidence $1-\alpha$ (see Acton [1], Halperin [4]). So, MUCI's are constructed by using the calibration data (i.e., by using the same estimates of β, σ^2) from a single calibration experiment $\mathscr{E}_n$ and have the property that at least a proportion γ of them contains the corresponding true x-value with confidence $1-\alpha$. The two-sided MUCI for the unknown x corresponding to a future observation Y_x is considered in Lieberman et al. [10], Scheffé [16], Mee et al. [13], Krishnamoorthy and Mathew [7], and Witkovský [17] in the closed form

$$\mathscr{I}(Y_x) = \{x \in \mathscr{X} : f^T(x)\hat{\beta} - g(x)S \leq Y_x \leq f^T(x)\hat{\beta} + g(x)S\}, \tag{1}$$

where $\hat{\beta}$ denotes the least squares estimator of β, S^2 denotes the residual mean square based on $n-q$ degrees of freedom, and $g(.)$ is a positive, unimodal function determined subject to requirements of MUCI's. It means, that the two-sided MUCI is also found as an intersection of horizontal line in $y = Y_x$ with a band around the fitted calibration curve $f^T(x)\hat{\beta} \pm g(x)S, x \in \mathscr{X}$ (see Fig.1.). If an observation Y_{x^*} is captured by the band $[f^T(x^*)\hat{\beta} - g(x^*)S, f^T(x^*)\hat{\beta} + g(x^*)S]$, then it is obvious that $\mathscr{I}(Y_{x^*})$ will contain the true value x^*. Hence, a function $g(.)$ is to be chosen so as to satisfy the condition of MUCI's, which can be expressed as $P_{\hat{\beta},S}\left(\liminf_{K\to\infty} \frac{1}{K}\sum_{i=1}^{K} \delta(x_{n+i}) \geq \gamma\right) = 1-\alpha$, where $\delta(x) = 1$ if $f^T(x)\hat{\beta} - g(x)S \leq Y_x \leq f^T(x)\hat{\beta} + g(x)S$ and 0 otherwise, and $\frac{1}{K}\sum_{i=1}^{K} \delta(x_{n+i})$ is the proportion of the intervals $\mathscr{I}(Y_{x_{n+i}})$, $i = 1, 2, \ldots, K$ which contain the true corresponding x-value. The variable $\delta(x)$ is Bernoulli distributed with success probability conditional on given $\hat{\beta}, S$:

$$C(x;\hat{\beta},S) = \\ = P_{Y_x}(f^T(x)\hat{\beta} - g(x)S \leq Y_x \leq f^T(x)\hat{\beta} + g(x)S \mid \hat{\beta}, S). \tag{2}$$

Thus, for a large number K of future observations the property of MUCI's is simplified based on the strong law of large numbers to

$$P_{\hat{\beta},S}\left(\frac{1}{K}\sum_{i=1}^{K} C(x_i;\hat{\beta},S) \geq \gamma\right) = 1-\alpha, \tag{3}$$

see e.g. Mee and Eberhardt [12], Krishnamoorthy and Mathew [7]. The condition (3) can be rewritten for the one-sided MUCI's, see Krishnamoorthy et al. [8], Krishnamoorthy and Mathew [7], Han et al.[5].

The condition (3) is a rather difficult condition to work with. A sufficient condition to the property of MUCI's to hold is the condition of the $(1-\alpha,\gamma)$-simultaneous tolerance intervals (STI's) for a linear regression model (or equivalently the $(1-\alpha,\gamma)$-tolerance band), i.e. $P_{\hat{\beta},S}\left(\min_{x\in\mathscr{X}} C(x;\hat{\beta},S) \geq \gamma\right) = 1-\alpha$. Determination of the MUCI's accomplished by inverting the STI's has been exploited by several authors, see e.g., Lieberman et al. [10], Scheffé [16], Mee et al. [13], and Witkovský [17]. The two-sided STI's presented in Mee et al. [13] and the one-sided STI's presented in Odeh and Mee [14] are exact for a multiple linear regression model. For the considered model, where the covariates are assumed to have functional relationships, the STI's become conservative, except for the case of a simple linear regression. A simulation-based method for determining the exact one-sided STI's for our considered model is suggested in Han et al. [5]. Since the same fixed functional form of function $g(.)$ is used in Han et al. [5] as in Odeh and Mee [14], the computation of the resultant MUCI's is simple, a built-in function for finding root of a function is in usually used analytical software, e.g *fzero()* in MATLAB. The Han et al. method can be modified to the two-sided case, but the resultant MUCI's, as in the one-sided case, will be conservative and it means that they will be wider than necessary.

The layout of this paper is as follows. Section 2 deals with the construction of the MUCI's suggested from the marginal property (3) assuming a distribution of the explanatory variable. Section 3 provides a numerical comparison of the MUCI's based on the exact $(1-\alpha,\gamma)$-STI's and constructed by the suggested method for the case of a simple linear regression. The application of MUCI's is illustrated on an example. Section 4 contains discussion and conclusions.

2. New multiple use confidence intervals

A future observation, $Y_x = f^T(x)\beta + \varepsilon, Y_x \sim N(f^T(x)\beta, \sigma^2)$, corresponding to a value $x \in \mathscr{X}$ is assumed to be independent of a vector of observations $Y = (Y_{x_1}, \ldots, Y_{x_n})^T$ from the calibration experiment $\mathscr{E}_n$. Let X denote a $(n \times q)$-dimensional calibration experiment design matrix with rows $f^T(x_i), i = 1, \ldots, n$. Throughout, we shall assume that $rank(X) = q$. The least squares estimator $\hat{\beta} = (X^TX)^{-1}X^TY$ of β, and the estimator of the measurement error variance $S^2 = (Y - X\hat{\beta})^T(Y - X\hat{\beta})/(n-q)$ are independent. Under the model assumptions it holds $\hat{\beta} \sim N_q(\beta, \sigma^2(X^TX)^{-1})$ and $S^2(n-q)/\sigma^2 \sim \chi^2_{n-q}$, where χ^2_{n-q} denotes a central chi-squared random variable with $n-q$ degrees of freedom.

Define independent pivotal variables

$$B = \frac{\hat{\beta} - \beta}{\sigma} \sim N_q(0_q, (X^TX)^{-1}),\ U^2 = \frac{S^2}{\sigma^2} \sim \frac{\chi^2_{n-q}}{n-q}, \quad (4)$$

where 0_q denotes the q-dimensional vector of zeros. By using the pivotal variables, the probability of covering the observation Y_x (2) can be written as

$$\begin{aligned} C(x;\hat{\beta},S) &= \\ &= P_{Y_x}\left(f^T(x)B - g(x)U \leq \frac{Y_x - f^T(x)\beta}{\sigma} \leq f^T(x)B + g(x)U\right) \\ &= \Phi\left(f^T(x)B + g(x)U\right) - \Phi\left(f^T(x)B - g(x)U\right) = C(x;B,U), \end{aligned} \quad (5)$$

where $\Phi(.)$ denotes the cumulative distribution function of the standard normal distribution. Then, the condition (3) of the MUCI's can be expressed as

$$P_{B,U}\left(\frac{1}{K}\sum_{i=1}^{K} C(x_i;B,U) \geq \gamma\right) = 1 - \alpha. \quad (6)$$

Inspired by a connection between MUCI's and a prediction interval in a linear regression, we will consider the function $g(.)$ in the following form

$$g_{new}(x) = \nu\{1 + d^2(x)\}^{1/2},\ d^2(x) = f^T(x)(X^TX)^{-1}f(x) \quad (7)$$

where the constant $\nu > 0$ will be chosen to satisfy the calibration condition. Note that for the case $K = 1$ it holds $\nu = t_{n-q}(1-\alpha/2)$, where $t_{n-q}(1-\alpha/2)$ denotes the $(1-\alpha/2)$-quantile of the Student's t-distribution with $n-q$ degrees of freedom. For other possibilities for setting $g(.)$ see Witkovský [17]. Since there is arbitrariness in the choice of the sequence $\{x_{n+i}\}$ it can be assumed that the sequence $\{x_{n+i}\}$ is randomly generated with a probability distribution on the interval $\mathscr{X}$. Here, we suggest to assume the uniform distribution of the x's on $\mathscr{X}$. For a specified range of possible values of the explanatory variable, this is a natural choice of the distribution of the explanatory variable. Then, the scalar ν is a solution of the following integral equation

$$P_{B,U}\left\{(x_{max} - x_{min})^{-1}\int_{\mathscr{X}} C(x;B,U)dx \geq \gamma\right\} = 1 - \alpha. \quad (8)$$

The equation (8) is a population counterpart to (6) with the average replaced by the expected value. The multiple integration is required for solving equation (8). Since the computation of constant ν depends on $\mathscr{X}$ and also on X, the tabulations of its values are difficult for various α, γ. Hence, the value of ν is calculated for each problem anew. The unknown constant ν for the MUCI's can be estimated with adequate accuracy for practical work by a simulation. The detailed algorithm of calculation ν is shown in Algorithm 1. The code in MATLAB is available from the author upon request.

Table 1. Algorithm for calculating ν for the new MUCI's.

Algorithm 1

1: **Input**: X, $\mathscr{X} = [x_{min}, x_{max}]$, α, γ, N - number of runs (n is the number of rows of X, q is the number of columns of X)
2: Generate N times $B \sim N_q(0_q, (X^TX)^{-1})$, and $U \sim \sqrt{\chi^2_{n-q}/(n-q)}$ (e.g. $N = 500{,}000$)
3: Find roots of the equation $\sum_{i=1}^{N} Ind(cov_i \geq \gamma)/N = 1 - \alpha$,
where $Ind(cov_i \geq \gamma) = 1$, if $cov_i \geq \gamma$ and 0 otherwise
$cov_i = (x_{max} - x_{min})^{-1} \int_{\mathscr{X}} C(x;B_i,U_i)dx$
4: **Output**: ν

For example, suppose the simple linear regression, i.e. $f^T(x) = (1,\ x)$, $q = 2$, $B = (B_0, B_1)^T$,

$$\begin{pmatrix} B_0 \\ B_1 \end{pmatrix} \sim N_2\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \frac{1}{S_x}\begin{pmatrix} \frac{\sum_{i=1}^n x_i^2}{n} & -\bar{x} \\ -\bar{x} & 1 \end{pmatrix}\right),\ U \sim \sqrt{\frac{\chi^2_{n-2}}{n-2}}, \quad (9)$$

where $\bar{x} = \sum_{i=1}^n x_i/n$, and $S_x = \sum_{i=1}^n (x_i - \bar{x})^2$. Further, we shall assume that $\bar{x} = 0$, $\sum_{i=1}^n x_i^2 = n$, $n = 30$, and $\mathscr{X} = [-3, 3]$. We calculated ν by the algorithm by taking $\gamma = 0.90$, and $\alpha = 0.05$ for 50 times, the average equaled 2.150 and the standard deviation equaled 0.001. Note that the exact value of ν for the setting parameters equals 2.151, see Table 2. The Monte-Carlo approach is widely used in the development of statistical methods, and it was also used in Han et al. [5]. The calculated value ν is used repeatedly for determining $\mathscr{I}(Y_{x_{n+1}}), \mathscr{I}(Y_{x_{n+2}}), \ldots$ corresponding to a sequence of additional responses $Y_{x_{n+1}}, Y_{x_{n+2}}, \ldots$. The MUCI's are computed by using a built-in function for finding the root of a function in analytical software, e.g *fzero()* in MATLAB.

3. Numerical results

We have numerically investigated the statistical properties of the MUCI's constructed by inverting the suggested band, i.e. with g_{new} and by inverting the exact simultaneous tolerance intervals for the case of a simple linear regression, see Mee et al. [13], Krishnamoorthy and Mathew [7] (page 76, (3.3.15)). Mee et al. [13], for constructing the

Table 2. The values of ν and λ for $\alpha = 0.05$ and selected combinations of n, τ, γ.

γ	n	ν			λ		
		$\tau = 2$	$\tau = 3$	$\tau = 4$	$\tau = 2$	$\tau = 3$	$\tau = 4$
	10	2.846	2.873	2.894	1.367	1.379	1.386
	20	2.297	2.325	2.364	1.149	1.158	1.164
.90	30	2.128	2.151	2.187	1.089	1.096	1.102
	40	2.042	2.059	2.090	1.063	1.068	1.073
	50	1.988	2.002	2.029	1.046	1.051	1.055
	10	2.010	2.063	2.133	1.245	1.264	1.276
	20	1.612	1.646	1.703	1.056	1.070	1.080
.75	30	1.491	1.514	1.557	1.010	1.020	1.029
	40	1.429	1.446	1.470	0.992	0.999	1.005
	50	1.391	1.404	1.431	0.983	0.988	0.993

two-sided STI's, supposed the function $g(x)$, $x \in \mathscr{X}$ in the fixed functional form $g_{STI}(x) = \lambda\{z_{(1+\gamma)/2} + \sqrt{(q+2)}d(x)\}$, where $z_{(1+\gamma)/2}$ denotes the $(1+\gamma)/2$-quantile of the standard normal distribution. The constant $\lambda > 0$ is chosen to satisfy the condition of the STI's for a multiple linear regression, where the first m components are common for all rows of X. In the case of a simple linear regression the first component equals 1 for all $f(x)^T$, i.e. $f^T(x) = (1,\ x)$ (i.e., $q = 2$) for all $x \in \mathscr{X}$. Under the assumption $\bar{x} = 0$ it holds $d^2(x) = (1,x)(X^TX)^{-1}(1,x)^T = 1/n + x^2/S^2_{xx}$, where $S^2_{xx} = \sum_{i=1}^n x_i^2$. Mee et al. [13] suggested a procedure for determining λ over the range of $d(x)$ given $[d_{min}, d_{max}]$. The values of λ reported in Mee et al. [13] and in Krishnamoorthy and Mathew [7] were calculated for a double regression and assuming $d_{min} = n^{-1/2}$ and $d_{max} = ((1+\tau^2)/n)^{1/2}$, $\tau = \{2,3,4\}$. It implies $d^2_{max} = 1/n + \tau^2/n$. For simplicity and to obtain the same range, we considered $\mathscr{X} = [-\tau, \tau]$, i.e. $x^2_{max} = x^2_{min} = \tau^2$ and $S^2_{xx} = n$. Under the above assumptions the distributions of the variables $B = (B_0, B_1)$, U are the same as in (9). Table 2. provides the values of ν and λ computed for $n = \{10,20,30,40,50\}$, $\alpha = .05$, $\gamma = \{.75, .90\}$, $\tau = \{2,3,4\}$ over $\mathscr{X} = [-\tau, \tau]$. The values of ν and λ were determined by direct computation (i.e., three-dimensional quadrature). Note that the values of λ presented in Table 2. are slightly smaller than the values reported in [7] and [13]. The difference between the values of λ is caused by the fact that the values of λ tabulated in [7], [13] were determined assuming a double regression (i.e., $Y_{x_0,x_1} = \beta_0 x_0 + \beta_1 x_1$), while the values of λ in Table 2. were determined for the case of a simple linear regression (i.e., $Y_{1,x_1} = \beta_0 + \beta_1 x_1$, $x_0 = 1$).

In what follows, the statistical properties of the two-sided MUCI's are numerically investigated for the considered settings of parameters n, α, γ, τ in Table 2. and by using the values of ν and λ from Table 2.

3.1. *Estimated confidence*

Three different sequences of $\{x_{n+i}\}_{i=1}^K$ were considered to investigate the confidence of the considered MUCI's, see

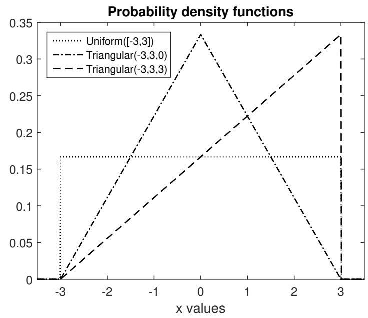

Fig. 2. Probability density functions of the considered distributions in the numerical experiment.

Fig.2. The first sequence ($S1$) consists of x_{n+i}'s generated from $U(\mathscr{X})$, where $U(a,b)$ denotes the uniform distribution on the interval $[a,b]$. Since ν is calculated by assuming the uniform distribution for x on a $\mathscr{X}$, we considered two triangular distributions for x of a different shape to analyse the behaviour of the suggested MUCI's when this assumption is not correct. The second sequence ($S2$) consists of x_{n+i}'s generated from $Tr(\mathscr{X}, 0)$, where $Tr(I,b)$ denotes the triangular distribution on an interval I with parameter of non-centrality (mode) b. The third sequence ($S3$) consists of x_{n+i}'s generated from $Tr(\mathscr{X}, \tau)$. In addition, we considered three ranges of possible values given as $\mathscr{X} = [-\tau, \tau]$, $\tau = \{2,3,4\}$ for each sequence. The distribution of $\hat{\beta}$ depends on the design matrix X through the fitted value $S^2_{xx} = n$ in our setting. By considering three different $\mathscr{X}$ for the fixed value of S^2_{xx}, we tried to investigate the influence of X on the confidence of MUCI's. The empirical confidences (6) are based on $N = 100,000$ generated triples $(b_0, b_1, u)^T$ of the random variables B_0, B_1, U and the mean coverage is analysed for $K = 10,000$ x_{n+i}'s on $\mathscr{X}$ corresponding to the selected sequence. The values of λ and of ν reported in Table 2. were used.

The estimated confidences are presented in Table 3. The estimated confidence of the MUCI's based on the suggested band around the fitted calibration curve is satisfactory close to the prescribed level for all considered sequences of x_i. As we expected, the MUCI's constructed based on the exact STI's are conservative, the estimated confidence level is over the prescribed level and their empirical confidences grow by increasing the values of τ for all sequences.

3.2. *Average band width*

By inverting the narrower band, the narrower MUCI's are obtained which provide more accurate information about the unknown value x. Because the new band and STI's around the fitted calibration curve differ in the functional form of function $g(x)$, $x \in \mathscr{X}$ it is not possible to compare the bands based only on the values in Table 2. The functions $g_{STI}(x)$, $g_{new}(x)$, $x \in [-4,4]$ for $\gamma = 0.9$ with the values of ν and λ from Table 2. are shown in Fig.3. For the case $n = 10$, a band constructed with g_{new} for a $\hat{\beta}$, S^2 would be uniformly narrower on all $\mathscr{X}$, while for the case $n = 50$ there is an interval on $\mathscr{X}$, where the tolerance band would be narrower.

Table 3. The estimated confidences of the two-sided MUCI's constructed by inverting the suggested band (ν) and by the exact STI's (λ), respectively. Precribed level $1-\alpha = 0.95$.

	γ	n	ν			λ		
			τ					
			2	3	4	2	3	4
S_1	.90	10	.950	.950	.951	.972	.976	.980
		20	.949	.950	.950	.979	.986	.988
		30	.950	.949	.953	.983	.989	.991
		40	.952	.952	.952	.984	.992	.993
		50	.952	.952	.950	.982	.990	.999
	.75	10	.950	.952	.952	.977	.982	.984
		20	.949	.950	.951	.986	.991	.992
		30	.950	.950	.952	.987	.993	.994
		40	.951	.952	.952	.989	.995	.996
		50	.952	.951	.951	.988	.995	.995
S_2	.90	10	.949	.952	.953	.968	.972	.975
		20	.953	.955	.959	.974	.981	.986
		30	.952	.957	.962	.974	.984	.988
		40	.951	.957	.964	.975	.986	.991
		50	.953	.957	.963	.974	.983	.989
	.75	10	.950	.956	.96	.972	.979	.982
		20	.953	.958	.965	.978	.987	.992
		30	.952	.959	.968	.970	.989	.993
		40	.952	.960	.960	.980	.990	.994
		50	.954	.959	.966	.979	.989	.994
S_3	.90	10	.949	.950	.950	.971	.977	.979
		20	.949	.949	.949	.978	.985	.988
		30	.950	.949	.950	.981	.988	.990
		40	.949	.950	.951	.982	.991	.993
		50	.950	.948	.949	.981	.990	.993
	.75	10	.948	.947	.949	.976	.982	.984
		20	.949	.948	.947	.983	.999	.991
		30	.949	.948	.949	.986	.992	.992
		40	.949	.950	.949	.989	.994	.995
		50	.950	.948	.948	.987	.995	.995

For the considered combinations of parameters n, γ, τ value of the function $g_{new}(.)$ is greater than value of the function $g_{STI}(.)$ for x close to $\bar{x} = 0$, if there is an intersection of both functions. A percentage of the range $\mathscr{X}$, where value of the function $g_{STI}(.)$ is less than the value of the suggested function $g_{new}(.)$ is presented in Table 4. in brackets. In the majority of the considered combinations of parameters n, γ, τ in Table 4., the suggested band is narrower than STI's on the whole $\mathscr{X}$.

Here, we also considered the average width of a band as an optimality criterion for a comparison of the considered two forms of MUCI's. The average width of a band over $\mathscr{X}$ is defined as $\xi = \int_{\mathscr{X}} g(x)dx/(x_{max} - x_{min})$. Table 4. provides values of ξ for the suggested band and for the STI's for the combinations of parameters n, τ, γ from Table 2., and the values of ν and λ reported in Table 2. were used. The average band width of the suggested band is smaller than that of the STI's for all considered combinations of parameters n, τ, γ.

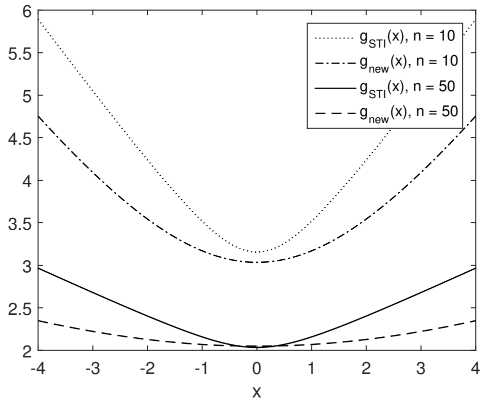

Fig. 3. Illustration of function g for the suggested band (g_{new}) and for the exact STI's (g_{STI}).

Table 4. Average width of the suggested band (ξ_ν) and of STI's (ξ_λ).

	γ	n	$\tau = 2$	$\tau = 3$	$\tau = 4$
ξ_ν	.90	10	6.315 (0%)	10.152 (0%)	14.641 (0%)
		20	4.853 (0%)	7.629 (0%)	10.81 (0%)
		30	4.418 (0%)	6.863 (0%)	9.606 (5.4%)
		40	4.200 (0%)	6.476 (0%)	8.988 (7.7%)
		50	4.066 (0%)	6.239 (0%)	8.606 (8.6%)
	.75	10	4.460 (0%)	7.292 (0%)	10.793 (0%)
		20	3.405 (0%)	5.400 (0%)	7.787 (7.9%)
		30	3.095 (0%)	4.830 (0%)	6.841 (9.9%)
		40	2.940 (0%)	4.547 (0%)	6.362 (10.5%)
		50	2.846 (0%)	4.375 (3.9%)	6.070 (10.5%)
ξ_λ	.90	10	7.056	11.732	17.262
		20	5.298	8.638	12.495
		30	4.759	7.673	10.991
		40	4.487	7.177	10.208
		50	4.318	6.867	9.717
	.75	10	5.193	8.881	13.368
		20	3.828	6.398	9.461
		30	3.416	5.625	8.223
		40	3.210	5.232	7.581
		50	3.084	4.989	7.182

3.3. *An Example*

For a numerical illustration we considered a controlled experiment that was conducted at the National Biological Service, Louisiana, to predict the amount of sodium chloride solution in dionized water (ASCS) based on electric conductivity (EC). The calibration data given in Johnson and Krishnamoorthy [6] involved 31 pairs of (x_i, y_i), where x_i is precisely known ASCS in dionized water and y_i is corresponding EC measurement obtained by using the Fisher conductivity meter $i = 1,2,\ldots,31$. The calibration data can be used repeatedly to construct MUCI's for ASCS corresponding to all future measurements of *EC*. In the analysis that followed, we used 28 randomly chosen measurements (out of 31) to estimate the parameters of a model. The omitted 3 measurements are used to construct MUCI's for corresponding ASCS. Because the three true ASCS in dionized water are known, we can see how well constructed MUCI's captured the true value.

A polynomial regression of the second order fits data well. Based on an analysis of residuals the distribution of the response can be modeled as normal, i.e. $Y_x \sim N(\beta_0 + \beta_1 x + \beta_2 x^2, \sigma^2)$, where $\beta = (\beta_0, \beta_1, \beta_2)$ and $\sigma^2 > 0$ are unknown parameters. The ordinary least squares estimate $\hat{\beta}$ of β, and the residual mean square S^2 estimate of σ^2, are $\hat{\beta} = [1.5911, 0.4158, -0.0043]'$ and $S^2 = 0.0007$. More over $\bar{x} = 8.5893$, $s_x^2 = \sum_{i=1}^{28} x_i^2/28 = 110.5089$, and $d^2(x) = 1/28 + 0.00972(x-8.5893)^2 + 0.000019(x^2-110.5089)^2 - 0.00082(x-8.5893)(x^2-110.5089)$. For given $q = 3$, $n = 28$, and chosen $\gamma = 0.90$, $x_{min} = 0$, $x_{max} = 24$, and the confidence level $\alpha = 0.05$, we evaluated $\lambda = 1.0607$ and $\nu = 2.1735$. Both determined bands are very close to each other ($\xi_\nu = 55.56$ and $\xi_\lambda = 59.46$), the suggested band is narrower than the tolerance band over the range of possible values of ASCS in the example. Table 5. gives the MUCI's based on the three omitted measurements of EC and the corresponding true ASCS in dionized water.

Table 5. The multiple use confidence intervals from the example, where $\mathscr{I}_\lambda$ denotes MUCI based on STI's, and $\mathscr{I}_\nu$ denotes the new MUCI. The value x is in the artificial example known and given for comparison.

y	2.4	3.8	7.5
x	2.0	5.5	17.0
$\mathscr{I}_\lambda$	(1.8137, 2.155)	(5.469, 5.806)	(17.001, 17.513)
$\mathscr{I}_\nu$	(1.8296, 2.141)	(5.472, 5.802)	(17.024, 17.488)

All MUCI's constructed based on inverting the suggested band are narrower than the MUCI's constructed by inverting the STI's. Although both MUCI's determined for EC equaled 7.5 missed the true ASCS value 17, it should be pointed out that they do provide accurate information on the true value.

4. Discussion and Conclusion

The procedure for constructing the multiple use confidence intervals is derived directly from the calibration condition (3) assuming a large number of future observations K and a uniformly distributed explanatory variable. The proposed multiple use confidence intervals are constructed by inverting a symmetric band around the fitted calibration curve of the fixed functional form, the width of the band is proportional to a scalar ν. The value of ν computed for given parameters $1-\alpha, \gamma, n, q, X$ is repeatedly used for determining all future multiple use confidence intervals. It was demonstrated that the condition of the multiple use confidence intervals is satisfied quite well, and based on the provided numerical investigation it is concluded that the proposed MUCI's are narrower than the MUCI's constructed based on the STI's. We can recommend to use our MUCI's in the case of a calibration, where the range of possible values is spanned in the calibration experiment. The procedure for computing the value ν can be modified appropriately to a known distribution of the explanatory variable.

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