A simulation study on an approximate confidence region of parameters of a quadratic calibration function

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Abstract. The goal of the paper is to derive the approximate confidence region of parameters of a quadratic calibration function in a one-dimensional replicated calibration model and to verify the accuracy of this approximate confidence region by a simulation study. We view calibration as a method for describing a relationship between two imprecise measurements. The relationship is called calibration function, we suppose this function in a quadratic form. There are two approximations in deriving the confidence region. First is replacement the nonlinear model by a linear one using a first-order Taylor series. Second is using Kenward-Roger approach for approximation the variance-covariance matrix of the estimators of parameters of the calibration function. The simulation study will be performed in the computer system Matlab. It will be concentrated on the validity of expression of the approximate confidence region depending on the number of measurement objects, on the number of replications and on the covariance matrix.

Keywords: one-dimensional calibration model, quadratic calibration function, MINQUE method, Kenward-Roger approach, simulation study.

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1 Introduction

We view calibration as a relationship between two measurements provided that both are imprecise. Sometimes, such a calibration is called comparative. The main purpose of calibration is to estimate the unknown parameters of a function describing such a relationship, called a calibration function.

Assuming a calibration function to be quadratic is a natural generalization of the assumption of a linear one motivated also by practical reasons since there may be situations in which a quadratic function describes the relationship better.

Moreover replicating a measurement makes it possible to estimate the unknown parameters of a model's covariance matrix. To this end, the paper uses a MINQUE method. An estimate of the covariance matrix is not sufficient for establishing a confidence region for the parameters to be estimated. However, Kenward-Roger's procedure can be used to derive a Wald-type statistic along with its approximate F-distribution to construct an approximate confidence region.

This paper contains two parts. First part is concetred on deriving the approximate confidence region. Second part describes results of a small simulation study, which should verify the validity of the aproximate confidence region.

Our motivation for this model was to calibrate two measurements of moisture in corn. We have two replicated measurements from two methods, one is standard and one is quicker. We consider a quadratic calibration function because we know that both devices measure well on a scale from 10 % to 15 % and anything below and above is less precise. We can verify this relation by testing the significance of the parameters of the calibration function.

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2 Deriving a model

Suppose that a single value is measured for n objects using two different methods each time with a series of m independent measurement made. We may also assume independence of the first and second measurement series and of the measurements of individual objects.

Let then the result of the j-th repetition of the first-series measurement is the realization of an n-dimensional random vector for which

$$\mathbf{X}^j \sim N_n(\boldsymbol{\mu}, \sigma_x^2 \mathbf{I}_n) \text{ for } j = 1, \ldots, m.$$

The result of the j-th repetition of the second-series measurement is the realization of an n-dimensional random vector for which

$$\mathbf{Y}^j \sim N_n(\boldsymbol{\nu}, \sigma_y^2 \mathbf{I}_n) \text{ for } j = 1, \ldots, m.$$

The results of all the measurement may be summarized as

$$\begin{pmatrix} \mathbf{X}^1 \\ \mathbf{Y}^1 \\ \vdots \\ \mathbf{X}^m \\ \mathbf{Y}^m \end{pmatrix} \sim N \left[\mathbf{1}_m \otimes \begin{pmatrix} \boldsymbol{\mu} \\ \boldsymbol{\nu} \end{pmatrix}, \mathbf{I}_m \otimes \begin{pmatrix} \sigma_x^2 \mathbf{I}_n & \mathbf{0}_n \\ \mathbf{0}_n & \sigma_y^2 \mathbf{I}_n \end{pmatrix} \right].$$

Further, let us assume that the relationship between the actual (error-free) measurement values (the calibration function) is quadratic:

$$\boldsymbol{\nu} = a \mathbf{1}_n + b \boldsymbol{\mu} + c \, \mathrm{Diag}^2(\boldsymbol{\mu}) \mathbf{1}_n,$$

where $a, b, c \in R$, $\mathrm{Diag}(\boldsymbol{\mu})$ is a diagonal matrix with entries on the diagonal given by the components of vector $\boldsymbol{\mu}$, $\mathbf{1}_n = (1, \ldots, 1)' \in R^n$.

As the calibration function is non-linear (involving products of the unknown parameters), we linearize it using a Taylor series expansion around b_0, c_0, $\boldsymbol{\mu}_0$. Neglecting terms of order two and higher, we have

$$\boldsymbol{\nu} \doteq \mathbf{1}_n a + \boldsymbol{\mu}_0 b + \mathrm{Diag}^2(\boldsymbol{\mu}_0) \mathbf{1}_n c + \mathrm{Diag}(b_0 \mathbf{1}_n + 2c_0 \boldsymbol{\mu}_0) \delta \boldsymbol{\mu},$$

where $\delta \boldsymbol{\mu} = \boldsymbol{\mu} - \boldsymbol{\mu}_0$. In terms of the vectors of unknown parameters, the calibration function may be rewritten as

$$(\mathrm{Diag}(b_0 \mathbf{1}_n + 2c_0 \boldsymbol{\mu}_0), -\mathbf{I}_n) \begin{pmatrix} \delta \boldsymbol{\mu} \\ \boldsymbol{\nu} \end{pmatrix} + (\mathbf{1}_n, \boldsymbol{\mu}_0, \mathrm{Diag}^2(\boldsymbol{\mu}_0) \mathbf{1}_n) \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \mathbf{0}$$

and this form thought of as conditions for the unknown parameters.

Thus, we get the model

$$\begin{pmatrix} \mathbf{X}^1 - \boldsymbol{\mu}_0 \\ \mathbf{Y}^1 \\ \vdots \\ \mathbf{X}^m - \boldsymbol{\mu}_0 \\ \mathbf{Y}^m \end{pmatrix} \sim N \left[\mathbf{1}_m \otimes \begin{pmatrix} \delta \boldsymbol{\mu} \\ \boldsymbol{\nu} \end{pmatrix}, \mathbf{I}_m \otimes \begin{pmatrix} \sigma_x^2 \mathbf{I}_n & \mathbf{0}_n \\ \mathbf{0}_n & \sigma_y^2 \mathbf{I}_n \end{pmatrix} \right]$$

with the following parameter conditions

$$(\mathrm{Diag}(b_0 \mathbf{1}_n + 2c_0 \boldsymbol{\mu}_0), -\mathbf{I}_n) \begin{pmatrix} \delta \boldsymbol{\mu} \\ \boldsymbol{\nu} \end{pmatrix} + (\mathbf{1}_n, \boldsymbol{\mu}_0, \mathrm{Diag}^2(\boldsymbol{\mu}_0) \mathbf{1}_n) \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \mathbf{0}.$$

We call this model a one-dimensional replicated calibration model with a quadratic calibration function.

2.1 Estimators of model parameters

Next we will be concerned with expressing estimators of the unknown parameters using this model. Note that estimators of the unknown parameters in a one-dimensional non-replicated calibration model ($m = 1$) with a quadratic calibration function can be found in [3].

Supposing known covariance matrix (known parameters σ_x^2, σ_y^2), denoting $\mathbf{D} = \mathrm{Diag}(b_0\mathbf{1}_n + 2c_0\boldsymbol{\mu}_0)$, $\mathbf{A} = (\mathbf{1}_n, \boldsymbol{\mu}_0, \mathrm{Diag}^2(\boldsymbol{\mu}_0)\mathbf{1}_n)$, $\mathbf{W} = \sigma_x^2\mathbf{D}^2 + \sigma_y^2\mathbf{I}_n$ and using the relationships found in [1, p. 129], we will write the estimators:

$$\hat{\boldsymbol{\mu}} = \bar{\mathbf{X}} - \sigma_x^2\mathbf{D}(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+(\mathbf{D}(\bar{\mathbf{X}} - \boldsymbol{\mu}_0) - \bar{\mathbf{Y}}),$$

$$\hat{\boldsymbol{\nu}} = \bar{\mathbf{Y}} + \sigma_y^2(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+(\mathbf{D}(\bar{\mathbf{X}} - \boldsymbol{\mu}_0) - \bar{\mathbf{Y}}),$$

$$\begin{pmatrix} \hat{a} \\ \hat{b} \\ \hat{c} \end{pmatrix} = -(\mathbf{A}'\mathbf{W}^{-1}\mathbf{A})^{-1}\mathbf{A}'\mathbf{W}^{-1}(\mathbf{D}(\bar{\mathbf{X}} - \boldsymbol{\mu}_0) - \bar{\mathbf{Y}}),$$

where $\mathcal{P}_\mathbf{A}$ is projection matrix on the orthogonal complement of the columns of matrix $\mathbf{A}$ and $(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+ = \mathbf{W}^{-1} - \mathbf{W}^{-1}\mathbf{A}(\mathbf{A}'\mathbf{W}^{-1}\mathbf{A})^{-1}\mathbf{A}'\mathbf{W}^{-1}$ (a Moore-Penrose pseudoinverse). The covariance matrices of the estimators are

$$\mathrm{var}\begin{pmatrix} \hat{\boldsymbol{\mu}} \\ \hat{\boldsymbol{\nu}} \end{pmatrix} = \frac{1}{m}\begin{pmatrix} \sigma_x^2\mathbf{I}_n - \sigma_x^4\mathbf{D}(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+\mathbf{D} & \sigma_x^2\sigma_y^2\mathbf{D}(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+ \\ \sigma_x^2\sigma_y^2(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+\mathbf{D} & \sigma_y^2\mathbf{I}_n - \sigma_y^4(\mathcal{P}_\mathbf{A}\mathbf{W}\mathcal{P}_\mathbf{A})^+ \end{pmatrix},$$

$$\mathrm{var}\begin{pmatrix} \hat{a} \\ \hat{b} \\ \hat{c} \end{pmatrix} = \frac{1}{m}(\mathbf{A}'\mathbf{W}^{-1}\mathbf{A})^{-1},$$

$$\mathrm{cov}\left(\begin{pmatrix} \hat{a} \\ \hat{b} \\ \hat{c} \end{pmatrix}, \begin{pmatrix} \hat{\boldsymbol{\mu}} \\ \hat{\boldsymbol{\nu}} \end{pmatrix}\right) = -\frac{1}{m}(\mathbf{A}'\mathbf{W}^{-1}\mathbf{A})^{-1}\mathbf{A}'\mathbf{W}^{-1}(\sigma_x^2\mathbf{D}, -\sigma_y^2\mathbf{I}_n).$$

Note that if the covariance matrix is unknown and we have estimates of the parameters of this matrix, the estimators of the model are in the same form. However, the estimates $\hat{\sigma}_x^2$, $\hat{\sigma}_y^2$ are used instead of the true values σ_x^2, σ_y^2. One possibility to receive the estimates is the MINQUE method described in the part 3. In the last part of this paper, we will construct a approximate confidence region for the vector of the parameters of a calibration function, if the parameters of the covariance matrix are unkown.

2.2 Estimator of covariance matrix parameters

As mentioned above, using a replicated model, also estimates may be expressed of the covariance matrix unknown parameters. This can be done using a MINQUE method, see, for example, [1] or [5] for more information. This method has a local character requiring initial estimates. The covariance matrix of our model depends on two parameters only, σ_x^2, σ_y^2. Denote $\sigma_{x,0}^2$, $\sigma_{y,0}^2$ the initial estimates of the unknown parameters and $\mathbf{W}_0 = \sigma_{x,0}^2\mathbf{D}^2 + \sigma_{y,0}^2\mathbf{I}_n$. Then the $(\sigma_{x,0}^2, \sigma_{y,0}^2)'$-MINQUE estimate of the vector $(\sigma_x^2, \sigma_y^2)'$ is given by the equation

$$\begin{pmatrix} \hat{\sigma}_x^2 \\ \hat{\sigma}_y^2 \end{pmatrix} = \left[n(m-1)\begin{pmatrix} \sigma_{x,0}^{-4} & 0 \\ 0 & \sigma_{y,0}^{-4} \end{pmatrix} + \mathbf{S}\right]^{-1}\begin{pmatrix} \gamma_1 \\ \gamma_2 \end{pmatrix},$$

where

$$\gamma_1 = \sigma_{x,0}^{-4}\sum_{k=1}^{m}(\mathbf{X}^k - \overline{\mathbf{X}})'(\mathbf{X}^k - \overline{\mathbf{X}}) + m(\overline{\mathbf{X}} - \hat{\boldsymbol{\mu}})'(\overline{\mathbf{X}} - \hat{\boldsymbol{\mu}}),$$

$$\gamma_2 = \sigma_{y,0}^{-4}\sum_{k=1}^{m}(\mathbf{Y}^k - \overline{\mathbf{Y}})'(\mathbf{Y}^k - \overline{\mathbf{Y}}) + m(\overline{\mathbf{Y}} - \hat{\boldsymbol{\nu}})'(\overline{\mathbf{Y}} - \hat{\boldsymbol{\nu}}),$$

$$\overline{\mathbf{X}} = \frac{1}{m}\sum_{k=1}^{m}\mathbf{X}^k, \quad \overline{\mathbf{Y}} = \frac{1}{m}\sum_{k=1}^{m}\mathbf{Y}^k$$

and

$$\mathbf{S} = \begin{pmatrix} \mathrm{Tr}\left\{(\mathbf{D}(\mathcal{P}_{\mathbf{A}}\mathbf{W}_0\mathcal{P}_{\mathbf{A}})^{+}\mathbf{D})^2\right\} & \mathrm{Tr}\left\{(\mathbf{D}(\mathcal{P}_{\mathbf{A}}\mathbf{W}_0\mathcal{P}_{\mathbf{A}})^{+})^2\right\} \\ \mathrm{Tr}\left\{((\mathcal{P}_{\mathbf{A}}\mathbf{W}_0\mathcal{P}_{\mathbf{A}})^{+}\mathbf{D})^2\right\} & \mathrm{Tr}\left\{((\mathcal{P}_{\mathbf{A}}\mathbf{W}_0\mathcal{P}_{\mathbf{A}})^{+})^2\right\} \end{pmatrix}.$$

The estimator's covariance matrix is

$$\mathrm{var}\begin{pmatrix} \hat{\sigma}_x^2 \\ \hat{\sigma}_y^2 \end{pmatrix} = 2\left[n(m-1)\begin{pmatrix} \sigma_{x,0}^{-4} & 0 \\ 0 & \sigma_{y,0}^{-4} \end{pmatrix} + \mathbf{S}\right]^{-1}.$$

2.3 Approximate confidence region

We will use a procedure by Kenward and Roger (see [2]) to construct an approximate confidence region for the calibration function's parameter vector applying it to the model

$$\begin{pmatrix} \hat{a} \\ \hat{b} \\ \hat{c} \end{pmatrix} \sim N\left[\begin{pmatrix} a \\ b \\ c \end{pmatrix}, \left(\mathbf{A}'\left(\frac{1}{m}\mathbf{W}\right)^{-1}\mathbf{A}\right)^{-1}\right].$$

Using the notation from [2] we denote the covariance matrix

$$\mathbf{\Phi} = \frac{1}{m}(\mathbf{A}'\mathbf{W}^{-1}\mathbf{A})^{-1}.$$

Based on the above paper, we will write an adjusted covariance matrix:

$$\hat{\mathbf{\Phi}}_A = \hat{\mathbf{\Phi}} + 2\hat{\mathbf{\Phi}}\{\sum_{x,y}\sum_{x,y}\mathbf{V}_{ij}(\mathbf{Q}_{ij} - \mathbf{P}_i\hat{\mathbf{\Phi}}\mathbf{P}_j)\}\hat{\mathbf{\Phi}},$$

where

$$\mathbf{V} = \begin{pmatrix} V_{xx} & V_{xy} \\ V_{yx} & V_{yy} \end{pmatrix} = 2\left[n(m-1)\begin{pmatrix} \sigma_{x,0}^{-4} & 0 \\ 0 & \sigma_{y,0}^{-4} \end{pmatrix} + \mathbf{S}\right]^{-1},$$

$$\mathbf{P}_x = -\frac{1}{m}\mathbf{A}'\mathbf{W}^{-1}\mathbf{D}^2\mathbf{W}^{-1}\mathbf{A}, \quad \mathbf{P}_y = -\frac{1}{m}\mathbf{A}'\mathbf{W}^{-1}\mathbf{W}^{-1}\mathbf{A},$$

$$\mathbf{Q}_{xx} = \frac{1}{m^2}\mathbf{A}'\mathbf{W}^{-1}\mathbf{D}^2\mathbf{W}^{-1}\mathbf{D}^2\mathbf{W}^{-1}\mathbf{A}, \quad \mathbf{Q}_{xy} = \frac{1}{m^2}\mathbf{A}'\mathbf{W}^{-1}\mathbf{D}^2\mathbf{W}^{-1}\mathbf{W}^{-1}\mathbf{A},$$

$$\mathbf{Q}_{yx} = \frac{1}{m^2}\mathbf{A}'\mathbf{W}^{-1}\mathbf{W}^{-1}\mathbf{D}^2\mathbf{W}^{-1}\mathbf{A}, \quad \mathbf{Q}_{yy} = \frac{1}{m^2}\mathbf{A}'\mathbf{W}^{-1}\mathbf{W}^{-1}\mathbf{W}^{-1}\mathbf{A}$$

and $\hat{\mathbf{\Phi}}$ has the same form as $\mathbf{\Phi}$, with the estimates $\hat{\sigma}_x^2$, $\hat{\sigma}_y^2$ calculated by the MINQUE method used for the unknown parameters σ_x^2, σ_y^2.

After some rather lengthy calculations we get

$$A_1 = \sum_{x,y}\sum_{x,y} V_{ij}\,\mathrm{Tr}\{\mathbf{P}_i\hat{\mathbf{\Phi}}\}\mathrm{Tr}\{\mathbf{P}_j\hat{\mathbf{\Phi}}\}, \quad A_2 = \sum_{x,y}\sum_{x,y} V_{ij}\,\mathrm{Tr}\{\mathbf{P}_i\hat{\mathbf{\Phi}}\mathbf{P}_j\hat{\mathbf{\Phi}}\},$$

$$B = \frac{1}{6}(A_1 + 6A_2),$$

$$g = \frac{4A_1 - 7A_2}{5A_2},$$

$$c_1 = \frac{4A_1 - 7A_2}{8A_1 + 31A_2}, \quad c_2 = \frac{-4A_1 + 22A_2}{8A_1 + 31A_2}, \quad c_3 = \frac{-4A_1 + 32A_2}{8A_1 + 31A_2},$$

$$E^* = (1 - \frac{A_2}{3})^{-1},$$

$$V^* = \frac{2}{3}\frac{1 + c_1 B}{(1 - c_2 B)^2(1 - c_3 B)},$$

$$\rho = \frac{V^*}{2{E^*}^2},$$
$$u = 4 + \frac{5}{3\rho - 1},$$
$$\lambda = \frac{u}{E^*(u-2)}.$$

Then we can derive that the λ-multiple of the statistic

$$F = \frac{1}{3}\left(\begin{pmatrix} \hat{a}-a \\ \hat{b}-b \\ \hat{c}-c \end{pmatrix}' \hat{\mathbf{\Phi}}_A^{-1} \begin{pmatrix} \hat{a}-a \\ \hat{b}-b \\ \hat{c}-c \end{pmatrix} \right)$$

has an approximate F-distribution with degrees of freedom of 3 and u. The approximate confidence region for the calibration function parameters vector is a set of vectors $(a, b, c)'$ which fulfill the inequality:

$$P(F \leq \frac{1}{\lambda} F_{3,u}(1-\alpha)) = 1 - \alpha. \tag{1}$$

3 Small simulation study

We verified the validity of the aproximate confidence interval (1) for the calibration function parameters vector $(a, b, c)'$ by simulations in software Matlab, in which we implemented the derived formulas. Values of the first-series and the second-series measurement have been generated at fixed values of the model parameters, particularly at fixed values of the first measurement mean values $\boldsymbol{\mu}$, quadratic calibration function parameters a, b , c, a number of replications m and variances σ_x^2, σ_y^2. We chose parameters of the calibration function as follows $a = 1$, $b = 2$, $c = 3$. For the number of replications m we selected numbers 3, 5 and 10. Standard deviations (variances) have been chosen in different ways (see below), as well as the mean values vector of the first measurement $\boldsymbol{\mu}$ has been chosen in several ways, but always elements of the vector were symmetrically and equidistantly around the parabola's minimum. As an estimate of the confidence, we calculated the ratio the generated values satisfying the inequality (1) to all generated values.

Standard deviations effect

For the standard deviations (variances) effect research, we considered the mean values vector of the first measurement $\boldsymbol{\mu} = (-10, -9, .., 8, 9)'$ and the number of replications $m = 3$. For each choice of two standard deviations we carried out 10 000 repetitions.

$\sigma_x = \sigma_y$	$\sigma_x = 0.05$ $\sigma_y = 0.05$ 94.12 %	$\sigma_x = 0.01$ $\sigma_y = 0.01$ 94.01 %	$\sigma_x = 0.1$ $\sigma_y = 0.1$ 93.59 %	$\sigma_x = 0.5$ $\sigma_y = 0.5$ 94.55 %			94.07 %
$\sigma_x < \sigma_y$	$\sigma_x = 0.01$ $\sigma_y = 0.05$ 94.32 %	$\sigma_x = 0.01$ $\sigma_y = 0.1$ 94.72 %	$\sigma_x = 0.01$ $\sigma_y = 0.5$ 96.66 %	$\sigma_x = 0.1$ $\sigma_y = 0.5$ 94.06 %	$\sigma_x = 0.05$ $\sigma_y = 0.1$ 94.56 %	$\sigma_x = 0.05$ $\sigma_y = 0.5$ 94.41 %	94.79 %
$\sigma_x > \sigma_y$	$\sigma_x = 0.1$ $\sigma_y = 0.05$ 93.38 %	$\sigma_x = 0.5$ $\sigma_y = 0.05$ 87.83 %	$\sigma_x = 0.5$ $\sigma_y = 0.1$ 88.64 %				89.95 %

Table 1 The simulation results of standard deviations effect

The best results are when the first measurement standard deviation is less than the standard deviation of the second measurement ($\sigma_x < \sigma_y$) and reaches almost 95 %. We can say, that the bigger differences the better results are. Percentage of the confidence for the same values of standard deviations is around 94 %. If $\sigma_x > \sigma_y$, the confidence is only about 90 %. The obtained results may cause the fact that the values of the second measurement are from a wider interval than the values of the first measurement.

Effect of replications

Effect of measurement replications, we considered for the the mean values vector of the first measurement $\boldsymbol{\mu} = (-10, -9, .., 8, 9)'$ and for four cases of standard deviations $\sigma_x = 0.1$, $\sigma_y = 0.5$; $\sigma_x = 0.5$, $\sigma_y = 0.5$; $\sigma_x = 0.01$, $\sigma_y = 0.5$; $\sigma_x = 0.1$, $\sigma_y = 0.1$. For all cases, we carried out 10 000 repetitions and we got results:

$m = 3$	$m = 5$	$m = 10$
94.43 %	94.61 %	94.69 %

Table 2 The simulation results of replications effect

As you can see in the table 2, the confidence is around 94.5 %, probably due to we chose only the cases of two variances, for which we achieved "good" results in the previous part. With a growing number of replications increases the confidence, but not particularly striking.

Number of measument objects effect

In the last part we focuse on the effect of measurement objects number. We suppose that all objects (points) are located equidistantly and symmetrically around the minimum of the parabola. We set values of other parameters as $\sigma_x = 0.1$, $\sigma_y = 0.5$ and $\sigma_x = 0.5$, $\sigma_y = 0.5$ for standard deviations and $m = 10$ for the number of replications.

$n = 10$	$n = 20$	$n = 40$
94.05 %	94.39 %	94,48 %

Table 3 The simulation results of effect of measurement objects number

The resulting values show that the increasing number of measurement objects cause the increasing confidence. All the same the confidence only get closer to 95 %. The diference between confidences for 10 and 20 measurement objects are stronger than the diference of confidences between 20 and 40 measurement objects.

4 Conclusion

Globally we could say that the confidence obtained by the simulation is approximatly around 94.5 %, which is lower than it should be according to the inequality (1). These results are an inspiration to other simulation studies with a different choice of the calibration function parameters and possibly to modify the derived formula.

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