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AN EXTENSION OF THE BAYESIAN EXPRESSION FOR RECALIBRATION OF A MEASUREMENT DEVICE

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Abstract – The Bayesian method of estimating is applied to the problem of recalibration of a measurement device. Recalibration of the device is considered within the Bayesian approach and earlier expressions for estimates of the interesting quantities are generalized to the case when the measurement device incorporates several calibrated reference quantities.

The obtained new expressions take into account the result of a previous calibration of the reference quantities and give a posteriori estimates.

Keywords: traceability in metrology, Bayesian approach, recalibration

1. INTRODUCTION

In evaluation of measurement results the Bayesian inference methods [1] can be used to take into account prior information about the measurand. Application of the Bayes approach to the recalibration of measurement device has been presented earlier [2]. The process of recalibration has been considered for a measurement device which incorporates a reference quantity. It was assumed that prior estimate for this reference quantity is known. This prior information has been transformed into the form which is appropriate for the Bayesian approach. Namely, a prior probability density function (PDF) has been associated with the prior estimate. The PDF for the case has been taken Gaussian [3]. It has been assumed that the recalibration itself consists in measuring a quantity whose value is known before the measurement.

A simple measurement model has been introduced in consideration for description of the above recalibration. This model amounts to the equation of measurement

$$K = X / X_R \tag{1}$$

which is equivalent to measuring the ratio K of two quantities X and X_R. In the calculation of the task (1) different cases were considered. A special choice of initial values, which are equal to prior values, was used [4] in linearization to simplify the linear equations defining resulting expressions. The case of unspecified linearization was considered in [2] where simple numerical example was given to illustrate the difference between two approaches to recalibration. One of the approaches is usual replacement of the reference value by the new one and the second of the approaches, which is Bayesian, takes into account the prior information about the reference quantity.

The model (1) describes only simple measurement configurations. An extended model can be presented by the following equation

$$K = (X_1)^{n_1} (X_2)^{n_2} ... (X_m)^{n_m} \tag{2}$$

with exponents $n_o = \pm 1$ (α = 1,…,m). The model (2) corresponds to a measurement device which includes several reference quantities involved in the calibration chain. For the case of the special linearization the task (2) was considered in [5]. In the calculation the prior values were supposed independent. Below generalization of previous expressions is presented for the extended model (2) of measurement device including an arbitrary number of reference quantities with correlated prior values.

2. LINEAR FORM OF THE EQUATION

Linearization

$$X_\alpha \to x_\alpha = X_\alpha / X_{o\alpha} - 1,\; K \to k = K / K_o - 1$$

which can be performed with appropriate arbitrary initial values $X_{o\alpha}$ and calculated value

$$K_o = (X_{o1})^{n_1} (X_{o2})^{n_2} ... (X_{om})^{n_m} ,$$

gives a linear equation correspondent to original equation (2). Further simplification can be achieved by the following replacement of variables

$$x_\alpha \to q_\alpha = n_\alpha x_\alpha .$$

Then the final linear form of the equation correspondent to (2) has view

$$k(q_1,...,q_m) = \sum_1^m q_\alpha . \tag{3}$$

For quantity k a set of measured values $\mathbf{k} = (k_1,...,k_n)^T$ is supposed to be obtained in the process of recalibration. For quantities q_α a set of correlated prior estimates

$$q_{o\alpha}, V_{o\alpha\beta} \;\; (\alpha, \beta = 1,...,m) \tag{4}$$

is supposed to be available. Symbols $q_{o\alpha}$ and $V_{o\alpha\beta}$ denotes elements of vector

$$\mathbf{q}_o = (q_{o1},...,q_{om})^T . \tag{5}$$

and correspondent covariance matrix $\mathbf{V}_o$.

It should be noted that the subscript '$_o$' has different sense for the original and relative quantities. For the original quantities it denotes the arbitrary and calculated initial values used for the linearization. And for the relative quantities it denotes prior values which are to be calculated from known prior values for the original reference quantities.

3. SOLUTION FOR THE EXTENDED MODEL

3.1. Description of the Model

As in the case of the simple model [2], the prior PDF, which is correspondent to the set (4), is taken Gaussian. For the present case the PDF is multivariate

$$f_o(\mathbf{q}) = N(\mathbf{q};\mathbf{q}_o,\mathbf{V}_o) = \\ = \frac{1}{(2\pi)^{m/2}\,|\mathbf{V}_o|^{1/2}} e^{-\frac{1}{2}(\mathbf{q}-\mathbf{q}_o)^T \mathbf{V}^{-1}{}_o(\mathbf{q}-\mathbf{q}_o)} . \qquad (6)$$

The likelihood has former view

$$f_L(\mathbf{k}\,|\,\mathbf{q}) = \frac{1}{(2\pi\sigma^2)^{n/2}} e^{-\frac{1}{2\sigma^2}(\mathbf{k}-k(\mathbf{q})\mathbf{1})^T(\mathbf{k}-k(\mathbf{q})\mathbf{1})} \qquad (7)$$

where $\sigma = u(k_i)$ is uncertainty of measured values k_i and $\mathbf{1}$ denotes the unit n-vector $\mathbf{1} = (1,1,...,1)^T$.

Application of the Bayes theorem to the model gives the posterior PDF $f_{post}(\mathbf{q})$ which has to be calculated now according to relationship

$$f_{post}(\mathbf{q}) = C f_L(\mathbf{k}\,|\,\mathbf{q})\, f_o(\mathbf{q}) . \qquad (8)$$

The inverse of the normalization factor C

$$C^{-1} = \int ... \int dq_1 ... dq_m\, f_L(\mathbf{k}\,|\,\mathbf{q})\, f_o(\mathbf{q}) \equiv f(\mathbf{k}) \qquad (9)$$

gives prior distribution $f(\mathbf{k})$ of vector $\mathbf{k}$.

3.2. Expressions for the posterior values

Calculation of (8) can be done by the same method as used for the simple model. The posterior PDF is multivariate Gaussian

$$f_{post}(\mathbf{q}) = N(\mathbf{q};\hat{\mathbf{q}},\hat{\mathbf{V}}) = \\ = \frac{1}{(2\pi)^{m/2}\,|\hat{\mathbf{V}}|^{1/2}} e^{-\frac{1}{2}(\mathbf{q}-\hat{\mathbf{q}})^T \hat{\mathbf{V}}^{-1}(\mathbf{q}-\hat{\mathbf{q}})} . \qquad (10)$$

The expectations $\hat{\mathbf{q}}$ can be calculated

$$\hat{\mathbf{q}} = \mathbf{q}_o + \delta\mathbf{q} \equiv \\ \mathbf{q}_o + \frac{\bar{k} - k_o}{\mathrm{Var}(\bar{k}) + \mathrm{Var}(k_o)} \mathrm{Cov}(\mathbf{q}_o, k_o) . \qquad (11)$$

In (11) $\mathrm{Cov}(\mathbf{q}_o, k_o)$ denotes vector composed of m components which are the covariances

$$\mathrm{Cov}(q_{o\alpha}, k_o) = \sum_{\beta=1}^{m} V_{o\alpha\beta}\ , \alpha = 1,...,m \qquad (12)$$

calculated for m components of vector (5)

$$\mathrm{Cov}(\mathbf{q}_o, k_o) = (\mathrm{Cov}(q_{o1}, k_o),...,\mathrm{Cov}(q_{om}, k_o))^T .$$

Also, denotations $\bar{k}$ and k_o have been introduced in (11) for the average

$$\bar{k} = \frac{1}{n}\sum_{i=1}^{n} k_i \qquad (13)$$

of measured values k_i and for the prior estimate

$$k_o = \sum_{\alpha=1}^{m} q_{o\alpha} \qquad (14)$$

of k given by (3), reciprocally.

The covariance matrix $\hat{\mathbf{V}}$ in the posterior PDF $f_{post}(\mathbf{q})$ (10) is given by the expression

$$\hat{\mathbf{V}} = \mathbf{V}_o - \\ \frac{1}{\mathrm{Var}(\bar{k}) + \mathrm{Var}(k_o)} \mathrm{Cov}(\mathbf{q}_o, k_o)\, \mathrm{Cov}(\mathbf{q}_o, k_o)^T . \qquad (15)$$

The inverse $\hat{\mathbf{V}}^{-1}$ matrix for (15) can be straightforwardly calculated with the result

$$\hat{\mathbf{V}}^{-1} = \mathbf{V}_o^{-1} + \frac{1}{\mathrm{Var}(\bar{k})}\Pi_m . \qquad (16)$$

In (16) Π_m denotes the $m \otimes m$-matrix whose elements are equal to 1. The variances $\mathrm{Var}(\bar{k})$ and $\mathrm{Var}(k_o)$ of quantities (13) and (14) are given by

$$\mathrm{Var}(\bar{k}) = \sigma^2 / n , \qquad (17)$$

$$\mathrm{Var}(k_o) = \sum_{\alpha,\beta=1}^{m} \mathbf{V}_{o\alpha\beta} , \qquad (18)$$

reciprocally, according to (7) and (4).

3.3. Expression for prior distribution $f(\mathbf{k})$

Prior distribution (9) is also Gaussian. It is given by the expression

$$f(\mathbf{k}) = \frac{1}{(2\pi)^{n/2}\,|\mathbf{B}|^{1/2}} e^{-\frac{1}{2}(\mathbf{k}-k_o\mathbf{1})^T \mathbf{B}^{-1}\,(\mathbf{k}-k_o\mathbf{1})} \qquad (19)$$

where matrix $\mathbf{B}$ has the form

$$\mathbf{B} = \sigma^2 + \mathrm{Var}(k_o)\Pi_n . \qquad (20)$$

The inverse matrix for the matrix (20) can be found by use of the previous relationships ([2], Eqs. (44) and (45)). Thus, it is given by expression

$$\mathbf{B}^{-1} = \frac{1}{\sigma^2} - \frac{\mathrm{Var}(k_o)}{n\mathrm{Var}(\bar{k})[\mathrm{Var}(\bar{k}) + \mathrm{Var}(k_o)]}\Pi_n . \qquad (21)$$

3.4. Calculations of the exponents

To prove the equality

$$f_o(\mathbf{q}) * f_L(\mathbf{k}\,|\,\mathbf{q}) = f_{post}(\mathbf{q}) * f(\mathbf{k}) \qquad (22)$$

for initial expressions for the PDF (6) and (7), supposed expression (19) for $f(\mathbf{k})$ with parameters (14), (20) and deduced expression (10) for $f_{post}(\mathbf{q})$ with parameters (11), (15) the equality of the exponents and the factors in (22) can be proved. The comparison of the exponents has been done with transformation of the exponent for the right side of (22) to the exponent of the left side of this equation. Use of the above expressions gives for the exponent in (10) when the factor “-1/2” is dropped

$$\sum_{\alpha,\beta=1}^{m}(q_\alpha - \hat{q}_\alpha)\hat{V}_{\alpha\beta}^{-1}(q_\beta - \hat{q}_\beta) =$$

$$\sum_{\alpha,\beta=1}^{m}(q_\alpha - q_{o\alpha})V_{o\alpha\beta}^{-1}(q_\beta - q_{o\beta}) + \Delta_1 \, , \qquad (23)$$

where

$$\Delta_1 = \frac{1}{\mathrm{Var}(\bar{k})}[\sum_{\alpha=1}^{m}(q_\alpha - q_{o\alpha})]^2 +$$

$$\sum_{\alpha,\beta=1}^{m}\delta q_\alpha \hat{V}_{\alpha\beta}^{-1}(\delta q_\beta - 2q_\beta + 2q_\beta) \ . \qquad (24)$$

For the exponent in (19) we have analogously

$$\sum_{i,j=1}^{n}(k_i - k_o)B_{ij}^{-1}(k_j - k_o) =$$

$$\sum_{i=1}^{n}(k_i - k \ )^2/\sigma^2 + \Delta_2 \qquad ,$$

(25)

where

$$\Delta_2 = \frac{n}{\sigma^2}(2\bar{k}k - k^2 - 2k^2 + k_o^2) -$$

$$\frac{(\bar{k} - k_o)^2\,\mathrm{Var}(k_o)}{\mathrm{Var}(\bar{k})[\mathrm{Var}(\bar{k}) + \mathrm{Var}(k_o)]} \ . \qquad (26)$$

From the above expressions (24) and (26) for Δ_1 and for Δ_2, reciprocally, one can straightforwardly obtain relationship

$$\Delta_1 + \Delta_2 = 0 \, .$$

This relationship proves that the exponents in both sides of (22) are equal.

3.5. Calculations of the factors

Then the equality of the factors in (22) should be verified. These factors are equal if the following determinant relationship

$$|\mathbf{B}| = \sigma^{2n} \cdot |\hat{\mathbf{V}}^{-1}| \cdot |\mathbf{V}_o| \qquad (27)$$

is valid. One can verify the validity of (27) by straightforward calculation also. For the determinant $|\mathbf{B}|$ of matrix $\mathbf{B}$ the previous expression (this expression is given by (46) in [2]) can be used. A simple change of notations in this equation ((46) in [2]) gives the following expression for the determinant of matrix (20)

$$|\mathbf{B}| = n(\sigma^2)^{n-1} \cdot (\mathrm{Var}(\bar{k}) + \mathrm{Var}(k_o)) \, . \qquad (28)$$

To calculate the right side of (27) the determinant of matrix $\hat{\mathbf{V}}^{-1}\mathbf{V}_o$

$$|\hat{\mathbf{V}}^{-1}\mathbf{V}_o| = |\hat{\mathbf{V}}^{-1}| \cdot |\mathbf{V}_o|$$

has been considered. The explicit form of the product $\hat{\mathbf{V}}^{-1}\mathbf{V}_o$ can be written. Use of the relationship (16) gives for this product

$$\mathbf{U} = \hat{\mathbf{V}}^{-1}\mathbf{V}_o = 1 + b \cdot \Pi_{\mathbf{m}}\mathbf{V}_o \qquad (29)$$

where denotation

$$b = 1/\,\mathrm{Var}(\bar{k}) \qquad (30)$$

is introduced. The determinant $|\mathbf{U}|$

$$|\mathbf{U}| = |\, 1 + b \cdot \Pi_{\mathbf{m}}\mathbf{V}_o \,|$$

of matrix (29) can be calculated by the following transformation

$$|\mathbf{U}| =$$

$$\begin{vmatrix} 1 + b\sum\limits_\gamma V_{o\gamma 1} & b\sum\limits_\gamma V_{o\gamma 2} & \dots & b\sum\limits_\gamma V_{o\gamma m} \\ b\sum\limits_\gamma V_{o\gamma 1} & 1 + b\sum\limits_\gamma V_{o\gamma 2} & \dots & b\sum\limits_\gamma V_{o\gamma m} \\ \dots & \dots & \dots & \dots \\ b\sum\limits_\gamma V_{o\gamma 1} & b\sum\limits_\gamma V_{o\gamma 2} & \dots & 1 + b\sum\limits_\gamma V_{o\gamma m} \end{vmatrix} =$$

$$\begin{vmatrix} 1 & 0 & \dots & -1 \\ 0 & 1 & \dots & -1 \\ \dots & \dots & \dots & \dots \\ b\sum\limits_\gamma V_{o\gamma 1} & b\sum\limits_\gamma V_{o\gamma 2} & \dots & 1 + b\sum\limits_\gamma V_{o\gamma m} \end{vmatrix} =$$

$$= 1 + b\sum_{\alpha\gamma} V_{o\gamma\alpha} = 1 + \mathrm{Var}(k_o)/\mathrm{Var}(\bar{k}) \, . \qquad (31)$$

Thus the right side of (27) is given by

$$\sigma^{2n} \cdot |\hat{\mathbf{V}}^{-1}| \cdot |\mathbf{V}_o| =$$

$$n(\sigma^2)^{n-1} \cdot (\mathrm{Var}(\bar{k}) + \mathrm{Var}(k_o))$$

and the equality of the factors in both sides of (22) is also proved. This proves also the validity of the relationship (22) for the considered functions and parameters.

3.6. Some consequent of the calculation

As some corollary of the above calculation we can write the result for definite integral

$$J = \int_{\infty}^{\infty} .. \int_{-\infty}^{\infty} dq_1 .. dq_m e^{-\frac{1}{2}(\mathbf{q}-\mathbf{q}_o)^T \mathbf{V}^{-1}{}_o(\mathbf{q}-\mathbf{q}_o) - \frac{1}{2\sigma^2}\sum\limits_i (k_i - \sum\limits_\alpha q_\alpha)^2} \qquad (32)$$

in the following form

$$J = \frac{(2\pi)^{m/2}\,|\mathbf{V}_o|^{1/2}}{[1 + n(\sum\limits_{\alpha\beta} V_{o\alpha\beta})/\sigma^2]^{1/2}} e^{-\frac{1}{2}(\mathbf{k} - k_o\mathbf{l})^T \mathbf{B}^{-1} \ (\mathbf{k} - k_o\mathbf{l})} \qquad (33)$$

because the solution of the above task is equivalent to calculation of the definite integral (32).

It follows also that the a priori function (19) for values k_i is the same for the considered models which involved one or more reference quantities correlated or noncorrelated [2,4]. Some explanation of this will be given below from metrology standpoint.

4. APPLICATION TO MEASUREMENT DEVICES

4.1. The recalibration process

The obtained solution can be used in many metrological situations. Figure 1 presents a scheme of measurement process which can be either measuring a quantity X or recalibrating a measurement device. Both cases are described by (1)-(2). In case of the measurement value of quantity X is supposed to be unknown. In case of the recalibration value of quantity X is supposed to be known.

X – ***measurand or quantity for recalibration*** **→ ($\mathbf{q_1}$)**
R – ***reference quantity*** **→ ($\mathbf{q_2,\dots,q_m}$)**
D – ***divider*** **→ ($\mathbf{k_1,\dots,k_n}$)**

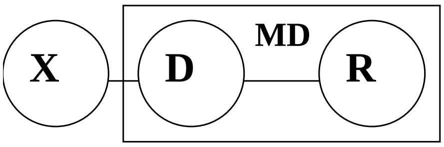

Fig. 1. Scheme of the measurement process

Calibrated measurement device (MD) includes a divider (D) and reference quantities (R) whose a priori values $q_{o2},\dots,q_{om}$ are result of a calibration. The most simple case (1), which is considered in [2], involves only one reference quantity X_R. To recalibrate the measurement device one can use a quantity whose value q_{o1} is a priori known from another source. There are several different approaches to recalibrate the measurement device. Some of the approaches may need a measurement with the device to be performed. Below the three approaches are given:

- Recalibration of MD by replacement of the reference quantity or its value;
- Recalibration of MD by measuring a quantity whose value q_{o1} is known to assign new value to the reference quantity;
- Recalibration of MD by measuring a quantity whose value q_{o1} is known to assign new value to the reference quantity when the result of previous calibration $q_{o2},\dots,q_{om}$ are turned to account.

The above approaches to recalibration can be referred as replacement, direct recalibration and Bayesian approach to recalibration, reciprocally. The last two approaches demand to perform measurements with the divider involved in the measurement device. The result of the measurements is a set of values $k_1,\dots,k_n$. Any of considered approaches to recalibration changes reference value from q_o to $\hat{q}$ which depends on the available information:

- Replacement (R):
$$\hat{q} = \hat{q}(q_{o1}) ;$$
- Direct recalibration (DR):
$$\hat{q} = \hat{q}(q_{o1};k_1,..,k_n) ;$$
- Bayesian approach (BA):
$$\hat{q} = \hat{q}(q_{o1},..q_{om};k_1,..,k_n) .$$

The simple model (1) divides explicitly the quantities involved into the reference quantity X_R and the measurand X. The generalised model (2) is an unified scheme which does not divide explicitly the quantities into the reference quantities and the measurand. The model (2) is applicable, for example, to measurements performed with the bridge method, to the Josephson installation which realizes the volt on base of measurements of the fundamental constants, etc.

As have been remarked above, the prior distribution (19) has the same view for the different considered models which can include one or more reference quantities. According to the scheme presented at Fig.1 the function (19) coincides in form with the distribution of measured values when the measurement device is used to measure quantity X. In this case matrix $\mathbf{B}$ gives variances and covariances of values obtained in the measurement. This matrix has view

$$\mathbf{B}_o = \sigma^2 + (\sum_{\alpha,\beta=2}^{m} V_{o\alpha\beta})\Pi_n \tag{34}$$

before the recalibration, and

$$\hat{\mathbf{B}} = \sigma^2 + (\sum_{\alpha,\beta=2}^{m} \hat{V}_{\alpha\beta})\Pi_n \tag{35}$$

after the recalibration. The second term in (34) and (35) describes the correlations that is due to the systematic error from use of the same reference quantities. The correlations are to be taken into account when the results of measurements with the measurement device are combined in calculations. Thus, the $m \otimes m$-matrix Π_m can be named the unit systematic matrix.

4.2. A graphical consideration

The final expressions (11), (15), (20) can be reduced to the correspondent expressions given in previous publications [2,4] where different models were considered. From practical standpoint the comparison of results which can be obtained with application of the considered approaches to recalibration is important. A simple graphical consideration can be given for the simple case where the numbers of reference quantities and measurements by the divider are the following $m = 2, n = 1$.

For $m = 2$ expressions (11) and (15) describe situation given in [2]. For $n = 1$ matrices (34), (35) become scalars. To characterize the result of recalibration of the measurement device a ratio of uncertainties $u = \sqrt{\hat{B}/B_o}$, which involves uncertainty $\sqrt{B_o}$ of the device before the recalibration and uncertainty $\sqrt{\hat{B}}$ of the device after the recalibration, can be considered. Dependence of this ratio u on the ratio $r = \sigma/\sqrt{V_{o22}}$, which involves uncertainty σ from the divider and uncertainty $\sqrt{V_{o22}}$ from the reference quantity, is presented by Fig.2 for considered methods of recalibration. The curves ($m = 2, n = 1$) have been plotted at the value of the parameter $p = V_{o11} / V_{o22}$ =0,8. It is clear from Fig.2 that the most advantage in application of the Bayesian approach to recalibration takes place for small values of r.

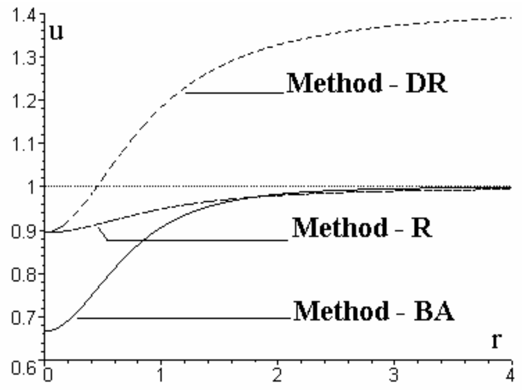

Fig. 2. A comparison of methods “R”,”DR” and “BA”.

For more complicate case (2) analogous analysis can be performed numerically at the stage of planning of the experiments.

5. CONCLUSION

Posterior estimates (11) and correspondent covariance matrix (15) contain the total information about the measurement device after the recalibration. These expressions give final values and uncertainties for the reference values used in the recalibration. These expressions generalize previous expressions for the estimates obtained for more simple models. The above consideration is equivalent to taking a definite integral. This definite integral gives prior distribution $f(\mathbf{k})$ (19) which have the very same form as the distribution of values obtained in measurements with the measurement device.

It should be noted that the interpretation of the model (3) as a recalibration process classifies the all m quantities q_α $(\alpha = 1,....,m)$ into two parts. One part includes $m-1$ quantities that are reference quantities involved in the measurement device. Their prior values are obtained in a previous calibration of the measurement device. Another part includes one quantity which is usually measured with the measurement device. In the case of measurement value of this quantity is supposed to be unknown. However, when the recalibration measurement is carried out value of this quantity is supposed to be known and included in set (5).

Finally, a remark has to be done about the scope of the above approaches. When dominant contribution to the uncertainties of values, which are obtained with the measurement device, comes from the divider (σ) then the ratio u, which is ratio of these uncertainties after and before the recalibration, does not depend practically on uncertainties of values of the reference quantities. For this case the advantage from application the Bayesian approach (BA) is not sensible.

However, if for the measurement device the contribution from the reference quantities to the total budget of uncertainties of the measured values and the contribution from the divider are comparable then the Bayesian approach can have a sensible advantage. In the last case the Bayesian approach is similar to weighting all available data in gaining the final estimates.

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