XIX IMEKO World Congress
Fundamental and Applied Metrology
September 6−11, 2009, Lisbon, Portugal

BAYESIAN ANALYSIS OF A CALIBRATION MODEL

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Abstract − A Bayesian analysis of a calibration model was presented in *Metrologia*, **43** (2006) S167-S177, wherein two approaches were considered to obtain the probability density function associated with the measurand. In one of them, Bayes' theorem was applied directly to an input quantity for which measurement data were available. In the other approach, that same input quantity was expressed in terms of the measurand and the other input quantities. Since the forms of the likelihood function used in each approach were not the same, different prior functions were needed. In this paper we show that both approaches produce the same final results if the prior function to be used in the second approach is derived from that applicable to the first approach. By following this procedure, both prior functions are assured to encode the same initial information.

Keywords: Bayesian analysis, prior functions

1. INTRODUCTION

At the time the GUM [1] appeared, there was some debate among metrologists about the merits and drawbacks of conventional and Bayesian statistics to evaluate measurement data. Since no agreement was reached, both viewpoints were mixed in that document, making it somewhat confusing for theoreticians and practitioners alike [2]. Currently, the conflict seems to have been resolved in favor of the Bayesian treatment. The recent publication of the Supplement 1 to the GUM [3], which is entirely based on Bayesian ideas, supports this assertion.

Yet, it appears that some misunderstanding about fundamental Bayesian concepts still prevails. In this paper we address the apparent paradox raised in [4], where it was stated that two approaches for doing a Bayesian analysis are possible. These approaches were designated as

(i) Bayesian analysis applied to the type A input quantities only;
(ii) Bayesian analysis treating all unknown quantities as statistical parameters.

When applied to a simple calibration model, it was found in [4] that the results of both approaches were different. It was later suggested [5] and proved [6] that the discrepancy was to be attributed to the use of different prior functions in the two approaches. In the present article we show that if both priors encode the same initial state of knowledge, the two approaches are reconciled.

2. ANALYSIS

Consider a measurand Y modeled as

$$Y = \frac{X - B_0}{B_1}, \tag{1}$$

and assume that the three input quantities X, B_0 and B_1 are independent from each other. X is a quantity that is repeatedly measured during calibration yielding independent data $D_X = \{x_1, \ldots, x_n\}, n \geq 2$, while B_0 and B_1 are characterized by known probability density functions (PDFs) $g_{B_0}(\beta_0)$ and $g_{B_1}(\beta_1)$.[1] It is assumed that no prior knowledge about the measurand is available.

2.1. Approach (i)

In approach (i) Bayes' theorem is applied to the quantity X, giving

$$g_{X,\boldsymbol{P}}(\xi, \boldsymbol{\pi} | D_X) \propto l(\xi, \boldsymbol{\pi}; D_X) g_{X,\boldsymbol{P}}(\xi, \boldsymbol{\pi}), \tag{2}$$

where $\boldsymbol{P}$ designates the set of parameters that may appear in the sampling distribution from which the likelihood function $l(\xi, \boldsymbol{\pi}; D_X)$ is constructed. The function $g_{X,\boldsymbol{P}}(\xi, \boldsymbol{\pi} | D_X)$ is the joint PDF of the quantity X and parameters $\boldsymbol{P}$ after the data are obtained; the prior function $g_{X,\boldsymbol{P}}(\xi, \boldsymbol{\pi})$ encodes whatever information is available about X and $\boldsymbol{P}$ before the data are gathered.

It is frequently appropriate to assume that the data D_X are explained by the action of a Gaussian random mechanism with standard deviation S. In this case, the likelihood becomes

[1] The notation in [3] is followed here: the subscripted letter g denotes PDFs (either joint or marginal) or prior functions, and lower case Greek letters denote the possible values of the corresponding upper case Roman letters that designate quantities. All PDFs and prior functions should be regarded as encoding states of knowledge, not as sampling distributions.

$$l(\xi,\sigma;D_X)\propto\frac{1}{\sigma^n}\exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(\xi-x_i)^2\right),\qquad(3)$$

or equivalently, since $\bar{x}=\Sigma\, x_i/n$ and $s^2=\Sigma\,(x_i-\bar{x})^2/(n-1)$ are sufficient statistics,

$$l(\xi,\sigma;D_X)\propto\frac{1}{\sigma^n}\exp\left(-\frac{(n-1)s^2+n(\xi-\bar{x})^2}{2\sigma^2}\right).\qquad(4)$$

In the absence of prior information about one or more quantities or parameters, it is today widely accepted that reference prior functions should be adopted for them [7,8]. In the present circumstances, if nothing is previously known about X and S, the reference prior becomes the improper noninformative function [9]

$$g_{X,S}(\xi,\sigma)\propto\frac{1}{\sigma}.\qquad(5)$$

By inserting this prior and the likelihood (4) into (2), and integrating out the standard deviation, the posterior PDF $g_X(\xi|D_X)$ is found to be a scaled *t*-distribution with $n-1$ degrees of freedom centered at $\bar{x}$ [10].

The next step is to express the joint PDF about the input quantities after taking into account the data but before using the measurement model. Since the input quantities are independent, this PDF is given by

$$g_{X,B_0,B_1}(\xi,\beta_0,\beta_1|D_X)=g_X(\xi|D_X)g_{B_0}(\beta_0)g_{B_1}(\beta_1).\ (6)$$

It is now possible to introduce the measurand Y instead of one input quantity that may be chosen arbitrarily. This is done by expressing the latter in terms of the measurand and the other input quantities with the help of the model (1). For example, solving for X gives

$$\xi=\beta_0+\beta_1\eta.\qquad(7)$$

The well-known transformation rules of probability calculus [11] then yield

$$g_{Y,B_0,B_1}(\eta,\beta_0,\beta_1|D_X)=$$
$$g_X(\beta_0+\beta_1\eta|D_X)g_{B_0}(\beta_0)g_{B_1}(\beta_1)\left|\frac{\partial\xi}{\partial\eta}\right|.\qquad(8)$$

The last step is to marginalize the PDF (8) by integrating out all remaining input quantities. In this way we get

$$g_Y^{(i)}(\eta|D_X)=$$
$$\int|\beta_1|g_{B_1}(\beta_1)\int g_X(\beta_0+\beta_1\eta|D_X)g_{B_0}(\beta_0)\,\mathrm{d}\beta_0\,\mathrm{d}\beta_1.\qquad(9)$$

Using the same reasoning, the following two equivalent expressions are obtained

$$g_Y^{(i)}(\eta|D_X)=$$
$$\int|\beta_1|g_{B_1}(\beta_1)\int g_X(\xi|D_X)g_{B_0}(\xi-\beta_1\eta)\,\mathrm{d}\xi\,\mathrm{d}\beta_1\qquad(10)$$

and

$$g_Y^{(i)}(\eta|D_X)=$$
$$\int g_X(\xi|D_X)\int\frac{|\xi-\beta_0|}{\eta^2}g_{B_0}(\beta_0)g_{B_1}\left(\frac{\xi-\beta_0}{\eta}\right)\mathrm{d}\beta_0\,\mathrm{d}\xi.\qquad(11)$$

Fig. 1 depicts the PDF $g_Y^{(i)}(\eta|D_X)$ (solid curve) for the data D_X used in [4] ($n=5$, $\bar{x}=100{,}521$, $s=1{,}50227$). The PDFs $g_{B_0}(\beta_0)$ and $g_{B_1}(\beta_1)$ were taken as Gaussian distributions with expectations $b_0=0$ and $b_1=1$, and with standard uncertainties $u_{B_0}=0{,}25$ and $u_{B_1}=0{,}20$. The expectation of $g_Y^{(i)}(\eta|D_X)$ is $y^{(i)}=105{,}1$ and its standard uncertainty is $u_Y^{(i)}=24{,}5$. Arbitrary but consistent units are implied.

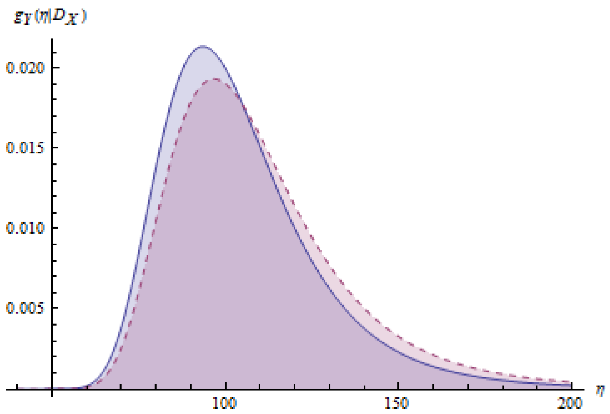

Fig. 1. Posterior PDFs for the measurand obtained with approach (i) (solid curve) and (ii) (dashed curve) for the data given in the text.

2.2. Approach (ii)

In approach (ii) Bayes' theorem is also applied to the quantity X, but expressed in terms of the measurand and the other input quantities through (7). This procedure gives

$$g_{Y,B_0,B_1,S}(\eta,\beta_0,\beta_1,\sigma|D_X)\propto$$
$$l(\eta,\beta_0,\beta_1,\sigma;D_X)g_{Y,B_0,B_1,S}(\eta,\beta_0,\beta_1,\sigma).\qquad(12)$$

where

$$l(\eta,\beta_0,\beta_1,\sigma;D_X)\propto$$
$$\frac{1}{\sigma^n}\exp\left(-\frac{(n-1)s^2+n(\beta_0+\beta_1\eta-\bar{x})^2}{2\sigma^2}\right)\qquad(13)$$

and

$$g_{Y,B_0,B_1,S}(\eta,\beta_0,\beta_1,\sigma)\propto g_{B_0}(\beta_0)g_{B_1}(\beta_1)g_{Y,S}(\eta,\sigma).\ (14)$$

This second approach needs the function $g_{Y,S}(\eta,\sigma)$. Since there is neither prior knowledge about Y nor about S, one might be tempted to assume, by analogy with (5), that the adequate noninformative prior would be

$$g_{Y,S}(\eta,\sigma) \propto \frac{1}{\sigma}. \tag{15}$$

By inserting this prior into (14) and the result, together with the likelihood (13), into (12), and by integrating over σ, we get

$$\begin{aligned} &g_{Y,B_0,B_1}(\eta,\beta_0,\beta_1|D_X) \propto \\ &t(\beta_0+\beta_1\eta|D_X)g_{B_0}(\beta_0)g_{B_1}(\beta_1), \end{aligned} \tag{16}$$

where $t(\beta_0+\beta_1\eta|D_X)$ is equal to the distribution $g_X(\beta_0+\beta_1\eta|D_X)$ above, namely, a scaled *t*-distribution with $n-1$ degrees of freedom centered at $\bar{x}$.

Finally, marginalization of (16) yields

$$\begin{aligned} &g_Y^{(ii)}(\eta|D_X) = \\ &k\int g_{B_1}(\beta_1)\int t(\beta_0+\beta_1\eta|D_X)g_{B_0}(\beta_0)\,\mathrm{d}\beta_0\,\mathrm{d}\beta_1, \end{aligned} \tag{17}$$

where k is a normalization constant to be found numerically.

Fig. 1 depicts the PDF $g_Y^{(ii)}(\eta|D_X)$ (dashed curve) for the same data and PDFs $g_{B_0}(\beta_0)$ and $g_{B_1}(\beta_1)$ as before. The expectation is $y^{(ii)}=110{,}8$ and the standard uncertainty is $u_Y^{(ii)}=28{,}6$. These results are manifestly different from those obtained with approach (i).

3. DISCUSSION

Both approaches follow from a straightforward application of Bayes' theorem and of the rules of probability calculus. The PDFs $g_Y^{(i)}(\eta|D_X)$ and $g_Y^{(ii)}(\eta|D_X)$ express the state of knowledge about the output quantity after taking into account the measurement model, the measurement data and all relevant prior information. So why are they different?

The culprit is clearly the prior function (15), because it does not encode the absence of prior information as intended. To see this, let us transform the prior $g_{X,B_0,B_1,S}(\xi,\beta_0,\beta_1,\sigma)$ from X to Y, as in (8). The result is

$$\begin{aligned} &g_{Y,B_0,B_1,S}(\eta,\beta_0,\beta_1,\sigma) = \\ &g_{B_0}(\beta_0)g_{B_1}(\beta_1)g_{X,S}(\beta_0+\beta_1\eta,\sigma)\left|\frac{\partial\xi}{\partial\eta}\right|. \end{aligned} \tag{18}$$

Inserting the partial derivative $\partial\xi/\partial\eta=\beta_1$ and the noninformative prior $g_{X,S}(\xi,\sigma)\propto 1/\sigma$ produces

$$g_{Y,B_0,B_1,S}(\eta,\beta_0,\beta_1,\sigma) \propto g_{B_0}(\beta_0)g_{B_1}(\beta_1)\frac{|\beta_1|}{\sigma} \tag{19}$$

which, in combination with the likelihood (13) followed by integration over σ and marginalization yields

$$\begin{aligned} &g_Y^{(ii\,\mathrm{m})}(\eta|D_X) = \\ &\int|\beta_1|\,g_{B_1}(\beta_1)\int t(\beta_0+\beta_1\eta|D_X)g_{B_0}(\beta_0)\,\mathrm{d}\beta_0\,\mathrm{d}\beta_1, \end{aligned} \tag{20}$$

where the superscript m stands for "modified". The PDF (20) is exactly equal to (9).

4. CONCLUSION

The simple (nonlinear) calibration model (1) was analyzed in [4] using two Bayesian approaches, yielding different results. It was shown that the discrepancy between those approaches is due to a differing choice of the prior functions: (5) in approach (i) and (15) in approach (ii). The prior (15) appears to be a noninformative, but it is not. To adequately reflect the available information, the prior to be used in approach (ii) is obtained by transforming the prior $g_{X,B_0,B_1,S}(\xi,\beta_0,\beta_1,\sigma)$ in (14) from X to Y, yielding (19). In this way the two approaches are reconciled.

ACKNOWLEDGMENT

The support of Fondecyt (Chile) research grant 1095160 is gratefully acknowledged.

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