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MEASUREMENT UNCERTAINTY EVALUATION ASSOCIATED WITH CALIBRATION FUNCTIONS

M, G Cox [1], A B Forbes [2], P M Harris [3], I M Smith [4]

[1] National Physical Laboratory, Teddington, UK, maurice.cox@npl.co.uk
[2] National Physical Laboratory, Teddington, UK, alistair.forbes@npl.co.uk
[3] National Physical Laboratory, Teddington, UK, peter.harris@npl.co.uk
[4] National Physical Laboratory, Teddington, UK, ian.smith@npl.co.uk

Abstract – Calibration procedures are widely implemented in metrology. This paper considers the evaluation of measurement uncertainty associated with the use of a calibration function. Three methods for uncertainty evaluation are described and the differences in the results returned are discussed. A simple calibration function is used to illustrate these differences.

Keywords: measurement uncertainty, calibration

1. INTRODUCTION

Calibration is an essential part of many measurement problems and often involves fitting to measurement data a calibration function that best describes the relationship between an independent (stimulus) variable and a dependent (response) variable.

The purpose of a calibration procedure is to determine estimates of the parameters of the calibration function on the basis of measurement data. The measurement data has associated uncertainty (and possibly covariance), which means that there will be uncertainty (and covariance) associated with the parameter estimates.

Having obtained estimates of the calibration function parameters and evaluated their associated uncertainties and covariances, the calibration function may subsequently be used for prediction, where an observation of the response variable and its associated standard uncertainty are used to estimate the corresponding value of the stimulus variable and evaluate its associated standard uncertainty.

In this paper, we consider three approaches to uncertainty evaluation related to the use of a calibration function: a) the GUM uncertainty framework [1], b) a Monte Carlo approach as described in GUM Supplement 1 [2], and c) a Bayesian approach. Results are illustrated for the case of a cubic calibration function.

2. MODELS FOR CALIBRATION

2.1 Functional model

The calibration function is a functional model that describes the mathematical relationship between the stimulus and response variables. The functional model can be a physical, empirical or hybrid model. A physical model is one where there is a theory about how the variables depend on each other. An empirical model is one in which a relationship between the variables is expected or observed but without any supporting theory. A hybrid model has both physical and empirical components. We assume a functional model of the form $\eta = \phi(\xi, \boldsymbol{\alpha})$ describing the response variable η as a function of the stimulus variable ξ and parameters $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)^{\mathrm{T}}$.

2.2 Statistical model

We assume the measurement data (x_i, y_i), $i = 1, \ldots, m$, arises according to the following statistical model:

$$x_i = \xi_i + d_i, \quad y_i = \phi(\xi_i, \boldsymbol{\alpha}) + e_i, \quad i = 1, \ldots, m, \qquad (1)$$

where d_i and e_i are realizations of random variables. The statistical model is completed by making statements about the expectations (almost always taken to be zero), variances and covariances (often taken to be zero) of the random variables and, possibly, the probability distributions characterizing them.

A common statistical model encountered in metrology is one where the uncertainties associated with the measured y-values are non-zero and those associated with the measured x-values can be regarded as negligible and all covariances are taken to be zero. Another is where the uncertainties associated with both the measured x- and y-values are non-zero and all covariances are taken to be zero.

3. DETERMING THE CALIBRATION FUNCTION FROM DATA

The aim of the calibration procedure is to determine estimates $\mathbf{a}$ of $\boldsymbol{\alpha}$ and the covariance matrix $V_{\mathbf{a}}$ associated with the estimates, given the measurement data and associated uncertainty information. The algorithm used to determine the estimates depends on the nature of the functional and statistical models [3]. For the case in which the functional model is linear in $\boldsymbol{\alpha}$ and the uncertainties and covariances associated with the estimates x_i of ξ_i are all zero, the best estimates $\mathbf{a}$ are those that minimize

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$$\mathbf{f}^{\mathrm{T}} V_{\mathbf{y}}^{-1} \mathbf{f}, \quad \mathbf{f} \equiv \mathbf{f}(\boldsymbol{\alpha}) = \mathbf{y} - C\boldsymbol{\alpha}, \tag{2}$$

with respect to the α_j, where $f_i = y_i - \phi(x_i, \boldsymbol{\alpha})$, C is the matrix of partial derivatives of first order $\partial\phi(x_i, \boldsymbol{\alpha})/\partial\alpha_j$ of the model function with respect to the parameters $\boldsymbol{\alpha}$, evaluated at x_i, and V_y is the covariance matrix associated with the y_i in (1).

If $V_y = \sigma^2 I$, then

$$\mathbf{a} = \left(C^{\mathrm{T}} C\right)^{-1} C^{\mathrm{T}} \mathbf{y}, \quad V_{\mathbf{a}} = \sigma^2 \left(C^{\mathrm{T}} C\right)^{-1}, \tag{3}$$

that is, $\mathbf{a}$ is the solution of the normal equations derived from (2) and $V_{\mathbf{a}}$ is obtained using the general result for the relationship $\mathbf{w} = G\,\mathbf{v}$ that $V_{\mathbf{w}} = G V_{\mathbf{v}} G^{\mathrm{T}}$. If we make the further assumption that

$$y_i \in \mathrm{N}(\phi(x_i, \boldsymbol{\alpha}), \sigma^2), \tag{4}$$

meaning that y_i is a draw from the indicated distribution, then $\mathbf{a} \in \mathrm{N}(\boldsymbol{\alpha}, V_{\mathbf{a}})$. From a Bayesian point of view, assuming an uninformative prior $p(\boldsymbol{\alpha}) \propto 1$, the posterior distribution for $\boldsymbol{\alpha}$, given the measurement data, is $\mathrm{N}(\mathbf{a}, V_{\mathbf{a}})$.

4. USING THE CALIBRATION FUNCTION

We suppose that estimates $\mathbf{a}$ of $\boldsymbol{\alpha}$ and associated covariance matrix $V_{\mathbf{a}}$ have been determined. Given an observed response value y generated according to the model

$$y = \phi(\xi, \boldsymbol{\alpha}) + e, \tag{5}$$

where e is a realization of a random variable with expectation zero and variance σ^2, what is the best estimate x of ξ and its associated uncertainty? In the absence of any further information we invoke the principal of maximum entropy to characterize the random variable of which e is a realization by $\mathrm{N}(0, \sigma^2)$ [2].

The uncertainty associated with x will have two contributing factors: the uncertainty associated with the observed response value and the uncertainties and covariances associated with the estimates of the calibration function parameters. We give three approaches to answering the above question: the GUM uncertainty framework [1], the GUM Supplement 1 (GUMS1) approach [2] and a Bayesian approach. We note here that the GUMS1 and Bayesian approaches use distributional information while the GUM approach can be implemented on the basis of knowing only expectations, variances and covariances.

4.1 GUM uncertainty framework

In the GUM uncertainty framework the best estimate of ξ is the x that solves $y = \phi(x, \mathbf{a})$. This equation implicitly defines x as a function of y and $\mathbf{a}$. The GUM uncertainty framework requires the calculation of the sensitivity coefficients for x with respect to y and the parameters $\mathbf{a}$. Using a linear approximation, the calculations show that the standard uncertainty $u(x)$ associated with the estimate x is given by

$$\left(\frac{\partial\phi}{\partial x}\right)^2 u^2(x) = u^2(y) + \mathbf{c}_{\mathbf{a}}^{\mathrm{T}} V_{\mathbf{a}} \mathbf{c}_{\mathbf{a}}, \tag{6}$$

where $\mathbf{c}_{\mathbf{a}} = \left(\frac{\partial\phi}{\partial\alpha_1}, \ldots, \frac{\partial\phi}{\partial\alpha_n}\right)^{\mathrm{T}}$ is the vector of partial derivatives of first order of the model function with respect to the parameters $\boldsymbol{\alpha}$, evaluated at x, and $\partial\phi/\partial x$ is the partial derivative of first order of the model function with respect to the stimulus quantity parameter, evaluated at x and $\boldsymbol{\alpha}$. Equation (6) makes clear the contributions arising from y and $\mathbf{a}$.

4.2 GUM Supplement 1 approach

The Monte Carlo approach described in GUMS1 requires draws y_q and $\mathbf{a}_q$, for $q = 1, \ldots, M$, to be made from the distributions assigned to y and $\mathbf{a}$. The corresponding values x_q satisfying $y_q = \phi(x_q, \mathbf{a}_q)$ are then calculated. The values x_q, $q = 1, \ldots, M$, constitute a discrete representation of an approximation to the probability distribution for ξ. Statistics, namely the mean and standard deviation, are calculated for the M values x_q giving values for, respectively, the estimate of ξ and its associated standard uncertainty. Coverage intervals can also be calculated corresponding to prescribed coverage probabilities.

Whereas the GUM uncertainty framework approach assumes that a linear approximation to the model is sufficient, the Monte Carlo method makes no such assumption. It is therefore likely that the uncertainties returned by the GUM and Monte Carlo approaches will be different if nonlinearities are significant relative to the magnitudes of the uncertainties involved.

4.3 Bayesian approach

The Bayesian approach calculates a posterior distribution $p(\xi \mid y)$ for ξ based on the observed response y, the knowledge $p(\boldsymbol{\alpha})$ about $\boldsymbol{\alpha}$ gained from the prior calibration exercise and any prior information about ξ given in terms of a distribution $p(\xi)$. Applying Bayes' Theorem

$$p(\xi, \boldsymbol{\alpha} \mid y) \propto p(y \mid \xi, \boldsymbol{\alpha})\, p(\boldsymbol{\alpha})\, p(\xi), \tag{7}$$

the required distribution is given by marginalization, namely

$$p(\xi \mid y) = \int_{\Omega} p(\xi, \boldsymbol{\alpha} \mid y)\, \mathrm{d}\boldsymbol{\alpha}, \tag{8}$$

where Ω represents Euclidean n-space.

Markov chain Monte Carlo (MCMC) techniques [4, 5] can be used to generate samples from $p(\xi, \boldsymbol{\alpha} \mid y)$ from which an estimate, standard deviation and coverage interval

can be calculated in the same way as for the GUMS1 approach.

For the case of linear models, the marginalization in (8) can be performed analytically (see annex A for details). Suppose $\phi(\xi, \boldsymbol{\alpha}) = \mathbf{c}^{\mathrm{T}}(\xi)\boldsymbol{\alpha}$ expresses $\phi(\xi, \boldsymbol{\alpha})$ as a linear combination of basis functions. If $y \mid \xi, \boldsymbol{\alpha} \sim \mathrm{N}(\phi(\xi, \boldsymbol{\alpha}), \sigma^2)$, $\boldsymbol{\alpha} \sim \mathrm{N}(\mathbf{a}, V_{\mathbf{a}})$ and $p(\xi) \propto 1$, then

$$p(\xi \mid y) \propto \frac{1}{\sigma(\xi)} \exp\left\{-\frac{1}{2}\left(\frac{y - \mathbf{c}^{\mathrm{T}}(\xi)\mathbf{a}}{\sigma(\xi)}\right)^2\right\}, \qquad (9)$$

with $\sigma^2(\xi) = \sigma^2 + \mathbf{c}^{\mathrm{T}}(\xi)V_{\mathbf{a}}\mathbf{c}(\xi)$. Equation (9) expresses the posterior distribution for ξ in terms of the calibration information $\mathbf{a}$ and $V_{\mathbf{a}}$ and the basis function values $\mathbf{c} \equiv \mathbf{c}(\xi)$. The constant of integration can be determined by numerical quadrature.

5. EXAMPLE: CUBIC CALIBRATION FUNCTION

We illustrate the behaviour of the three approaches for a calibration function of the form

$$\eta = \phi(\xi, \boldsymbol{\alpha}) = \alpha_1 + \alpha_2\xi + \alpha_3\xi^3. \qquad (10)$$

Calibration data has been simulated according to the model (4). Fig. 1 shows example data and the fitted calibration function for parameter vector $\boldsymbol{\alpha} = (0, 1, 1)^{\mathrm{T}}$ and $\sigma = 0.2$. The expanded uncertainties associated with the y_i are illustrated by vertical bars, centred on y_i and having extremities $y_i - 2\sigma$ and $y_i + 2\sigma$.

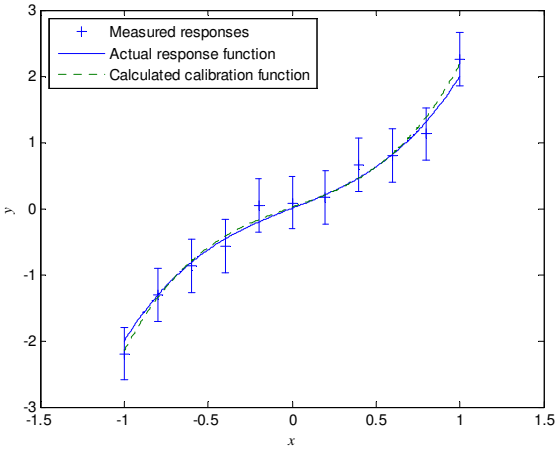

Fig. 1. Cubic calibration function generated from simulated data.

Given an observed response value $y \in \mathrm{N}(\phi(\xi, \boldsymbol{\alpha}), \sigma^2)$, the three methods described in section 4 are used to provide an estimate x of ξ and its associated standard uncertainty $u(x)$. In the current context, the GUMS1 approach assumes that the quantities of which y and $\mathbf{a}$ are realizations are characterized by normal distributions $\mathrm{N}(y, \sigma^2)$ and $\mathrm{N}(\mathbf{a}, V_{\mathbf{a}})$, respectively. The Bayesian approach is implemented using (9) with $\mathbf{c}^{\mathrm{T}}(\xi) = (1, \xi, \xi^3)$. A MCMC sampling method based on a version of the Metropolis-Hastings described in [5] has also been implemented.

The set of values returned by the GUMS1 and MCMC approaches may be assembled into histograms forming frequency distributions that, when normalized to have unit area, provide approximations to the probability density functions (PDFs) for ξ.

Figs. 2 and 3 show the results of example calculations for two response values y and $\sigma = 0.2$. For both cases the three distributions are different. The Bayesian and GUM distributions have the same mode given by the ξ that solves $y = \phi(\xi, \mathbf{a})$.

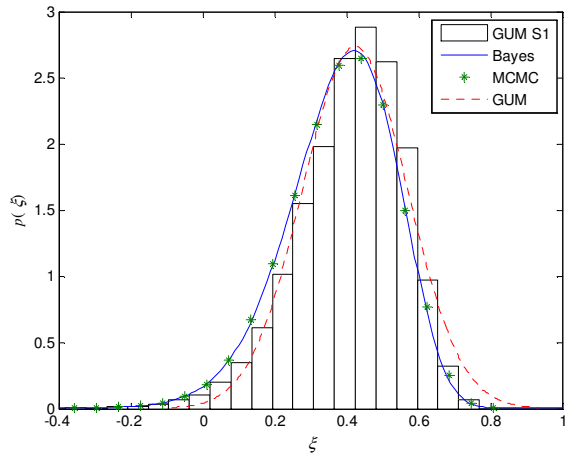

Fig. 2. Distributions for ξ from the three uncertainty evaluation methods and MCMC for $y = 0.5$ and $\sigma = 0.2$.

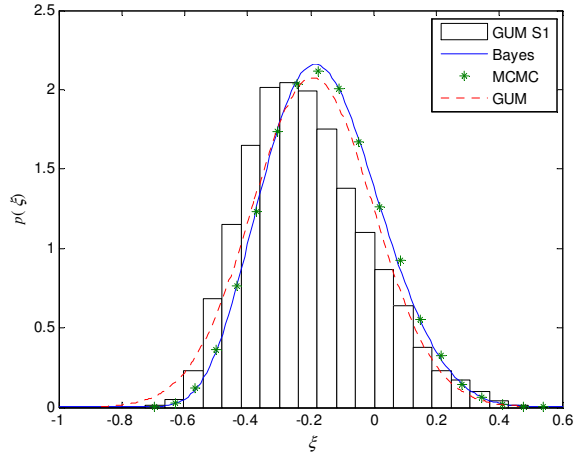

Fig. 3. As Fig. 2 but for $y = -0.2$.

6. DISCUSSION

The GUMS1 and Bayesian approaches clearly provide different distributions in the example of section 5. The differences between the distributions can be related to the roles of the observation equation and the measurement in the GUM [7]. From a Bayesian point of view, the difference can be described as follows. The observation model $y \in \mathrm{N}(\phi(\xi, \boldsymbol{\alpha}), \sigma^2)$ describes how the measurement process can produce an observation and specifies the probability $p(y \mid \xi, \boldsymbol{\alpha})$ of observing y, given parameter values ξ and $\boldsymbol{\alpha}$. We write $y \mid \xi, \boldsymbol{\alpha} \sim \mathrm{N}(\phi(\xi, \boldsymbol{\alpha}), \sigma^2)$, regarding y as the variable and ξ and $\boldsymbol{\alpha}$ as given. The data from the calibration experiment provides a distribution for $\boldsymbol{\alpha}$, namely $\mathrm{N}(\mathbf{a}, V_{\mathbf{a}})$. This distribution is the distribution posterior to gathering the calibration data, but we now regard it as the distribution prior to observing a response. Given a prior distribution $p(\xi)$ for the stimulus variable ξ, Bayes' theorem (7) and (8), defines the posterior distribution $p(\xi \mid y)$, where now ξ is regarded as the variable and y the fixed (observed) response value. Bayes' theorem can be regarded as probabilistic inversion, converting information about how an observation can arise to information about the system that gave rise to the observation.

The GUM approach is to recast the observation equation as the measurement function. The equation $\eta = \phi(\xi, \boldsymbol{\alpha})$ implicitly defines $\xi = \psi(\eta, \boldsymbol{\alpha})$ as a function of η and $\boldsymbol{\alpha}$. We term this "functional inversion" as opposed to "probabilistic inversion". By assigning distributions to η and $\boldsymbol{\alpha}$ on the basis of the measured response y and the calibration experiment, the relation $\xi = \psi(\eta, \boldsymbol{\alpha})$ defines a distribution for ξ. The GUM methodology implicitly propagates the distributions for η and $\boldsymbol{\alpha}$ through to that for ξ using the law of propagation of uncertainty based on first (or second) order approximations, while GUMS1 uses a Monte Carlo method, without any approximating assumptions. For both GUM and GUMS1 calculation methods, η is assigned the distribution $\mathrm{N}(y, \sigma^2)$ and $\boldsymbol{\alpha}$ the distribution $\mathrm{N}(\mathbf{a}, V_{\mathbf{a}})$. In the GUM approach, the best estimate of ξ is given by $x = \psi(y, \mathbf{a})$. The distribution assigned to η represents the predicted distribution of the responses for repeated measurement of the same stimulus using the same instrument. The propagation methodology provides a method for approximating the distribution of estimates $\tilde{\xi}$ that would be returned if the same calibration, measurement, and estimation procedure were repeated many times for the same artefact and using the same instrument. That is, the methodology provides an approximation for the distribution $p(\tilde{\xi} \mid \xi = x_0, \boldsymbol{\alpha} = \mathbf{a}_0)$, where x_0 and $\mathbf{a}_0$ are candidate values for ξ and $\boldsymbol{\alpha}$. In this sense, the GUM/GUMS1 methodology is aimed at characterizing the behaviour of the measuring system [8]. The candidate values usually chosen are those arising from the calibration and response measurement, $\mathbf{a}$ and $x = \psi(y, \mathbf{a})$.

The differences in the GUM/GUMS1 and Bayesian approaches can be analyzed more straightforwardly if the calibration parameters $\boldsymbol{\alpha}_0 = (0, 1, 1)^{\mathrm{T}}$, say, are known with negligible uncertainty. In this case, the uncertainty associated with the stimulus arises solely from the measurement of the response $\eta = \phi(\xi, \boldsymbol{\alpha}_0) = \xi + \xi^3$ modelled as $y \in \mathrm{N}(\phi(\xi, \boldsymbol{\alpha}_0), \sigma^2)$. The estimate x of ξ can be written implicitly as a function $x = \psi(y, \boldsymbol{\alpha}_0)$ of y. Given an observed y, the GUMS1 approach (as interpreted above) assigns the normal distribution $\mathrm{N}(y, \sigma^2)$ to "best estimate" y and propagates this distribution through to "best estimate" x via the function $\psi(y, \boldsymbol{\alpha}_0)$. From a Bayesian point of view, the assignment of the normal distribution to y is only justified if the prior distribution for observing y is uniform, that is, before the experiment is performed there is an equal probability of the response variable taking any value between –1 and 1, say. By contrast, the Bayesian approach (as interpreted above) assigns a uniform prior distribution to the stimulus variable.

Since the cubic calibration function is monotonic increasing, the relationship $\eta = \phi(\xi, \boldsymbol{\alpha}_0)$ represents a re-parameterization. A state-of-knowledge distribution for ξ defined by a PDF $p(\xi)$ defines a PDF $p(\eta)$ with

$$p(\eta) = p(\xi)\left|\frac{d\psi}{d\eta}\right| \quad \text{and} \quad p(\xi) = p(\eta)\left|\frac{d\phi}{d\xi}\right|.$$

The assignment of a prior for the response implies a prior for the stimulus and vice versa. In particular, a uniform prior for the response assigns the quadratic prior $p(\xi) \propto 1 + 3\xi^2 = \phi'(\xi)$ for the stimulus. The effect of this quadratic prior can be seen in Figs. 2 and 3. The effect is more pronounced for larger σ. Fig. 4 shows the Bayesian and GUMS1 distributions for σ = 0.5 and y = 0.0 and 0.5.

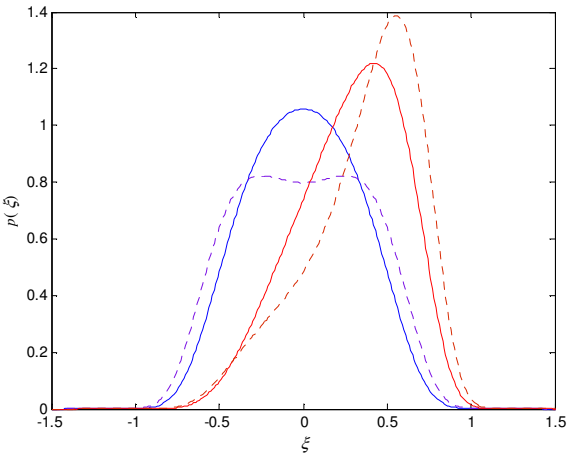

Fig. 4. Bayesian (solid) and GUMS1 (dotted) distributions for ξ associated with responses y = 0.0 (left hand pair) and 0.5 (right hand pair).

For this example, the GUMS1 distribution can only be interpreted as a state-of-knowledge distribution for the stimulus variable, posterior to the measurement data, if we believe the quadratic distribution summarizes the prior information available about the stimulus variable. This is unlikely to be the case; for example, it implies that the nominal value is the least probable value for the stimulus variable. More generally, assigning a uniform prior to the response variable is equivalent to assigning a prior $p(\xi) \propto |\phi'(\xi)|$ for the stimulus variable. For the case of a linear calibration function, the slope is constant and the stimulus variable is also associated with a uniform prior.

From a practical point of view, the differences in the GUM uncertainty framework, GUMS1 approach and Bayesian approach become apparent only when the uncertainty associated with the response measurement is appreciable relative to the curvature in the calibration function. In the numerical example considered in section 5, the standard uncertainty associated with the response measurement is approximately 10 % of the response range. If this standard uncertainty is reduced to 1 % of the range, the differences become negligible and a GUM uncertainty evaluation should be sufficient for practical purposes.

The computational requirements of the three evaluation schemes for obtaining the uncertainty associated with a measured value of the response are different. The GUM uncertainty framework requires the evaluation of a formula, the Bayesian approach requires one-dimensional numerical quadrature (for a linear model), while the GUMS1 approach requires a Monte Carlo calculation. If the standard uncertainty associated with the measured response value is known a priori, then means, standard uncertainties and coverage intervals can be calculated beforehand and stored for all three methods. Given a particular measured response value, the associated uncertainty information can be read from the stored calculations. Fig. 5 gives 95 % coverage intervals for the Bayesian and GUM approaches along with the mean of the distributions for the Bayesian distributions. The fact that the mode and mean for the distributions are generally different bring to the fore the question of what should be returned as the "best estimate" of the stimulus variable.

7. CONCLUSIONS

We have described GUM, GUMS1 and Bayesian methodologies for evaluating the uncertainty associated with the value of the stimulus variable corresponding to a measured value of the response variable. These methodologies take account of the uncertainties associated with the determination of the calibration function. For many practical situations, all three methods will give results that do not differ appreciably from each other. The GUM uncertainty framework uses linearizing approximations that can limit the validity of the results. Two alternative evaluation methods, the GUMS1 and Bayesian approaches, have been considered. Neither method relies on the linearizing approximations that form the basis of the GUM uncertainty framework. However, the two methods involve different distributions. The GUMS1 approach follows the GUM's use of the measurement function, a functional inversion of the observation equation, which allows the uncertainty to be evaluated using an implementation of the propagation of distributions. The propagated distribution characterizes the behaviour of the measuring system. From this point of view, the GUM approach makes an assumption of underlying normality, but the GUMS1 approach makes no such assumption. The Bayesian approach depends directly on the observation equation and uses probabilistic inversion to provide a state-of-knowledge distribution for the stimulus variable. In cases where the two distributions are different, it is important that inferences based on one or other of the distributions are made carefully. One of the issues arising in the revision of the GUM, now under way, is the role of the observation equations and measurement function in uncertainty evaluation.

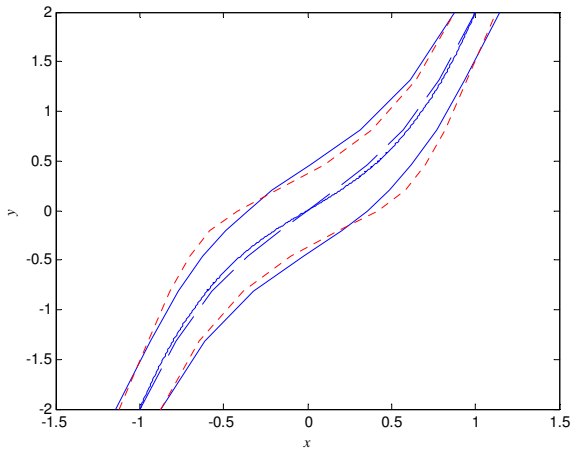

Fig. 5. Mode and 95 % coverage intervals based on a Bayesian uncertainty evaluation (solid). The GUM coverage intervals are given by the dotted curves. The dashed curve is the mean of the Bayesian distributions.

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ANNEX A

Suppose $\phi(\xi, \boldsymbol{\alpha}) = \mathbf{c}^{\mathrm{T}}(\xi)\boldsymbol{\alpha}$ expresses $\phi(\xi, \boldsymbol{\alpha})$ as a linear combination of basis functions. If $y \mid \xi, \boldsymbol{\alpha} \sim \mathrm{N}(\phi(\xi, \boldsymbol{\alpha}), \sigma^2)$, $\boldsymbol{\alpha} \sim \mathrm{N}(\mathbf{a}, V_{\mathbf{a}})$ and $p(\xi) \propto 1$, then

$$p(y \mid \xi, \boldsymbol{\alpha}) \propto \exp\left\{-\frac{1}{2}\left(\frac{y - \mathbf{c}^{\mathrm{T}}(\xi)\boldsymbol{\alpha}}{\sigma}\right)^2\right\}, \qquad \text{(A1)}$$

and

$$p(\boldsymbol{\alpha})\,p(\xi) \propto \exp\left\{-\frac{1}{2}(\mathbf{a}-\boldsymbol{\alpha})^{\mathrm{T}} V_{\mathbf{a}}^{-1}(\mathbf{a}-\boldsymbol{\alpha})\right\}. \qquad \text{(A2)}$$

If $V_{\mathbf{a}}$ is factored as $V_{\mathbf{a}} = (R_{\mathbf{a}}^{\mathrm{T}} R_{\mathbf{a}})^{-1}$, $\mathbf{z} = \begin{bmatrix} y/\sigma \\ R_{\mathbf{a}}\mathbf{a} \end{bmatrix}$ and $D \equiv D(\xi) = \begin{bmatrix} \mathbf{c}^{\mathrm{T}}(\xi)/\sigma \\ R_{\mathbf{a}} \end{bmatrix}$, then

$$p(\xi, \boldsymbol{\alpha} \mid y) \propto \exp\left\{-\frac{1}{2}(\mathbf{z}-D(\xi)\boldsymbol{\alpha})^{\mathrm{T}}(\mathbf{z}-D(\xi)\boldsymbol{\alpha})\right\}. \qquad \text{(A3)}$$

With ξ fixed, let $\hat{\mathbf{a}} \equiv \hat{\mathbf{a}}(\xi)$ minimize $(\mathbf{z}-D\boldsymbol{\alpha})^{\mathrm{T}}(\mathbf{z}-D\boldsymbol{\alpha})$ with respect to $\boldsymbol{\alpha}$ so that

$$(\mathbf{z}-D\boldsymbol{\alpha})^{\mathrm{T}}(\mathbf{z}-D\boldsymbol{\alpha}) =$$

$$(\mathbf{z}-D\hat{\mathbf{a}})^{\mathrm{T}}(\mathbf{z}-D\hat{\mathbf{a}}) + (\hat{\mathbf{a}}-\boldsymbol{\alpha})^{\mathrm{T}}(D^{\mathrm{T}}D)(\hat{\mathbf{a}}-\boldsymbol{\alpha}). \qquad \text{(A4)}$$

Since

$$\int \exp\left\{-\frac{1}{2}(\hat{\mathbf{a}}-\boldsymbol{\alpha})^{\mathrm{T}}(D^{\mathrm{T}}D)(\hat{\mathbf{a}}-\boldsymbol{\alpha})\right\} \mathrm{d}\boldsymbol{\alpha} \propto \left|D^{\mathrm{T}}D\right|^{-1/2}, \qquad \text{(A5)}$$

we have

$$p(\xi \mid y) \propto \exp\left\{-\frac{1}{2}(\mathbf{z}-D\hat{\mathbf{a}})^{\mathrm{T}}(\mathbf{z}-D\hat{\mathbf{a}})\right\}, \qquad \text{(A6)}$$

where $D \equiv D(\xi)$ and $\hat{\mathbf{a}} \equiv \hat{\mathbf{a}}(\xi)$ depend on ξ.

Continuing the analysis, $D^{\mathrm{T}}D = \frac{1}{\sigma^2}\mathbf{c}(\xi)\mathbf{c}^{\mathrm{T}}(\xi) + V_{\mathbf{a}}^{-1}$, and $\left|D^{\mathrm{T}}D\right| \propto \sigma^2(\xi)$, where $\sigma^2(\xi) = \sigma^2 + \mathbf{c}^{\mathrm{T}}(\xi)V_{\mathbf{a}}\,\mathbf{c}(\xi)$. It can be shown that

$$\hat{\mathbf{a}}(\xi) = \mathbf{a} + \left(\frac{y - \mathbf{c}^{\mathrm{T}}(\xi)\mathbf{a}}{\sigma^2(\xi)}\right) V_{\mathbf{a}}\mathbf{a}, \qquad \text{(A7)}$$

and

$$(\mathbf{z}-D\hat{\mathbf{a}})^{\mathrm{T}}(\mathbf{z}-D\hat{\mathbf{a}}) = \left(\frac{y - \mathbf{c}^{\mathrm{T}}(\xi)\mathbf{a}}{\sigma(\xi)}\right)^2, \qquad \text{(A8)}$$

so that (A6) simplifies to

$$p(\xi \mid y) \propto \frac{1}{\sigma(\xi)} \exp\left\{-\frac{1}{2}\left(\frac{y - \mathbf{c}^{\mathrm{T}}(\xi)\mathbf{a}}{\sigma(\xi)}\right)^2\right\}, \qquad \text{(A9)}$$

with $\sigma^2(\xi) = \sigma^2 + \mathbf{c}^{\mathrm{T}}(\xi)V_{\mathbf{a}}\mathbf{c}(\xi)$.

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