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A USER-FRIENDLY SOFTWARE FOR A SIMPLE AND VALIDATED IMPLEMENTATION OF GUM SUPPLEMENT 1

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Abstract – The Monte Carlo Method [3] requires computational resources to generate random numbers. LNE-MCM software was developed as user-friendly interface; it is validated and dedicated to the evaluation of measurement uncertainty using Monte Carlo simulations. Moreover, additional features are implemented: the case of multivariate models, sensitivity analysis and a goodness of fit test. LNE-MCM is scheduled to be freely available on LNE's website in 2015.

Keywords: measurement uncertainty, Monte Carlo Method, supplement 1 to the GUM, sensitivity analysis

1. INTRODUCTION

The method introduced in the Guide to the expression of Uncertainty in Measurement (GUM) for evaluating measurement uncertainty is based on the propagation of uncertainty [2]. However for a lot of common cases, the use of the Law of Propagation of Uncertainty (LPU) is not recommended. To take this limitation into account, one has to adopt a method with a broader scope like the method described in the GUM Supplement 1 [3] which is called Monte Carlo Method. The approach advocated in this Supplement 1 is based on the propagation of distributions instead of the propagation of uncertainty in the GUM. It is a stochastic procedure based on making random draws from the probability density function (PDF) for the input quantities. A pseudo-random number generator is needed to implement this Monte Carlo Method. Therefore we developed software, called LNE-MCM, coded in Matlab language with a user-friendly interface and dedicated to the evaluation of the measurement uncertainty using Monte Carlo simulations in the case of explicit mathematical models. The pseudo-random number generator is taken from Mersenne Twister's work [6]. This software provides the users with the possibility to choose between several probability distributions to represent the uncertainty of the input quantities. Correlations between input quantities are also taken into account when their marginal distributions are either Gaussian or Student. Moreover, many measurement problems involve more than one output quantity, LNE-MCM software is able to deal with such cases with respect to the GUM Supplement 2 [4]. Beyond the scope of GUM Supplement 1, LNE-MCM software provides an uncertainty budget with a sensitivity analysis. Two methods are available: the Spearman correlation coefficient for monotonic measurement models and Sobol' indices for more complex models [7]. The Kolmogorov-Smirnov goodness of fit test can be used to determine the probability distribution which is the closest to the obtained empirical PDF [5]. It is useful when the measurand of a measurement model is an input quantity for another measurement model. Furthermore, a numerical validation of the GUM uncertainty framework is proposed as recommended in the GUM Supplement 1. Illustration of LNE-MCM software will be based on the example of the GUM Supplement 1: the mass calibration model as shown in Fig. 1.

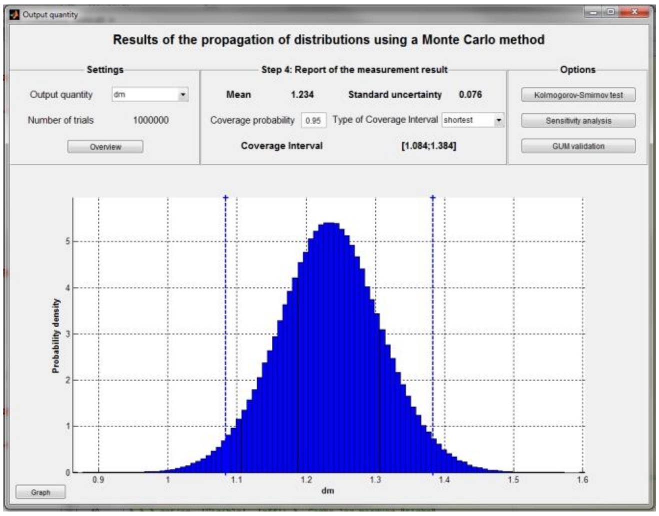

Fig. 1. PDF of the output quantity *dm* given by LNE-MCM software for the mass calibration example of the GUM Supplement 1.

In the following sections, we summarize the main principles of the Monte Carlo Method and we describe the additional features added in the LNE-MCM software.

2. MONTE CARLO METHOD (GUM S1)

As mentioned before, the Monte Carlo Method is an alternative method to the GUM when conditions to apply the GUM method are not fulfilled [1, 2]. Typical situations where Monte Carlo Method is recommended are when, the explicit mathematical measurement model is strongly non-linear, the partial derivatives of the model are difficult to compute, the best estimate and the uncertainty associated with the measurand have the same order of magnitude, the distributions for the input quantities are asymmetric... Additionally, when the PDF for the output quantity departs appreciably from a Gaussian distribution, coverage intervals are unrealistic. On the contrary, the Monte Carlo Method provides coverage intervals (either probabilistically symmetric or the shortest) which require no assumptions on the distribution of the output quantity. Basically the Monte Carlo Method can be summarized in four main steps as illustrated in Fig. 2. In the first step, the measurement process is analysed in order to precisely define the output quantity (measurand), to determine the input quantities upon which the output quantity depends and to develop the measurement model. Then, thanks to prior information, PDF are assigned to the input quantities. In the third step, the distributions of the PDF for the input quantities are propagated through the mathematical model using Monte Carlo simulations to obtain the PDF for the output quantity. Finally, the results are summarized using statistical parameters such as the mean, the standard deviation of the output quantity and a coverage interval containing the output quantity with a specified probability. In LNE-MCM software, it is first assumed that the analysis of the measurement process is being done. Indeed, before using LNE-MCM software the user should know the mathematical model, the input quantities and their PDF. Secondly, the use of LNE-MCM software is then intuitive and follows the previous steps.

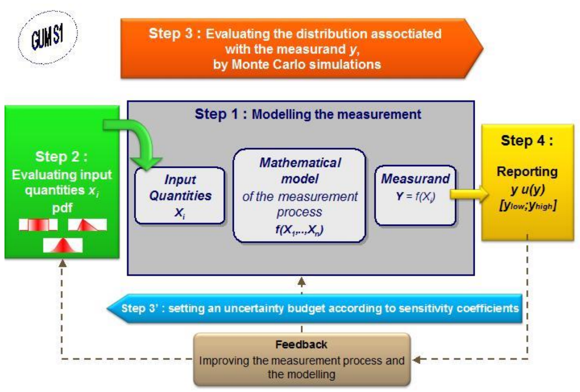

Fig. 2. Summary of procedure for evaluating and reporting uncertainty.

In order to increase its interest for the users, additional features were implemented that go beyond the GUM Supplement 1.

3. ADDITIONAL FEATURES

Indeed, LNE-MCM enables the user to consider measurement models with any number of output quantities [4], to perform a sensitivity analysis with two methods: Spearman rank correlation and Sobol' indices [7], to compare results given by the Monte Carlo Method and the LPU method using the validation procedure described in the GUM S1 and finally offers a goodness of fit test [5].

3.1. Multivariate models

The GUM and GUM Supplement 1 are focused on measurement models having a single output quantity. However, many measurement problems have more than one output quantity depending on a common set of input quantities. It happens for example when the measurand is a complex number, in which case it can be split up into a real part and imaginary part for example. LNE-MCM software considers also the case of multivariate models according to GUM Supplement 2. The two-dimensional coverage region considered in LNE-MCM software is an ellipse centred at the best estimates for the two involved Gaussian output quantities.

3.2. Sensitivity analysis

Sensitivity analysis is used to determine how “sensitive” a model is to changes in the value of the parameters of the model. In the context of the evaluation of measurement uncertainty, it enables one to have a better knowledge on the contributions of the different input quantities to the variance of the output quantity (also called the uncertainty budget). Within the GUM Uncertainty Framework (GUF) this is provided by the partial derivatives of the measurement model, which is a local sensitivity analysis. On the contrary, there is no immediate counterpart of sensitivity with a Monte Carlo Method. The GUM Supplement 1 proposes to evaluate such contributions by holding all input quantities but one fixed at their best estimate and performing a new Monte Carlo simulation for each input quantity. This method provides a quantification of the effect of the given input quantity on the standard deviation of the output quantity but is not computationally efficient for monotonic models since it requires additional simulations. Furthermore, when only one input quantity varies, holding all the other input quantities fixed at their best estimate, potential interaction effects cannot occur and will not be considered in the sensitivity analysis. To address this issue, we propose a global sensitivity analysis in LNE-MCM software based on the two following methods: the Spearman correlation coefficients for the monotonic measurement model and the Sobol' indices for more complex models. The Fig. 3. shows a sensitivity analysis performed on the example of mass calibration, with the Sobol' indices.

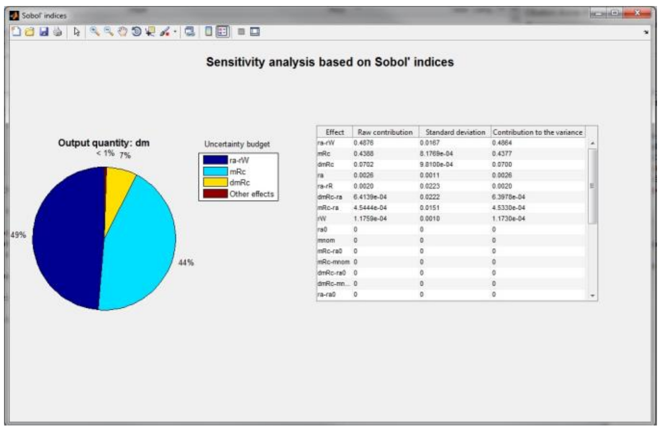

Fig. 3. Sensitivity analysis based on Sobol' indices for the example of mass calibration.

The main advantage of these two previous methods is that they are global in the sense that all over the range of the different input quantities are taken into account whereas with the GUF only the sensitivity around the best estimate of the input quantities is considered. Thereafter, are briefly summarized the two methods. For more details we refer to [7]. In practice, for a sample of size M, we consider the ranks of each simulated value for the input X_j and for the output quantity Y_k. For each ranked pair (X_j, Y_k), the difference d_i between the ranks is computed and the Spearman rank correlation coefficient between X_j and Y_k is calculated as in (1)

$$\rho_{j,k} = 1 - \frac{6\sum_{i=1}^{M} d_i^2}{(M^3 - M)} \tag{1}$$

This correlation coefficient is normalized in order to obtain an estimation of the contribution of the input quantity X_j to the variance of the output quantity Y_k according to (2):

$$S_{j,k} = \frac{\rho_{j,k}^2}{\sum_{j=1}^{M} \rho_{j,k}^2} \tag{2}$$

When the measurement model is not monotonic, one has to use Sobol' indices for sensitivity analysis. Sobol' method is a global sensitivity analysis technique which determines the contribution of each input (or group of inputs) to the variance of the output. According to the total variance decomposition theorem, the variance of an output quantity Y may be decomposed as the sum of the variance of the conditional expectation of Y given X_i and the expectation of the conditional variance of Y given X_i according to (3).

$$V(Y) = V\left[E(Y \,\|\, X_i)\right] + E\left[V(Y \,\|\, X_i)\right] \tag{3}$$

The first term $V_i = V\left[E(Y \,\|\, X_i)\right]$ denotes the part of the variance of Y due to the variations of the input quantity X_i while the second term denotes the part of the variance of Y that is due to all the input quantities but X_i. The first order sensitivity index is then defined as (4)

$$S_i = \frac{V_i}{V(Y)} \tag{4}$$

A second order sensitivity index can also be obtained from the variance due to the couple of quantities X_i and X_j according to (5)

$$S_{i,j} = \frac{V\left[E(Y \,\|\, X_i, X_j)\right] - V_i - V_j}{V(Y)} \tag{5}$$

Higher order sensitivity indices can be obtained in the same manner, until n^{th}order (where n is the number of input quantities). In LNE-MCM software, Sobol' indices are estimated by Monte Carlo Method, and available up to the second order. Consider two M-samples $(x_{i,j})_{i=1,\dots,n;\, j=1,\dots,M}$ and $(x'_{i,j})_{i=1,\dots,n;\, j=1,\dots,M}$. The first order sensitivity index is estimated by (5)

$$\hat{S}_i = \frac{\hat{D}_i}{\hat{D}} \tag{6}$$

and $\hat{D}_i$ and $\hat{D}$ are given by (7) and (8)

$$\hat{D}_i = \sum_{j=1}^{M} \frac{f(x_{1,j},\dots,x_{n,j})\, f(x'_{1,j},\dots,x'_{(i-1),j},x_{i,j},x'_{(i+1),j},\dots,x'_{n,j})}{M} - \hat{f}_0^2 \tag{7}$$

$$\hat{D} = \frac{1}{M}\sum_{j=1}^{M} f^2(x_{1,j},\dots,x_{n,j}) - \hat{f}_0^2 \tag{8}$$

The quantity (9) denotes the empirical mean of y

$$\hat{f}_0 = \frac{1}{M}\sum_{j=1}^{M} f(x_{1,j},\dots,x_{n,j}) \tag{9}$$

First (S_i) and second order ($S_{i,j}$) sensitivity indices provide then an uncertainty budget in terms of ranked contributions to the variance associated with the best estimate of the measurand.

3.3. Validation of the GUM uncertainty framework using Monte Carlo Method

The GUM uncertainty framework can be expected to work well in many circumstances. However, the Monte Carlo Method can be used in cases of doubt to check whether the LPU is applicable. A validation procedure is provided for this purpose and is given in the Supplement 1 to the GUM. Since the domain of validity for the Monte Carlo Method is broader than the domain of the GUM method, it is recommended to use first method. Nevertheless, it is often simpler to apply the law of propagation of uncertainty (LPU) described in the GUM. In this case, the assumptions for a valid application of the GUF should be verified by comparing the results obtained with the Monte Carlo Method and with the LPU. If both results are similar, then the GUM uncertainty framework is considered to be valid. Otherwise, the Monte Carlo method should be applied. The GUM Supplement 1 defines a criterion based on a comparison of the absolute differences of the respective endpoints of the coverage intervals obtained with the two methods with respect to a stipulated numerical tolerance. Let $u(y) = c \times 10^l$ be the standard deviation of the output quantity $\boldsymbol{y}$ where l is an integer and c an integer expressed with 1 or 2 significant decimal digit $n_{\text{dig.}}$ The user chooses n_{dig} =1 or 2 if he wants to validate GUM method with 1 or 2 significant digit. Then the numerical tolerance δ is given by $\delta = 0.5 \times 10^l$. Let d_{low} and d_{high} be respectively the differences between the lower and upper bounds of the two coverage intervals given by (10) and (11)

$$d_{\text{low}} = \left| y - U - y_{\text{low}} \right| \tag{10}$$

$$d_{\text{high}} = \left| y + U - y_{\text{high}} \right| \tag{11}$$

where U is the 95% expanded uncertainty given by the LPU method and y_{low} , y_{high} are the bounds of the 95% coverage interval given by the Monte Carlo Method. If both d_{low} , d_{high} are no larger than δ, the comparison is favourable and the GUM uncertainty framework is considered to be validated. In LNE-MCM software, the user has to provide the result of the LPU method (best estimate, standard uncertainty, coverage factor) and n_{dig} then the validation is automatically done. The Fig. 4 shows the results of the validation procedure between the result obtained by the GUM-LPU method at the first order and the result obtained by the

Monte Carlo Method. The graph is similar to the one in the Supplement 1 to the GUM.

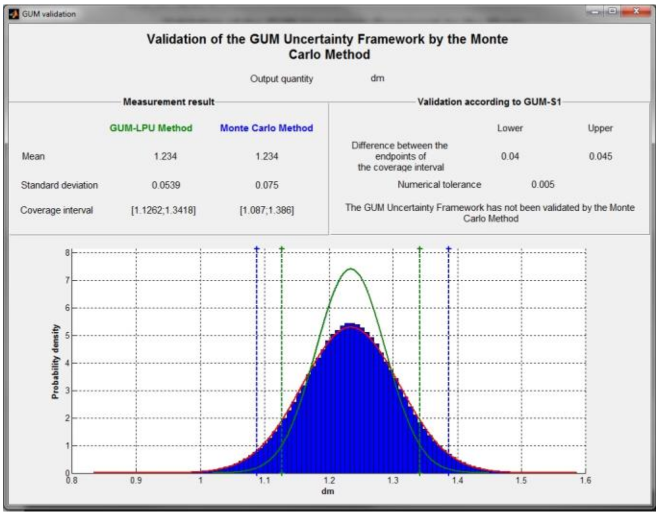

Fig. 4. Validation procedure of the GUM-LPU by the Monte Carlo Method for mass calibration example.

2.4. Goodness of fit test

The use of the Monte Carlo Method yields to a representation of the PDF associated with the output quantity. However, in cases where the output quantity is an input quantity of another measurement model, the PDF is needed in order to perform a new Monte Carlo simulation. To this extent, a goodness of fit test can be used to compare the empirical PDF resulting from the Monte Carlo simulation with the PDF from some usual probability distributions. First within LNE-MCM, parameters of classical probability distributions (Gaussian, Student, lognormal, gamma, beta,…) are provided by maximum likelihood estimation. Then Kolmogorov-Smirnov goodness of fit test is performed to select the theoretical distribution closest to the empirical one computed by Monte Carlo simulation.

3. CONCLUSION

To evaluate the measurement uncertainty with respect to the method described in the GUM Supplement 1, new software, LNE-MCM, with a user-friendly interface will be made freely available on LNE's website in 2015. Dedicated to the estimation of measurement uncertainty by the Monte Carlo Method, it goes beyond the scope of the Supplement 1 to the GUM by offering additional features to meet wider needs of practitioners in metrology. With LNE-MCM software, the user can consider measurement models having more than one output quantity with the formalism described in the Supplement 2 to the GUM. Due to the limitation of the sensitivity analysis proposed in the Supplement 1 to the GUM, two global methods of sensitivity analysis are implemented in LNE-MCM. Each of them have their domain of validating and are complementary. To validate the measurement uncertainty obtained by the GUM-LPU, the comparison procedure described in the Supplement 1 to the GUM is available in LNE-MCM. Finally, as an output quantity for a measurement model may be an input quantity for another measurement model, LNE-MCM proposes a goodness of fit test in order to guide the choice of the PDF for this quantity.

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