Some considerations on a Monte-Carlo method for evaluating measurement uncertainty

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Abstract* – *Uncertainty calculation task is discussed in the paper. Monte-Carlo method for uncertainty evaluation is covered. It is used for uncertainty evaluation of a proposed measurement scenario. In order to validate the Monte-Carlo method, long-run success rate estimation procedure is presented. Application of such procedure showed unexpected invalid results of uncertainty evaluation. A modification of the Monte-Carlo method is proposed that appears to deliver more valid results.

Key words – measurement uncertainty, valid solution, numerical methods, Monte-Carlo.

I. Introduction

A statement of the result of a measurement is only complete if it provides an estimate of the quantity concerned (often known as the measurand) and a quantitative measure of the reliability of that estimate, namely, the uncertainty associated with it.

Generally, several approaches to provide an estimate of the measurand, and the associated uncertainty (e.g. a coverage interval) for the measurand that is needed for conformity assessment and other decision making can be used. These approaches include Principle of Maximum Entropy, Bayesian treatment (probabilistic modeling) and Propagation of distributions (functional modeling) [1]. The latter is used to relate the measurand to model input quantities about which information is available, and is the basis of obtaining the probability density function (PDF) for the measurand from the PDFs assigned to the input quantities. In some simplest cases the PDF for the measurand can be obtained analytically. Otherwise, approximate and numerical implementations of the propagation of distributions are available, such as the ISO Guide's uncertainty framework [2] and a Monte Carlo method (MCM) [3]. The preferred use of MCM comparing to approximate analytical methods is shown in a number of studies[3,4,5].

In this paper, it is assumed that a model and PDFs for all input quantities are given. Thus, the second phase "calculation" of uncertainty evaluation procedure is discussed.

The goal of this paper is to highlight invalid solution of a simple measurement scenario by the MCM and therefore a need for its (possible) improvement and independent validation of usability of all candidate solution approaches.

Section II gives an account of MCM in brief. Section III covers the measurements scenario and uncertainty evaluation results by the MCM. Section IV presents modification of MCM intended to provide more valid results. Summary and draws of some conclusions are given in the Conclusions.

II. Monte-Carlo method

Regardless of the field of application, the physical quantity of concern, the model output quantity, can rarely be measured directly. Rather, it is determined from a number of contributions, or input quantities, that are themselves estimated by measured values or other information available.

The fundamental relationship between the input quantities and the output quantity is considered to be the model[6]. The input quantities, n, say, in number, are denoted by $X = (X_1,...,X_n)^T$ and the output quantity by $Y = (Y_1,...,Y_n)^T$. The model $Y = f(X)$ can be a mathematical formula, a step-by-step calculation procedure, numerical software or other prescription. Let us assume that PDF for $X = (X_1,...,X_n)^T$ and $f(X)$ are known. Estimate y of quantity Y is the measurement result. Then, the problem of uncertainty evaluation is the estimation of PDF of the output value $g(y)$ (or the distribution function $G(y)$) and therefore the estimation of moments and coverage regions(intervals for scalar) for y. The latter are needed for conformity assessment and decision making purposes, so its evaluation is the main result of uncertainty evaluation procedure.

According to the so-called Markov formula, if $\delta(\cdot)$ denotes the Dirac delta function and $g_{in}(x)$ denotes the joint PDF of input quantities, the PDF $g(y)$ could be generally found as[3]:

$$g(y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} g_{in}(x)\delta(y - f(x))dx_n dx_{n-1}...dx_1 \quad (1)$$

It would rarely be a practical proposition to use the integral expression (1) as the basis for the numerical determination of the PDF for the output quantity. A multivariate quadrature rule would need to be devised that was capable of delivering a prescribed numerical accuracy for each choice of y. Rather than attempting to evaluate the expression (1), an application of a MCM [3] encompasses an entirely different approach, based on the following considerations.

MCM uses pseudorandom numbers to obtain representative draws of possible values of the input quantities in order to generate a discrete representation of the output quantities via the given model[3]. The MCM computes from these draws the expectations and covariance matrix for the output quantities and a frequency distribution that approximates the joint PDF for the output quantities, the use of which provides best estimates of the output quantities and the associated uncertainty matrix (covariance matrix). Furthermore, the marginal PDF for any output quantity can be approximated accordingly and used to form coverage intervals for that quantity. If rules are given, MCM can also be used to determine, from the joint PDF, coverage regions for the output quantities. MCM provides approximations to the exact results that would be provided by analytical methods[4].

As stated in a number of studies[3,4,5], the quality of these approximations generally improves with the number of draws, and therefore a check on the convergence of MCM and careful ‘validation’ of the procedure are required. Some criteria and recommendations that come out in an adaptive MCM with reduced computing complexity are given[7].

III.The measurement scenario and MCM calculation

Let us consider a measurement of the magnitude of a complex valued quantity $\Omega = \Omega_1 + i\Omega_2$ [8]. Measurements of the real and imaginary components yield $z = z_1 + iz_2$, from which an estimate of $|\Omega|$ can be found:

$$|z| = \sqrt{z_1^2 + z_2^2} \quad (2)$$

We further consider that z_1 and z_2 are independent and have standard uncertainties equal to a known value u associated with a Gaussian distribution.

Application of the adaptive MCM[7] is used here. The application of this method here can be described in a series of steps.

1) Generate a sequence of samples z_{1i} and z_{2i}, where = $i = 1,..,L$ by drawing from a Gaussian distribution with mean z_1 and z_2,and variance u^2 for both of them. L is not chosen a prior but adaptively by means of procedure, described in[] for a required accuracy for estimates. In our scenario case, we require $\varepsilon = 0.01$ accuracy, that shall be enough for purposes described later in this section.

2) Calculate $|z_i|$ according to Eq. (2) for $i = 1,..,L$.

3) Sort the values of $|z_i|$ in ascending order.

4) Take the 0.025Lth value of $|z_i|$ as the lower bound of the uncertainty interval; Take the 0.975Lth value of $|z_i|$ as the upper bound of the uncertainty interval.

The result is an interval said to have 95% probability of containing $|\Omega|$[3]. Other coverage probabilities can also be applied with use of respective quantiles in step 4).

In order to assess the long-run success rates of the MCM, a series of simulated measurement results is processed. Pairs of data ($z_1[j]$, $z_2[j]$), $j = 1,..,10000$, are simulated and each pair is used as if it were the data obtained from an independent measurement of the same fixed measurand. The procedure is as follows.

1) A value for $\Omega = \Omega_1 + i\Omega_2$ is selected.

2) A sequence of pairs ($z_1[j]$, $z_2[j]$) is drawn from independent Gaussian distributions with means Ω_1 and Ω_2 , respectively, and variances u^2.

3) For each pair, a 95% uncertainty interval is calculated as described above and a counter is incremented if that interval contains $|\Omega|$.

4) The success rate of a procedure is estimated from the respective counter value divided by the total number of runs and multiplied by 100%.

These steps assess the success rate of a procedure at one fixed value of the measurand. In order to investigate a procedure's performance over a range of values, the method should be repeated with different measurand values, selected at step 1.

The symmetry of the scenario means that performance will be independent of the radial coordinate of the measurand in the complex plane. So, without loss of generality, ten $|\Omega|/u$ values lying along the real axis were chosen. For each measurand value, simulated experiments provided 10000 sets of input data for the MCM uncertainty estimation. The results are summarized in Table I. The second column of this table report the percent of successes. We should note, that some variability in the percent of successes observed can be expected. For a success rate of p = 0.95, the standard deviation of the percent of successes observed is $100\% * \sqrt{Np(1-p)}/N$, which is approximately equal to 0.22% in our case.

TABLE 1

PERCENT OF SUCCESSES FOR THE MCM

$\|\Omega\|/u$	Success rate
0.01	0%
0.05	0%
0.1	0%
0.2	0%
0.4	66,34%
1.0	90.25%
2.0	93.44%
4.0	95.12%
10.0	94.94%
100.0	95.17%

An unexpected fall in the success percents occurs when the measurand is close to the origin. The method fails to reach the required percents of success for $|\Omega|/u < 2.0$ and fails on every occasion when $|\Omega|/u < 0.224$. The core of this problem seems to be in asymmetry of the $|\Omega|$ PDF, if we use MCM with $z_1 = 0$ and $z_2 = 0$ and a standard uncertainty u = 1. The lower bound of the 95% uncertainty interval for this data is $|z_i| = 0.224$, and we should expect this bound to increase for any other MCM sample, so any measurand $|\Omega| < 0.224$ will fall outside the uncertainty intervals that can be generated. This explains the success rate of zero in the first four rows of Table I.

With the importance of traceability in metrology, methods used to calculate uncertainty should perform well in an event-based paradigm[2,8], because it is ultimately the accuracy of measurement and calibration events that is required. Failure of a method to do so is surely of concern. Consequently, valid methods of uncertainty calculation must achieve acceptable rates of success in the intended measurement scenarios.

What metrological meaning should be given to a nominal 95% coverage interval that is unlikely to contain the value of the quantity intended to be measured? We consider such a solution interval to be invalid in terms of long-run success rate. For our measurement scenario MCM should be treated as valid only with defined limits of usability, that is if $|\Omega|/u > 2$ in our case, e.g. if standard uncertainty is twice less the measurand value. It may be useful to note, that if we increase dimensionality of the magnitude measurement problem that "usability limit" is intended to increase.

IV. Modified adaptive MCM

A modification of the MCM is proposed in attempt to overcome the problem described above. It is proposed to find a coverage interval such as the shortest interval that contains pL MCM trials, where p is a coverage probability. Such interval should be used instead of one found at step 4) of the MCM procedure. Such approach is expected to take asymmetry of PDFs into account.

It should be clear that such an interval could be not unique(e.g. for rectangular distribution). Such cases should be treated properly. For example, we can take the interval that is most closest to the center of all sample values of the MCM.

Because the array of MCM samples is sorted, the problem can be simplified to finding the argument value of the minimum difference. It can be written as:

$$\underset{k=1..\frac{2L}{1-p}}{\arg\min}(z_{k+pL} - z_k) \tag{3}$$

Appropriate intuitive algorithm for solution of Eq.(3) can be implemented straightforward. Solution of this task will not invest a computing problem. It is obvious that computing time is $O(L)$, that will slightly increase overall computing time of the MCM[3,7]. We should also note that MCM(even adaptive, the one we use here) is a comprehensive computational task[7,9], method improvements to decrease computational time should be developed.

If $k=1$ gives the solution of Eq.(3), thus, the lower bound of uncertainty interval is the smallest MCM sample, application of the adaptive procedure[] could cause difficulties. Consequent discussion and possible solution is beyond the scope of this paper.

To assess the long-run success rates of the proposed modification of the MCM, the procedure, described in Section III is implemented for the same measurement scenario for ten values of $|\Omega|/u$. The results are summarized in Table II.

TABLE 2

PERCENT OF SUCCESSES FOR THE MODIFIED MCM

$\|\Omega\|/u$	Success rate
0.01	0%
0.05	0%
0.1	5.09%
0.2	59.11%
0.4	82,34%
1.0	92.31%
2.0	94.99%
4.0	94.85%
10.0	95.13%
100.0	95.19%

An increased performance of the modification comparing to MCM results can be observed. The modification should be treated as valid with $|\Omega|/u > 1$ limit of usablity in our case that is wider then for the MCM. Better performance should be expected in general case of a measurement problem, that is to be investigated in future work.

The result obtained means that modification can be used even if standard uncertainty and the measurand value are approximately equal and will yield invalid results if uncertainty is greater than measurand value.

Conclusions

In this paper, an adaptive MCM procedure for uncertainty calculation is used to evaluate coverage intervals for measurement scenario of magnitude measurement of a complex valued quantity.

The validation procedure for the MCM is proposed and implemented for the measurement scenario. Results of such validation discovered invalid results of coverage intervals calculation for the values close to the origin with comparitevly big uncertainty.

Modification of the MCM is presented. Modification is based on finding the smallest interval that contains respective number of MCM samples. Validation of such approach showed significantly better performance results, with appropriate wider scope. Such modified MCM should be used in practice as a more valid one instead of original MCM.

Further work will include wider research of the modified adaptive MCM, improvements of the method and its implementation on multiple processor and distributed computing systems.

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