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COMPUTATIONAL INTENSIVE METHOD FOR THE UNCERTAINTY ANALYSIS IN A MULTIVARIATE MODEL

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Abstract – In this work we want to address a computer-intensive approach for the uncertainty estimation in a measurement process. A multivariate model is considered and the level of confidence of a probability region, associated with the uncertainty of the measurement process, has been evaluated, using Monte Carlo computational method. The adopted simulation procedure is fully compatible with the conventional uncertainty estimation methods reported in the ISO/GUM [1] and it is adaptable to a large range of practical situations.

Keywords: Uncertainty, Monte Carlo method.

1 INTRODUCTION

The evaluation of uncertainty is an unavoidable part of any measurement result. A proper evaluation of uncertainty is a good professional practice and can provide laboratories and customers with valuable information about the quality and the reliability of the result in the measurement process.

Notions such as probability models, standard errors, confidence limits are all intended to formalise uncertainty.

In simple situations, the uncertainty of an estimate, in a measurement process, may be evaluated by analytical calculation based on an assumed probability model for the available data, as suggested in the key document "ISO Guide to the expression of uncertainty in measurement (GUM)" [1].

In more complicated problems the analytical approach suggested by the Guide, can be difficult and its results are potentially misleading if inappropriate assumptions have been made to simplify the process.

In this paper, we analyse the uncertainty expression in a measurement process for a multivariate model using a computer intensive technique: the Monte Carlo method. The performance of the adopted procedure is analysed in a practical situation too.

2 THE CONVENTIONAL UNCERTAINTY ESTIMATION

The aim and objective of a measurement is to attribute a value to a measurand Y. From the operational point of view, this is possible by comparing the measurand Y with a known quantity or with a quantity formed by other quantities $X_1, X_2, ..., X_N$, which are easy to determine. For this a model of evaluation is needed which expresses this assignment of a value to the measurand in mathematical terms (i.e. a functional relationship or equation):

$$Y = f(X_1, X_2, ..., X_N) \quad (1)$$

In particular, the function f includes corrections for systematic effects, accounts for sources of variability, such as those due to different instruments, observers, laboratories and so on. Thus, the general functional relationship represents not only a physical law but also a measurement process.

The result, or output quantity Y, is obtained by (1) using input estimates $x_1, x_2, ..., x_N$ for the values of the N input quantities $X_1, X_2, ..., X_N$ and it is reported as $Y = y \pm U$ where y is the estimate (or expectation) of Y and U is the expanded uncertainty defined by $U = ku_c(y)$. Here $u_c(y)$ is the combined standard uncertainty representing the estimated standard deviation of the result Y and k is a coverage factor chosen to produce an interval having a level of confidence close to the expectation value.

The standard uncertainties of measurement to be attributed to the input values are obtained as square roots from the variances of the distributions:

$$u(x_i) = \sqrt{Var[X_i]},\ \mathrm{i} = 1,...\mathrm{N}$$

The combined standard uncertainty of the measurement result y is the positive square root of the estimated variance $u_c^2(y)$ obtained from:

$$u_c^2(y) = \sum_{i=1}^{N} A_i + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} B_{ij} \tag{2}$$

where the terms $A_i = \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i)$ are weighted variances associated with x_i $\mathrm{i} = 1,2,...,\mathrm{N}$ and $B_{ij} = \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j)$ are weighted covariances associated with x_i, x_j $\mathrm{i, j} = 1,2,..., \mathrm{N}$ respectively. The terms A_i, B_{ij}, $\mathrm{i, j} = 1,...\mathrm{N}$ depend on the probability distributions that characterize one's knowledge of the input quantities.

The weight coefficients $\frac{\partial f}{\partial x_i}$ $\mathrm{i} = 1,...,\mathrm{N}$, referred to as sensitivity coefficients, are equal to $\frac{\partial f}{\partial X_i}$ evaluated at $X_{\mathrm{i}} = \mathrm{x_i}$ $\mathrm{i} = 1,...,\mathrm{N}$.

Equation (2) derives from the following considerations: if the function f, used to calculate the output estimate $y = f(x_1, x_2,..., x_N)$, of the measurand Y, is supposed to be a continuous function of the input estimate $x_1, x_2,..., x_N$, it can be approximated using a 2nd order Taylor's series expansion about the means:

$$y = f(\underline{x}) + \sum_{i=1}^{N}\left(\frac{\partial f(\underline{X})}{\partial x_i}\right)_{\underline{X}=\underline{x}} (X_i - x_i) + W \tag{3}$$

where $\underline{X} = (X_1, X_2,..., X_N)$ and $\underline{x} = (x_1, x_2,..., x_N)$. W is the remainder expressed by:

$$W = \frac{1}{2!}\left[\sum_{i=1}^{N} a_i (X_i - x_i)^2 + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} b_i (X_i - x_i)(X_j - x_j)\right] \tag{4}$$

where:

$$a_i = \left(\frac{\partial^2 f}{\partial x_i^2}\right)_{\underline{X}=\underline{x}+\theta(\underline{X}-\underline{x})},\quad 0 < \theta < 1$$

and

$$b_i = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)_{\underline{X}=\underline{x}+\theta(\underline{X}-\underline{x})},\quad 0 < \theta < 1$$

When $\underline{X} \to \underline{x}$, the remainder approaches zero more quickly than the first order terms in (3), so W and all the higher terms are normally neglected provided that the uncertainties in $X_1, X_2,..., X_N$ are small and the vector $\underline{X} = (X_1, X_2,..., X_N)$ is close to $\underline{x} = (x_1, x_2,..., x_N)$. For linear model W and all the higher terms are equal to zero.

Equation (2) is commonly referred to as the law of propagation of uncertainty and it is based on the first-order Taylor series approximation of (1). Actually, assuming $W = 0$ in (3) we have :

$$u(y) = \sqrt{\sum_{i=1}^{N}\frac{\partial f(\underline{X})}{\partial x_i} u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{\partial f(\underline{X})}{\partial x_i}\frac{\partial f(\underline{X})}{\partial x_j} u(x_i, x_j)} \tag{5}$$

where $u(x_i, x_j) = \rho_{ij} u(x_i) u(x_j)$, being ρ_{ij}, $i, j = 1,...\mathrm{N}$ the correlation coefficients.

The correlation coefficients are the measure in which potential dependencies of the knowledge of the input quantities for the evaluation are expressed. Their value lies in the range: $|\rho_{ij}| \le 1$. In the most frequent case that the knowledge of the input quantities can be considered non-correlated, the correlation coefficients have the values:

$$\rho_{ij} = \begin{cases} 0 & \text{if } i \ne j \\ 1 & \text{if } i = j \end{cases}$$

3 THE MEASUREMENT STATEMENT AND THE MONTE CARLO METHOD

The multivariate model

The measurand or output quantity Y, depends upon a number, say n, of input quantities M_i $(i = 1,...n)$. The row vector $\underline{M} = (M_1,..., M_n)$ is supposed to represent the set of measured quantities, having each a measurement uncertainty and the multivariate function $Y = f(\underline{M})$, is the mathematical model describing not only a physical law but also the measurement process. All the quantities, which are not exactly known, are treated as random variables, including the influence quantities which may affect the measured value.

If a probability region, say $C^{(n)} \subset R^n$, is chosen to represent the variability of the random variable $\underline{M}$, its level of confidence, p, satisfies the following relationship:

$$\mathrm{P}\{\underline{M} \in C^{(n)}\} = \mathrm{p}$$

By introducing an n-th dimensional joint probability density function: $f_{\underline{M}}(\underline{m})$, it is possible to evaluate the level of confidence of the probability region $C^{(n)} \subset R^n$ following the identity relation:

$$\mathrm{P}\{\underline{M} \in C^{(n)}\} = \int_{C^{(n)}} \cdot\cdot \int f_{\underline{M}}(\underline{m})\, dm_1 \cdot\cdot dm_n = \mathrm{p} \tag{6}$$

being $m = (m_1, m_2, ... m_n)$ a realization of the random variable $\underline{M} = (M_1, ..., M_n)$.

The Monte Carlo Method

The class of algorithms that solve problems probabilistically are known by the name of Monte Carlo methods (MCM). At the present MCM are the most competitive approaches in many computational problems when the numerical analytic algorithms become too heavy as in the multiple integral computation, or in the optimization and functional approximation in multidimensional spaces.

Here the purpose is to look at using Monte Carlo methods to evaluate the confidence region in a measurement process, that is to evaluate the n-dimensional integral in (6).

By defining a function $g(\underline{m}) = g(m_1, ..., m_n)$ as:

$$g(\underline{m}) = \begin{cases} 1 & \text{if } \underline{x} \in C^{(n)} \\ 0 & otherwise \end{cases} \qquad (7)$$

the integral in (6) can be written:

$$p = \frac{1}{V} \int_{C^{(n)}} \cdot \int f_{\underline{M}}(m_1, ... m_n) \, g(m_1, ... m_n) V dm_1 \cdot \cdot dm_n \qquad (8)$$

where V is the measure of the region $C^{(n)} \subset R^n$.

Equation (8) can be interpreted as the expectation of the function

$$h(\underline{m}) = f_{\underline{M}}(\underline{m}) g(\underline{m}) V$$

for the n-dimensional random variable $\underline{m} = (m_1, ..., m_n)$ which is uniformly distributed within the domain $C^{(n)}$.

This then gives an approximate procedure:

$$p \approx \frac{1}{N} \sum_{i=1}^{N} h(\underline{m}_i) = \frac{V}{N} \sum_{i=1}^{N} f_{\underline{M}}(\underline{m}_i) = \frac{V}{N} \sum_{i=1}^{N} f_{\underline{M}}(m_{i1}, m_{i2}, ..., m_{in}) \quad (9)$$

4. CASE STUDIES

A theoretical tri-dimensional model is examined and the level of confidence of the parallelepipedon having sides equal to the marginal confidence intervals of the three input variables is evaluated analytically and compared with the level of confidence of the probability region having minimal surface that is the ellipsoid with axes equal to the marginal confidence intervals of the three input variables computed by Monte Carlo method.

The three random variables M_i $i = 1,2,3$ are supposed to have normal distribution $M_i = \mathrm{N}(\mu_i, \sigma_i^2)$, $\sigma_i = \sqrt{\mathrm{Var}\{M_i\}}$ $i = 1,2,3$ can be used to evaluate the expanded uncertainty, u_i of the measure M_i as specified in (GUM) [1], being $\mu_i \pm u_i = \mu_i \pm k_i \sigma_i$ $i = 1,2,3$ where k_i is a coverage factor.

The correlation coefficients are:

$$\rho_{ij} = \left[E\{M_i M_j\} - \mu_i \mu_j \right] / \sigma_i \sigma_j \quad i, j = 1,2,3 \text{ with } |\rho_{ij}| \le 1$$

In the hypothesis of normal distribution for the output variable $Y = f(\underline{M})$ we have:

$$f_{\underline{M}}(\underline{m}) = (2\pi)^{-\frac{3}{2}} \left(det \underline{\underline{D}} \right)^{-\frac{1}{2}} exp\left[-\frac{1}{2} (\underline{m} - \underline{\mu}) \, \underline{\underline{D}}^{-1} \, (\underline{m} - \underline{\mu})^T \right] \quad (10)$$

where $\underline{\underline{D}}$ is the dispersion matrix (see Appendix).

Assuming $C^3 = I_1 \times I_2 \times I_3$ where $I_i = [\mu_i \pm k_i \sigma_i]$ $i = 1,2,3$ and following the procedure described in the Appendix, it is possible to obtain an analytical relation in terms of the characteristic parameters of the model and the level of confidence p of the region C^3 as follows:

$$\left(det \, \underline{\underline{D}} \right)^{-½} \left| det \, \underline{\underline{Q}} \right| \prod_{i=1}^{3} \frac{1}{\sqrt{\lambda_i}} \mathrm{erf}\left(\sqrt{\frac{\lambda_i}{2}} \, k_i^* \right) = p \qquad (11)$$

where $k_i^* = \sum_{j=1}^{3} q_{ij} k_j$ $i = 1,2,3$ are the transformed coverage factors, and erf(-) is the error function.

An Experimental Model

The three dimensional model concerns a circuit element in which the resistance R and the reactance X can be determined (following the Ohm's laws) by measuring simultaneously:

1. the amplitude V of a sinusoidally-alternating potential difference across its terminals

2. the amplitude I of the alternating current passing through it

3. the phase-shift angle ϕ of the alternating potential difference relative to the alternating current.

The characteristic parameters of the experimental model are reported in table (1), the correlation coefficients ρ_{ij} $i, j = 1,2,3$ are subjected to the following constraints:

$$1 + 2\rho_{12}\rho_{13}\rho_{23} \ge \rho_{12}^2 + \rho_{13}^2 + \rho_{23}^2$$

being the dispersion matrix $\underline{\underline{D}}$ positive semi-definite.

An experimental model is examined whose characteristic parameters are reported in table (1). The level of confidence is evaluated for different values of the coverage factors assuming that $k_i^* = k^*$ $i = 1,2,3$. The results, based on the Monte Carlo application are computed assuming an ellipsoid probability region

$$\overline{C}^3 \subset C^3 = I_1 \times I_2 \times I_3 \text{ where } I_i = [\mu_i \pm k_i\sigma_i] \quad i = 1,2,3$$

having volume $V = \frac{32}{3}\pi\prod_{i=1}^{3} k_i\sigma_i$ and $N = 10^5$.

The results are compared in table (2):

Table (1): characteristic parameter of the model

$\mu_1 = 4{,}999\ 57$ V	$\mu_2 = 19{,}661\ 01$ mA	$\mu_3 = 1{,}044\ 46$ rad
$\sigma_1 = 0{,}003\ 2$ V	$\sigma_2 = 0{,}009\ 5$ mA	$\sigma_3 = 0{,}000\ 75$ rad
$\rho_{12} = -0{,}36$	$\rho_{13} = 0{,}86$	$\rho_{23} = -0{,}65$

Table (2): the level of confidence

k^*	p_1	p_2
2	0.9634	0.9782
3	0.9866	0.9919
4	0.9993	0.9998

p_1 : is referred to the region $\overline{C}^3$

p_2 : is referred to the region $C^3 = I_1 \times I_2 \times I_3$

APPENDIX

In the hypothesis of *normal distribution* the n-th dimensional joint probability density assumes the form:

$$f_{\underline{M}}(\underline{m}) = (2\pi)^{-\frac{n}{2}} (det\,\underline{\underline{D}})^{-\frac{1}{2}}\, exp\left[-\frac{1}{2}(\underline{m}-\underline{\mu})\underline{\underline{D}}^{-1}(\underline{m}-\underline{\mu})^T \right] \quad (11)$$

with $\underline{\mu} = E\{\underline{M}\} = (E\{M_1\},..., E\{M_n\})$ is the expectation vector, and

$$\underline{\underline{D}} = E\{(\underline{M}-\underline{\mu})^T(\underline{M}-\underline{\mu})\} \quad (12)$$

is the $n \times n$ dispersion or covariance matrix that can be generically written:

$$\underline{\underline{D}} = \begin{bmatrix} \sigma_i^2 & cov(M_1, M_2) & ... & cov(M_1, M_n) \\ cov(M_2, M_1) & \sigma_2^2 & ... & cov(M_2, M_n) \\ ... & ... & ... & ... \\ cov(M_n, M_1) & cov(M_n, M_2) & ... & \sigma_n^2 \end{bmatrix} \quad (13)$$

The diagonal elements are the variances of the individual variables that is $\sigma_i^2 = E\{[M_i - \mu_i]^2\}$. It is a positive semi-definite matrix (no eigenvalue is negative).

It is possible to apply the diagonalization procedure to the matrix $\underline{\underline{D}}$, because of its properties, so that a unitary non singular matrix $\underline{\underline{Q}}$ exist, ($\underline{\underline{Q}}^{-1} = \underline{\underline{Q}}^T$), such that $\underline{\underline{Q}}^T\underline{\underline{D}}\,\underline{\underline{Q}} = \underline{\underline{\Lambda}}$ where $\underline{\underline{\Lambda}}$ is a diagonal matrix with the nonull elements equal to the eigenvalues of the matrix $\underline{\underline{D}}$.

Now applying a standardization procedure introducing the linear transformation

$$L(\underline{M}) = \underline{W} \quad \text{with} \quad \underline{W} = (\underline{M} - \underline{\mu})\underline{\underline{Q}} \quad (14)$$

the equation (2), taking into account the (11) and (14), assumes the following form:

$$p = P\{\underline{M} \in C^n\} = P\{\underline{W} \in B^n\} =$$
$$\int_{B^n} \cdot \int (2\pi)^{-\frac{n}{2}} (\det \underline{\underline{D}})^{-\frac{1}{2}} \exp\left[-\frac{1}{2}\underline{W}\,\underline{\underline{\Lambda}}\,\underline{W}^T\right] |(\det \underline{\underline{Q}})|\, d\,w_1 \cdot d\,w_n \quad (15)$$

where $B^n = L(C^n)$ is the transformed domain according to (14).

CONCLUSION

The present research has to be considered as an approach to understand the behaviour of the uncertainty expression, in a measurement process, concerning multivariate models.

To check the potentiality of the proposed method, different situations have been examined in a three dimensional model and the level of confidence of the probability regions has been evaluated and compared.

The results are appreciable enough to believe that the method could deserve further attention inside more complicated models.

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