Uncertainty evaluation in general including simple artificial applications and Monte Carlo uncertainty evaluation

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Abstract: A short introduction of the general bottom-up uncertainty evaluation approach according to the ISO-GUM, JCGM 100 was presented [1, 3]. The Monte-Carlo Method (MCM) for the evaluation of the measurement uncertainty was outlined [2]. An application of the Monte-Carlo technique to the standard addition method using a simple excel-spreadsheet was explained in order to encourage the use of this important and powerful approach. A four and a five point standard addition method were compared for different sets of uncertainties of input variables and represented graphically.

Measurement uncertainty evaluation using the bottom-up approach method outlined in the ISO-GUM (identical to JCGM 100) and recommended by a number of leading international member organisations is now in use successfully for about a generation in all fields of measurements. The recently revised laboratory accreditation standard ISO/IEC 17025:2017 again requires that laboratories evaluate the measurement uncertainty for their reported measurement values [4]. In order to extend the use of the ISO-GUM the Joint Committee for Guides in Metrology (JCGM) under the guidance of the BIPM (Bureau International des Poids et Mesures, Paris) and its member organisations have published the supplement 1 [2], which explains the use of the Monte Carlo Method to evaluate the measurement uncertainty. It is especially useful as the method gives access to the distribution of the measurand values. No partial derivatives have to be calculated. In case of a non-linear model equation for the measurand the method is very much to be recommended as the full information of the input variables is reflected in the distribution of the measurand values and not only a the most probable value for the measurand and the corresponding combined standard uncertainty.

This contribution focusses on giving some detailed practical information on how to perform MCM using excel. The random number generator and also the number of possible sampling points in excel have been improved by Microsoft and are now fit for purpose, which was not the case in the past.

A procedure to perform MCM using excel for uncertainty evaluation is outlined as follows [5]:

1. The model equation for the measurand needs to be created using all available knowledge about the measurement system. This is generally the most demanding task.

2. For each input quantity (either type A or type B) in the model equation we need either a measured or an assumed probability density function characterised by the defining parameters for the distributions. Most commonly these distributions are the rectangular, symmetric triangular and the Gaussian distributions. The above mentioned distributions are given by two
parameters which are the central value and the second moment (standard deviation). For further distributions see chapter 6.4 in JCGM 101.

3. If we have to consider a bias (sum of all systematic influences) our model equation needs a proper adaption. The bias is a value with a sign and has a corresponding uncertainty. Mostly the bias correction can be characterised as a simple distribution with a value and a standard deviation. The measurand is corrected for if the bias is large enough.

4. For each of the input quantities \( x_i \) we calculate a simulated random value \( x_{i,j} \) that reflects the distribution characteristics of that input quantity \( x_i \). From the set of these realisations \( x_{i,j} \) of each input quantity \( x_i \) we now calculate the values \( y_i \) of the measurand and repeat this procedure for say 100'000 times. JCGM 101 gives advice on the number of simulations (chapter 7.2 of JCGM 101). Now we have a vector \( y_i \) for the measurand with all realisations from the many simulations \( i \).

Sampling from a rectangular distribution with limits \( a_r, b_r \):

\[
x_{i,j} = m_{r,j} - \frac{r_{r,j}}{2} + \text{RAND()} \cdot r_{r,j} = a_{r,j} + \text{RAND()} \cdot \frac{b_{r,j} - a_{r,j}}{2}
\]

\( i \): MCM simulation number, \( j \): input quantity number

\( m_{r,j} \): mean value of rectangular distribution, \( \text{RAND()} \): random number \([0,1]\)

\( r_{r,j} = [b_{r,j} - a_{r,j}] \): range

The excel function \( \text{RAND()} \) produces a 15 digit random number in the range \([0,1]\). The values \( a_r, b_r \) characterise the minimum and the maximum of the rectangular distribution with the mean value \( 0.5 \cdot (a_r + b_r) \).

Sampling from a symmetric triangular distribution with limits \( a_t, b_t \):

\[
x_{i,j} = m_{t,j} - \frac{r_{t,j}}{2} + \{\text{RAND()} + \text{RAND()}\} \cdot \frac{r_{t,j}}{2} = a_{t,j} + \{\text{RAND()} + \text{RAND()}\} \cdot \frac{b_{t,j} - a_{t,j}}{2}
\]

Whenever the random number function is called a new value is created. That means the above two random number functions are independently evaluated with generally different numbers.

Sampling from a Gaussian distribution sampling:

\[
x_{i,j} = \text{NORMINV}\{\text{RAND()}, m_{g,j}, s_{g,j}\}
\]

\( m_{g,j} \): mean of Gaussian distribution of input variable \( j \)

\( s_{g,j} \): standard deviation of Gaussian distribution of input variable \( j \)

5. These simulated values \( y_i \) of the measurand \( Y \) have to be analysed to get the values for the measurand expectation and the expanded measurement uncertainty. The mean value is the expectation value for the measurand. Two times to calculated standard deviation is nearly identical to the expanded measurement uncertainty. Mostly the distribution is not totally symmetric and also not perfectly Gaussian. Therefore we can use the calculated, cumulative probability distribution where we have to extract the 2.5% value and the 97.5% value to get the 95% range, that we attribute to the expanded measurement uncertainty.

6. The cumulative probability distribution is calculated as follows :
a) First create a class vector with the numbers 1 to the maximum class number (e.g. 1 to 100). Calculate the values of the classes using the following expression repeatedly over all class numbers:

\[
\text{value(class)}_i = \min(y_{\text{simul}}) + \left[N^{\text{class}}_i - 1\right] \cdot \frac{1}{\left(N^{\text{class}}_{\text{max}} - 1\right)} \cdot \left\{ \max(y_{\text{simul}}) - \min(y_{\text{simul}}) \right\}
\]

The class values will start from the minimum of the simulated values (\(\min(y_{\text{simul}})\)) and the values (\(\text{value(class)}_i\)) with (total number \(N^{\text{class}}_{\text{max}}\)) will be evenly distributed between the minimum and the maximum of the simulated \(y_i\) values.

b) From the simulated values for the measurand \(y_i\) we count the frequency (that is the number of values in each class) for each of the said hundred equally distributed classes using the following excel-function:

\[
\text{FREQUENCY}(y_1 : y_{100000} ; \text{class1 : class100})
\]

(for e.g. 100'000 simulations and 100 classes in which \(y_1\) is the field of the first simulated value and \(y_{100000}\) is the field of the last simulated values and class1 the field containing the value for the first class and class100 the field containing the value for the last class.). The \(\text{FREQUENCY}\) function has two arguments: the vector of the simulated measurand values (\(y_1 : y_{100000}\)) and the vector for the calculated class values. Here we chose as an example 100 classes. The function returns a vector and it must be entered using CTRL+shift+enter. Corrections are made by pressing F2, edit→erase-all. The use of the \(\text{FREQUENCY}\)-function needs some training.

c) From the number of values in each class the cumulative frequency is calculated for each class by adding the number of values for all preceding classes. Subsequently also the percentage values of the cumulative frequency are calculated.

d) From the cumulative frequency distribution the expanded measurement uncertainty \(U\) is evaluated at the 2.5% and the 97.5% cumulative values.

7. The data are displayed graphically including the evaluated numbers for the expectation value and the expanded measurement uncertainty. Any change in the input quantity parameters are directly displayed in the excel table and the corresponding graph.

The MCM has been applied to the evaluation of the expanded measurement uncertainty estimation for an analyte value measured using the standard addition method, which is very common in analytical chemistry. By changing the input parameters the required expanded uncertainty can be simulated. For the five point calibration four samples have known amounts of analyte added. For high precision this is best done using a gravimetric approach and not a volumetric one.

The calibration curve is a linear function (eq. 1). Apart form the sample without added standard four additional samples with added known amounts of an analyte standard are measured (Fig. 1).

\[
y = f(x) = a + b \cdot x
\]

linear function

\[
a = \frac{\sum_{i=1}^{n} x_i y_i - \left(\sum_{i=1}^{n} x_i\right) \cdot \sum y_i}{n \cdot \sum x_i^2 - \left(\sum x_i\right)^2} \quad b = \frac{\bar{y} - a}{\bar{x}}
\]

(eq 1)

Best linear function from experimental values \(x_i, y_i\).

Uncertainties in \(x_i\) and \(y_i\) are taken into account. Gaussian distributions are used for all input variables using the sampling procedure described under point 4, above.
Tables 1, 2 & Figures 2, 3. Values and uncertainties for a 4-point and a 5-point standard addition.

Measurand values and expanded uncertainties estimated by MCM using Gaussian distributions for all input quantities. The expectation value for the measurand is the intersection point between the calibration line and the concentration axis.
Figure 5. Graphical display of the measurand distribution with a 5-point standard addition and the corresponding cumulative frequency distribution. Uncertainties improved for the $x_i$ and $y_i$ values compared to Fig. 1, 2.

Figure 6. Graphical display of the measurand distribution with a 4-point standard addition and the corresponding cumulative frequency distribution. Values for input quantities are different from Fig. 1 to 5. Compare result only with Fig. 7.

Figure 7. Graphical display of the measurand distribution with a 5-point standard addition and the corresponding cumulative frequency distribution. Values for input quantities are different from Fig. 1 to 5. Compare result only with Fig. 6. As expected a five point calibration reduces the expanded measurement uncertainty (cf. distribution of measurand in green).

Further improvement can be seen if the uncertainties of both $x_i$ and $y_i$ values are reduced.
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Expressions used often for MCM (see JCGM 101, p.19 ff)

**Rectangular distribution:** JCGM 101, Subclause 6.4.2.4
\[ x_i = m - \frac{r}{2} + z \cdot r = m - \frac{r}{2} + \text{RAND} \cdot r \]
\( m \) mean, \( r \) range, \( z \) random variable: \( \text{RAND}[0,1] \)

**Gaussian distribution:** JCGM 101, Subclause 6.4.7
\[ x_i = \text{NORMINV}(z, m, \text{std}) = \text{NORMINV}\{\text{RAND},m,\text{std}\} \]
\( z \) random variable [0,1], \( m \) mean, \( \text{std} \) standard deviation

**Triangular symmetric distribution:** JCGM 101, Subclause 6.4.5.4
\[ x_i = m - \frac{r}{2} + (z_1 + z_2) \cdot \frac{r}{2} = m - \frac{r}{2} + \{\text{RAND} + \text{RAND})\} \cdot \frac{r}{2} \]
\( z_1, z_2 \) random variables [0,1], \( m \) mean, \( r \) range

**Figure 8.** Further reduction of the uncertainty of the input quantity values reduces the expanded measurement uncertainty.
To achieve an expanded uncertainty of 1.2% for the measurand the mean relative uncertainties of the input quantity values have to be reduced to 0.25% and 0.43% (cf. title of the Fig.8), which is rather demanding. Compare Fig. 8 with Fig.9. In blue: calculated mean and expanded standard deviation (2 x std). In green: Expanded uncertainty from evaluation of cumulative frequency distribution.

**Figure 9.** Further reduction of the uncertainty of the input quantity values reduces the expanded measurement uncertainty.
To achieve an expanded uncertainty of 0.97% for the measurand the mean relative uncertainties of the input quantity values have to be reduced to 0.22% and 0.4% (cf. title of the Fig.9), which is rather demanding. Compare Fig. 9 with Fig.8. In blue: calculated mean and expanded standard deviation (2 x std). In green: Expanded uncertainty from evaluation of cumulative frequency distribution.

**Figure 10.** Most commonly used distribution for MCM sampling to evaluate the expanded measurement uncertainty. For further distributions see JCGM 101 [2], chapter 6.4.
References:

(all documents are accessible free of charge with the exception of [4]) :

[1] ISO-GUM, JCGM 100 :2008 (GUM 1995 with minor corrections).
[2] BIPM.JCGM 101 : 2008, Evaluation of measurement data – Supplement 1 to ‘Guide to the expression of uncertainty in measurement’ – Propagation of distributions using a Monte Carlo method., BIPM.
[3] EURACHEM/CITAC Guide (2012), https://www.eurachem.org/index.php/publications/ guides
[4] General requirements for the competence of testing and calibration laboratories, ISO/IEC 17025 :2017, Third edition 2017-11, ISO Geneva, Switzerland.
[5] Excel files are available from the author on request.