A Computer Program for a General Case Estimation of the Expanded Uncertainty

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Abstract
The ISO Guide to the Expression of Uncertainty in Measurement provides a uniform method for the estimation of combined standard uncertainty of a stationary measurand. However, the provided method for the expanded uncertainty is not complete. Particularly, it does not include the case where the contributing components are correlated. Also, the probability distribution of the combined uncertainty must be close to a student distribution otherwise a special scheme must be used to keep the error in the estimation reasonable. The method presented here is based on a combination of the ISO guide method and Monte-Carlo simulation. Some example results obtained by the computer program using both methods are compared and discussed.

1. Introduction.

The purpose of this project was to fill-in the gaps left by the ISO Guide [1], and provide a uniform approach to the estimation of expanded uncertainty. The ISO Guide is attempting to describe an analytical method to the estimation of the expanded uncertainty. The procedure makes an assumption that the measurand is stationary and that repeated measurements belong to the same well-behaved statistics. This is not always true and the best example is the metrology of time [2].

In the ISO Guide, the expanded uncertainty is estimated in two steps. In the first one, the combined (standard) uncertainty is estimated by a similar way variances are combined. In the second step, an assumption is made that the distribution of the combined uncertainties is a student distribution. This distribution is characterized by a shape factor, namely the degrees of freedom. In the absence of correlations, the degrees of freedom are estimated in the ISO Guide by means of the Welch - Satterthwaite equation [1]. In the general case (including correlated components and arbitrary distributions) the analytical estimation of the degrees of freedoms that may be used to approximate a student distribution is still an open problem.

The assumption that the combined distribution is a student distribution may not be correct in many practical cases. For example, if the dominant contributor in the uncertainty budget is assumed to have a finite range distribution, such as rectangular distribution. In such cases, the UK NAMAS recommends to use a different method [3]. According to this method, the expanded uncertainty in the dominant component is added to the expanded uncertainty obtained from all other components (assuming they well-behave).

2. Monte-Carlo simulation of uncertainty distribution

According to this method, each uncertainty contributor (component) is simulated by random numbers, which belong to a distribution similar to that of the contributor. The measurement equation is then computed for many realizations of the random numbers. A typical number of repetitions are 10000. The expanded uncertainty is estimated directly from the distribution of the outcomes of the measurement equation. As per the common interpretation of the VIM [4] definition of uncertainty, it encompasses a range of outcomes that constitutes a fraction of the total number of outcomes, which is equal to the required confidence level (e.g. 95%). If the correlations between the random numbers are similar to those between the contributors, one can obtain a correct estimate of the expanded uncertainty from the combined uncertainty distribution.

In contrast to the ISO Guide method, which can be, in principle, computed manually or with a calculator or a spreadsheet, because of the large number of repetitions, this method requires a dedicated computer program. A description and a comparison of the outcomes of the Evaluator program, which utilizes both, the ISO Guide and the Monte-Carlo methods, is given in the following sections.

3. The Evaluator program algorithms
The presently released version (1.54) of the Evaluator follows the above steps but has some shortcuts and approximations, which are described in the following sections.

3.1 The user has two options, to write a measurement equation or to assume that the linear approximation is good enough (that is, the combined standard uncertainty is the root-sum-of-squares of the contributing standard uncertainties). In the first option, only the Monte-Carlo expanded uncertainty is computed. In the second option we proceed with 3.2 to 3.4 below.
The program can display the uncertainty histograms for the two extreme correlation cases, which are used for inspection.

3.2 The combined uncertainty is computed for 3 cases, namely, for the case of maximum correlations between all contributors, zero correlations and for the actual correlations matrix. This is done using the ISO Guide method.

3.3 The degrees of freedom are computed using the Welch – Satterthwaite equation, however the correlation terms in the Taylor expansion are also included in the equation. Using the equation in such a way makes the error in the estimation of the degrees of freedom smaller. Also, the NAMS procedure for dominant component [3] is extended here to the case where there exists some correlation between components. The reason is that in many cases this improves the uncertainty estimates. The Expanded uncertainty according to the ISO (and NAMAS) methods is now computed.

3.4 The Monte-Carlo expanded uncertainty is computed for the case of maximum possible correlation between all the contributors and for the case where they all are uncorrelated. Note that the maximum possible correlation coefficient may be less than 1 if the correlated distributions are different. The expanded uncertainty with the actual correlation matrix is now estimated by using the proportions between the 3 cases in 3.2. That is, if $u_{c0} < u_{ca} < u_{cx}$ we assume that,

$$(U_a-U_x)/(U_0-U_x) = (u_{ca}-u_{cx})/(u_{c0}-u_{cx}) \quad \text{where,} \tag{1}$$

U_a is the required Monte-Carlo expanded uncertainty estimated for the actual correlation matrix,

U_x is the Monte-Carlo expanded uncertainty with the maximum correlation matrix,

U_0 is the Monte-Carlo expanded uncertainty with the zero correlation matrix,

u_{ca} , u_{cx} , and u_{c0} are the corresponding combined uncertainties from 3.2.

and if $u_{c0} > u_{ca}$ we use,

$$U_a / U_0 = u_{ca} / u_{cx} \qquad (2)$$

The Evaluator is used by labs either in its own right or as a safeguard against large errors that may result sometimes with the ISO Guide method.

4. Results and comparisons

In the following results all estimates were made for the 95% level of confidence.

4.1 We compare the expanded uncertainty estimates obtained by both methods with two uncorrelated contributors having rectangular distributions. Table 1 summarizes the results. The standard uncertainty of first component is 1 (arbitrary units) and that of the 2nd component is given in the table. The fluctuations in Monte-Carlo (MC) are about 0.02 units. Because both components are of type B, the degrees of freedom are very large. One can see that the NAMAS correction applied below 0.21 units, improves the estimate of the expanded uncertainty as compared to the ISO Guide. The difference between the methods can be as large as 18%. With some distributions the error may be as high as 48% (two equal components having each a two-peak distribution). The NAMAS column differs from the ISO in those cases where the NAMAS "dominant term" method applies.

Table 1. A comparison with two uncorrelated rectangle distributed contributions.

Value of 2nd	Combined u	ISO	NAMAS	MC	NAMAS-MC in %
0	1.0	1.96	1.65	1.65	0
0.01	1.0	1.96	1.67	1.65	1
0.1	1.0	1.96	1.84	1.64	12
0.21	1.02	2.0	2.06	1.74	18
0.22	1.02	2.01		1.75	15
0.3	1.04	2.05		1.82	13
0.5	1.12	2.19		2.06	6
1.0	1.41	2.77		2.7	2

4.2 Suppose we have two large, uncorrelated and equal contributions both having student distribution with the same number of degrees of freedom. Assume that the standard uncertainties of both contributors are 1 (arbitrary units). The combined uncertainty is 1.414 units for any degrees of freedom. What would be the error in the ISO estimation as a function of the degrees of freedom? Table 1 gives the estimates for several degrees of freedom. Note that as the distributions approach to the normal distribution the errors vanish.

Note that in this example the ISO estimate is too much optimistic when the number of degrees of freedom is small.

Table 2. Estimates of the expanded uncertainty of two uncorrelated contributions both having student distributions.

d.f.	ISO	MC	ISO-MC in %
1	6.08	27.3	-77
2	4.06	6.65	-39
3	3.63	4.59	-21
10	2.96	3.13	-5
1000	2.77	2.77	0

4.3 In this example we compare the expanded uncertainty estimates for the case of two equal contributors (standard uncertainty 1, arbitrary units), both having rectangular distributions, tabulated as a function of their correlation coefficient. It is expected that when two similar and correlated, with correlation coefficient r = 1, contributions are combined, the combined will have the same distribution. In line 1 of the Table 3, MC indeed has the correct value of 3.29 (at 95% confidence) expected from a rectangular distribution with a standard uncertainty of 2, as is the combined one. The difference in NAMS and ISO columns indicate where the NAMAS "dominant term" applies, considering the extension of the method to the case of correlated contributors.

Table 3. Estimates of expanded uncertainty of two equal and correlated components both having rectangular distributions.

<table>
<tr><th>Correlation c.</th><th>Combined u</th><th>ISO</th><th>NAMAS</th><th>MC</th><th>NAMAS-MC in %</th></tr>
<tr><td>1</td><td>2</td><td>3.92</td><td>3.61</td><td>3.29</td><td>10</td></tr>
<tr><td>0.45</td><td>1.7</td><td>3.33</td><td>3.61</td><td>3</td><td>20</td></tr>
<tr><td>0.4</td><td>1.67</td><td colspan="2">3.28</td><td>2.95</td><td>11</td></tr>
<tr><td>0</td><td>1.41</td><td colspan="2">2.77</td><td>2.7</td><td>3</td></tr>
<tr><td>-0.5</td><td>1</td><td colspan="2">1.96</td><td>1.91</td><td>3</td></tr>
<tr><td>-1</td><td>0</td><td colspan="2">0</td><td>0</td><td>0</td></tr>
</table>

5. Summary

We see that in many cases the ISO Guide and NAMS approaches may differ significantly from the correct values, by positive or negative values. In critical applications, intercomparisons or when best measurement capability is claimed, it may be important to check the simple estimates usually made using a spreadsheet with Monte-Carlo estimates.

References

[1] Guide to the Expression of Uncertainty in Measurement, BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML. ISO 1995.

[2] A. Lepek, Software for the prediction of measurement standards, NCSL International workshop and symposium 2001.

[3] NAMAS document M3003, The Expression of Uncertainty and Confidence in Measurement, 1997.

[4] VIM, International Vocabulary of Basic and General Terms in Metrology, BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, OIML. ISO 1993.