Uncertainty evaluation using a Monte Carlo method

Walter Bich

APAT IUPAC International Workshop on

Combining and reporting analytical results,

Rome, 6-8 March, 2006

Guide to the Expression of Uncertainty in Measurement

Supplement 1

Propagation of distributions using a Monte Carlo method

AIM: to overcome some of the limitations of the GUM, especially when an interval of confidence with a stipulated coverage probability is needed.

Formulation stage
(common to both GUM and Suppl. 1)

You decide a model

$$Y = f\left(X_1, X_2, \ldots, X_N\right)$$

in which each of the input quantities X_i (assumed for simplicity to be uncorrelated) and the output quantity Y are treated as random variables.

The GUM Method

One seeks for the following items of information

- An estimate x_i for each input quantity X_i
- Its standard uncertainty $u(x_i)$

You “propagate” x_i and $u(x_i)$ by using

$$y = f(x_1, x_2, \ldots, x_N)$$

and

The GUM Method

$$u^2(y) \approx \sum_{i=1}^{N} \left(\frac{\partial Y}{\partial X_i} u(x_i) \right)^2$$

This is a first-order approximation, good under weak conditions:

•The non-linearity of *f* to be negligible compared to the magnitude of the uncertainties.

•The probability density function (pdf) of each X_i to be symmetric about x_i.

The GUM Method

- In many cases one needs $U_p(y)$, where p is a prescribed coverage probability.
- In these cases more knowledge is necessary than simply the first (x_i) and second ($u^2(x_i)$) moments of X_i, namely

The pdf of Y.

The GUM Method

- The Central Limit Theorem helps, under rather strong conditions (GUM, G.2).
- If the conditions are met, then $(y - Y)/u(y)$ behaves like a Student's *t* distribution with n_{eff} degrees of freedom, where n_{eff} is determined with the Welch-Satterthwaite formula (GUM, G.4).

The GUM Method. Limitations

They are mostly in the determination of a coverage interval:

- If the conditions of the Central Limit Theorem are not met, other ways (e.g., analytical) must be explored. Little guidance is given in the GUM, only for a particular case (dominant uniform).
- The assignment of degrees of freedom to Type B evaluations looks “artificial”.

The GUM Method. Limitations

They exist also in the evaluation of the standard uncertainty, when:

- The input quantities are strongly asymmetric (e.g., cosine error).
- The measurement model is strongly nonlinear, or so complicated that the derivatives are difficult.

The Supplement 1 approach

- Instead of propagating only first and second moments of the input quantities X_i, their pdfs are propagated through the model.

  The method is more demanding in terms of amount of knowledge. One has to assign a pdf to each input quantity, based on the experimental data or other knowledge. Guidance is given on the assignment of a suitable pdf.

The Supplement 1 approach

Problem: given the pdfs of the N input quantities, find the pdf of the output quantity.

Solution 1:

Analytical, using the Jacobian method (see any textbook on mathematical statistics). A closed-form solution can be found only in the most simple (and therefore uninteresting) cases. In general, the integrals involved in this solution must be solved numerically. Not viable.

The Supplement 1 approach

Solution 2 (the one adopted in the Supplement):

- Purely numerical, by means of a numerical simulation.
- Method selected: Monte Carlo.
- Tools: suitable random number generators for the various pdfs, reasonable computing power.
- Outcome: a numerical approximation for the output distribution.

The Supplement 1 approach

- From the numerical approximation for the output distribution, the required statistics, such as the best estimate for the measurand, its standard uncertainty, and the endpoints of a prescribed coverage interval can be obtained.

The Supplement 1 approach

The method in a nutshell:

- From each input pdf draw at random a value x_i for the random variable X_i.
- Use the resulting vector $\boldsymbol{x}_j$ (j = 1,…M) to evaluate the model, thus obtaining a corresponding value y_j. The latter is a possible value for the measurand Y.
- Iterate M times the preceding two steps.

The Supplement 1 approach

The method in a nutshell (continued):

- Sort the M values y_j for Y in non-decreasing order.
- Use the sorted values to obtain a numerical approximation for the output distribution, in the form of a piecewise-linear function (details in the Supplement).

A comparison of the two approaches

- The Monte Carlo approach works in a broader class of problems than the GUM approach. In this sense, it is more general.
- Contrary to the GUM, the output distribution in general is asymmetric. Therefore, the coverage interval for a given coverage probability is not unique, and attention must be paid to this issue. Guidance is given in the Supplement.

A comparison of the two approaches (continued)

- Compared to the GUM, more emphasis is given to the expanded uncertainty (a coverage interval) than to the standard uncertainty.
- The best estimate (as the expectation of the numerical approximation for the output distribution) does not necessarily coincide with that provided by the GUM.
- Also the standard uncertainties do not coincide. The GUM value may be smaller. This is a consequence of the pdf recommended for sampled data (Student).

A comparison of the two approaches (continued)

- There is no longer any need for degrees of freedom. Actually, this approach is intrinsically Bayesian.

To go back to reality…

If your experiment needs statistics, you ought to perform a better experiment

(Lord Rutherford)

Or, if you prefer…

the only statistics you can trust are those you falsified yourself

(Churchill)