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METROLOGY SOFTWARE FOR EXPRESSING UNCERTAINTY BY PROBABILITY DENSITIES

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Abstract: The paper addresses development of metrology software for the evaluation and expression of measurement uncertainty. It is based on representing measurement results as a probability density over allowable values of the measurand. The architecture of a general code aiming at the treatment of any kind of measurement transformation is discussed and a first core module is presented, concerning linear time invariant processes. The output of the program is a probability density, which is calculated on the basis of available information, without using simulation. Standard and expanded uncertainty may be calculated at any required coverage level. Results are more accurate than provided by the Welch-Satterwaite method suggested in the GUM.

Keywords: evaluation of measurement uncertainty, metrology software, traceability, measurement theory.

1 INTRODUCTION

In the last years of the 20th century, a significant consensus on a worldwide basis has been reached on how to express measurement uncertainty. At the end of a process, which started at in the late 70s, the International “Guide for the expression of measurement uncertainty” was published, on 1993 (to be referred later as GUM) [1]. It was a milestone in providing a sound basis for a unified treatment of all sources of measurement uncertainty, thus satisfying the recommendations issued by the BIPM in the early 80s. After the publication of the GUM, a large debate has taken place on the several aspects of the problem, virtually relevant for all kind of measurements. Now the big challenge for the years to come is going beyond the GUM, in many senses.

In fact the following actions are in order.

A suitable *set of norms* should be devised, in order to provide a to-the-point answer to questions arising in practical application of uncertainty evaluation, especially in industry and services, including SMEs. Then a co-ordinated effort should be made in *education*, to ensure that all graduate students in scientific and technologic fields are able to evaluate measurement uncertainty, at least in standard cases. Such matters should also be highly recommended for students involved in medicine, economics, social or behavioural studies, due to the increasing impact of measurement in those fields. Moreover, *application in industry and services* should be highly supported. Some recent congresses have confirmed a great interest from industry in that sense [2-3]. Surely the development of software aiding in the evaluation of uncertainty is of great interest.

Finally, many *research* topics are strictly related to expression end evaluation of uncertainty, including:

- development of a general theory for the expression and evaluation of measurement uncertainty, compatible with general statements in the GUM [4-5];
- methods for uncertainty evaluation, based for instance on calculation (probability densities, intervals) or on simulation, and related metrology software (to be discussed thoroughly in the following paragraphs);
- systematic application of uncertainty evaluation to important classes of devices such as computer-based measuring chains [6];
- development of methods for specific highly complex devices, such as CMMs or interferometers[7-8].

In this scenario the research here considered takes place.

2 COMPUTER AIDED EVALUATION OF MEASUREMENT UNCERTAINTY

Studies on computer aided evaluation of measurement uncertainty and related software codes may be grouped in five main categories:

1. codes implementing the GUM procedure;
2. dedicated simulation for specific (usually complex) measuring systems [7-9];
3. general purpose simulation [10-13];
4. calculation of densities ;
5. calculation of non probabilistic uncertainty figures [6,14].

In the present paper the 4th approach is specifically addressed.

The goal to be pursued may be stated as follows: given a set of observations $\mathbf{y} = [y_1, y_2, ..., y_N]$, calculate probability density $p(x/\mathbf{y})$, that may be assigned to the measurand x, on the basis of all available knowledge, information on the measurement process and on data $\mathbf{y}$ themselves.

This complex problem may be efficiently faced if decomposed in sub-problems.

So let first consider a *single observation* y_i and look for an algorithm for the evaluation of $p(x/y_i)$. The evaluation is based on the following formula (dropping index i):

$$p(x/y) = \frac{p(y/x)p(x)}{p(y)} \propto p(y/x)p(x) \propto p(y/x) \tag{1}$$

having assumed a constant prior density on x, and provided proper scaling (see [5] for details).

So our problem reduce to the following:

for any value x in a set X calculate $p(y/x)$, with $y = y_i$

We may do that based on a proper *model* of the measuring process.

3 THE MODEL

Let then assume the following model:

$$y = f(x, \mathbf{v}) \tag{2}$$

where is $\mathbf{v}$ a vector of *n influence quantities*.

The associated probability density may be calculated, without using simulation, if f is linear or may be decomposed into a series of linear and non-linear transformations of the Hammerstein kind. Let then show how in both cases calculation of $p(y/x)$ may be reduced to operations on the densities of the array of variables $\mathbf{v}$. Then we will briefly mention how a set of observations $\mathbf{y}$ may be treated through a stochastic observation scheme.

Linear model

Assume function f in model (2) is differentiable. Since the evaluation of $p(y/x)$ is to be done *for each value of* x in many cases a local linearisation will be possible. In fact linearisation is the standard procedure considered in the GUM.

So, let consider a specific value of x, say x_0, and corresponding nominal or expected values of influence quantities, say $\mathbf{v_0}$, which may or may not depend on x.

The value of y will be a random variable due to possible variations of $\mathbf{v}$ around its nominal value $\mathbf{v_0}$:

$$y \cong kx_0 + \mathbf{a}^T(\mathbf{v} - \mathbf{v}_0) + b = y_0 + \mathbf{a}^T(\mathbf{v} - \mathbf{v}_0) \tag{3}$$

where $\mathbf{a}^T = [a_1 ... a_n]$; $a_i = \dfrac{\partial f}{\partial v_i}$ and b is a constant.

If we now introduce the auxiliary random variable d, which represents total deviation from nominal value y_0, $d = y - y_0 = \mathbf{a}^T(\mathbf{v} - \mathbf{v}_0)$, we have:

$$p(y/x_0) = p_d(y - y_0) \tag{4}$$

where dependence on x_0 is implicit as stated above, and $p_d(\cdot)$ may be calculated by a proper convolution integral. To see that, let further introduce the scaled variables:

$$z_i = a_i(v_i - v_{0i}) \;;\; \text{i=1,...n} \tag{5}$$

with densities:

$$p(z_i) = \frac{1}{|a_i|} p\left(\frac{z_i + a_i v_{0i}}{a_i}\right) \tag{6}$$

Each z_i represents the *contribution of variable* v_i *to the deviation of the output* so that:

$$d = \sum_{i=1}^{n} z_i \tag{7}$$

In the case of independent influence quantities, the density of d is simply the convolution of the densities of the z_i:

$$p(d) = \int \ldots \int p_{z_1}(d - x_2 \ldots - x_n) p_{z_2}(x_2 \ldots - x_n) \ldots p_{z_n}(x_n) dx_2 dx_3 \ldots dx_n \tag{8}$$

which may be calculated by a proper numerical procedure.

If there is a subset of correlated influence quantities, say the first n_1 variables, we may consider the following partitioning:

$$d = \sum_{i=1}^{n_1} z_i + \sum_{i=1}^{n_2} z_i = d_1 + \sum_{i=1}^{n_2} z_i \tag{9}$$

Density of d_1 may be obtained by the following formula, involving joint densities:

$$p(d_1) = \int \ldots \int p_{\mathbf{v}}(d - x_2 \ldots - x_{n_1}, x_2 \ldots - x_{n_1}, \ldots, x_{n_1}) dx_2 dx_3 \ldots dx_{n_1} \tag{10}$$

Then the final density of d, may be obtained by convolving the density of d_1 with the densities of the remaining n_2 variables, which are mutually independent.

It is worth noting anyway that in the case of gaussian correlated variables, which is the case considered in the previous paragraph, the result is again a gaussian with proper expectation and variance, so that the integral need not be calculated.

Non linear model.

Since the method works in term of densities, it is possible to deal with non linearities.

Let assume a model with non linearities in series with linear transformation such as the following:

$$y = y'' + \mathbf{a}''^T \mathbf{v}'' \tag{11a}$$

$$y'' = NL(y') \tag{11b}$$

$$y' = kx + \mathbf{a}'^T \mathbf{v} + b \tag{11c}$$

So the procedure will be:

1. calculate $p(y')$ by the procedure for linear transformations;
2. calculate $p(y'')$ by a dedicated procedure;
3. calculate $p(y)$ again by the procedure for linear transformations.

For many common non linearities (threshold, dead zone, polynomials,...) explicit solutions for step two are available.

Stochastic observation schema

Let consider now the general case, referring to the array of results $\mathbf{y} = [y_1, y_2, ... y_N]$. When iteration of measurement is in order, it is vital to distinguish between influence quantities actually varying, say vector $\boldsymbol{w}$, and those which are likely to remain constant during iteration, let call it J .

In the case of *independent variations* of measurement result, we simply have:

$$p(\mathbf{y}/x;\mathrm{J}) = \prod_{i=1}^{N} p(\mathrm{y_i}/x;\mathrm{J}) \tag{12}$$

In the general case we may consider the following factorisation of the conditioned probability density:

$$p(\mathbf{y}/x,\mathrm{J}) = p(y_N/y_{N-1},...,y_1;x,\mathrm{J})...p(y_2/y_1;x,\mathrm{J})p(y_1;x,\mathrm{J}) \tag{13}$$

Once $p(\mathbf{y}/x;\mathrm{J})$ is known, it may be inverted in much the same way as above:

$$p(x/\mathbf{y};\mathrm{J}) \propto p(\mathbf{y}/x;\mathrm{J}) \tag{14}$$

and the final restitution may be done, by taking the expected value with respect to J :

$$p(x/\mathbf{y}) = E_{\mathrm{J}}\, p(x/\mathbf{y};\mathrm{J}) = \int p(x/\mathbf{y};\mathrm{J})p(\mathrm{J})d\mathrm{J} \tag{15}$$

We will not pursued further this topic here, see [5] for details.

4 UNCERTAIN PARAMETERS AND POSTERIOR PARAMETER ESTIMATION

In the previous paragraph, evaluation of $p(y/x)$ has been addressed, as a set of operations over the densities of $\boldsymbol{v}$. Such densities may be calculated on the basis of available information, in much the same way as suggested in the GUM. Such information may be uncertain as well, typically depending upon some dispersion parameter, obtained by subjective evaluation or estimated from data themselves. This is sometimes called “uncertainty of uncertainty”.

In the GUM consideration of the equivalent degrees of freedom is recommended, for both type A and type B uncertainty, which may be combined by Welch-Satterwaite formula.

Here another approach is considered.

First note that dependence upon parameter σ may be expressed in the usual way:

$$p(y/x;s) \tag{16}$$

Then we may consider two cases:

1. a prior knowledge of σ is available as $p(\sigma)$, the we have:

$$p(x/y) = \int p(x/y;s)p(s)ds \tag{17}$$

2. we estimate σ on the basis of data $\boldsymbol{y}$ (in this case usually N>1 applies), so we have:

$$p(x/\mathbf{y}) = \int p(x/\mathbf{y};s)p(s/\mathbf{y})ds \tag{18}$$

5 THE CODE *UNCERT*

The implementation of a general purpose code, according to the above lines, is in progress.

Some previous work have been done, in Fortran. At present a *Matlab*-based implementation is considered (UNCERT), whose main features of the code are:

1. directly calculates densities;
2. allows for correlation between input variables;
3. directly accounts for uncertain dispersion parameters.

First the code asks from the user the characterising parameters of each influence (sensitivity coefficient, distribution type, dispersion parameter, uncertainty of dispersion parameter and, for correlated couples of variables, the correlation coefficient). Then the code computes the proper distribution for each input variable, accounting for uncertainty on the related dispersion parameter (17-18), if required. On the subset of correlated variables (9-10) a gaussian approximation is used.

Finally the density to be assigned to measurement results is calculated and plotted. Standard uncertainty and expanded uncertainty U at any required coverage levels are calculated, the latter being obtained by direct integration of the final distribution.

The code has been validated and tested with reference cases.

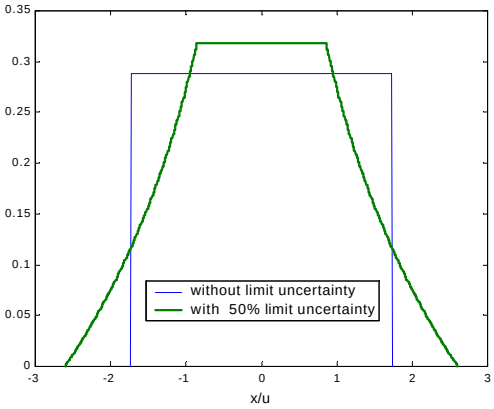

Figure 2

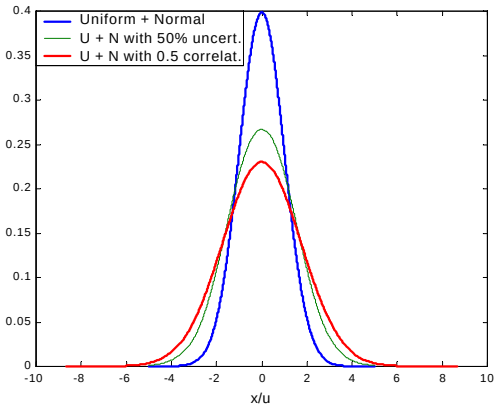

Figure 3

Figure 1 shows the effect of uncertainty of the dispersion parameter on a uniform density.

Figure 2 shows the result of two densities, one being normal, the other uniform, with the same variance. The effect of uncertainty on dispersion parameters is also shown, as well as the result of a 50% degree of correlation.

As a case study, example H.1 in the GUM has been treated (Figure 3). Standard uncertainty is 32 nm; expanded uncertainty at a 0,95 coverage level is 62 nm for ∞ degrees of freedom (to be compared with 63 nm from the GUM procedure) and 64 nm for actual degrees of freedom (against 68 nm).

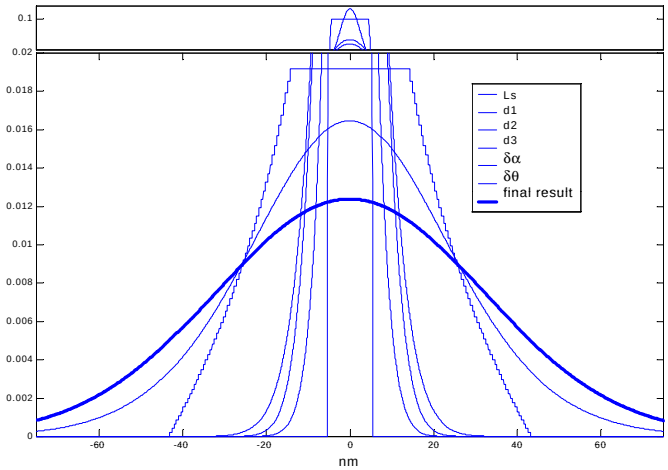

Figure 3

6 CONCLUSIONS

The research is a part of a series of studies undertaken by the authors in the last years, concerning the evaluation of uncertainty in terms of densities. It has been shown that, with the same information required by the GUM, it is possible to express the final result of measurement by a probability density, so including uncertainty in the most general way. This allows, if required, to evaluate both standard and expanded uncertainty, avoiding the rough approximation inherent to method of Welch - Satterwaite, suggested in the GUM. Moreover, the proposed approach goes beyond the GUM, allowing for evaluation also in cases where the Guide is not applicable, such as those involving non-linear transformations. On the basis of this theory, development of related metrological software is in progress. The software is arranged in a hierarchical structure, starting with linear time invariant transformations. Then non-linear algebraic functions will be included. Accounting for uncertainty in parameters is already possible. Direct calculation is used, instead of simulation, to reduce computation time and avoid convergence problems. The program is completely general and applicable to any kind of measurement (on a ratio scale). Self-testing options are included such as direct calculation of variance, to check more complicated calculations. Required input is the same as in the GUM, and the final result is expressed as a probability density. The standard and the expanded uncertainty, at whatever coverage level, may be calculated. Processing is more accurate than that provided by Welch-Satterwaite method and computation time is very low. It goes a step ahead than presently available codes, since it evaluates densities and provides a sound basis for future development.

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