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THE UNCERTAIN NUMBER: A DATA MODEL FOR MEASUREMENT

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Abstract – A simple model for data obtained by measurement is described. The data model satisfies requirements for evaluation and reporting of measurement uncertainty given in the *Guide to the expression of uncertainty in measurement* (GUM). The model supports what is called internally consistent and transferable calculations, which are qualities favoured by the GUM. In this way, more rigorous GUM-compliant digital data processing can be supported than the common reporting format of a single value for measurement uncertainty presently allows.

Keywords: Measurement uncertainty, metrological traceability, data model, abstract data-type, uncertain number

1. INTRODUCTION

The *Guide to the expression of uncertainty in measurement* (GUM) is recognised by the metrology community as describing a preferred approach to measurement data processing [1]. When data is obtained by measurement, the quantity intended to be measured (*measurand*) cannot be determined exactly. However, methods described in the GUM can be used to evaluate certain characteristics associated with a measurement, enabling an assessment of accuracy to be made: usually a statement can be made about the uncertainty in a measurement result as an estimate of the measurand.

The GUM was first published in 1993 and was not written with digital systems in mind. It describes the evaluation of measurement uncertainty in general mathematical terms. In metrology, measurement is a sequential process, in which laboratories cooperate to provide an infrastructure for traceability. National metrology institutes realise SI units and calibrate reference standards for the next tier of calibration laboratories. These laboratories, in turn, disseminate calibration information to their customers. The process goes on until an end-user completes the measurement. At the final stage, information is used to make an inference about a measurand that will inform a decision of some kind. The collaborative measurement process implements a metrological traceability chain to support decision-making by providing objective trustworthy information.

Each stage along a traceability chain must be appropriately documented. A lot of information is retained internally and only a very brief summary is reported between laboratories. However, independent control of laboratory quality systems and staff competencies ensures that adequate records are collected and retained and that the data reported is technically sound. The data that is shared is intended for skilled human interpretation and is in unspecified formats. However, the widespread digitalisation of metrological activities, which is intended to allow digital systems to act reliably on data without human intervention, requires a greater level of formal specification.

In this work, a data model suitable for exchange of information along a traceability chain is presented.[1] A data model is an abstract representation of key relationships between real-world entities and concepts. At a conceptual level, data models may specify the kinds of statement are meaningful in the problem domain. At a logical level, they can describe the semantics of classes and data structures used in representations; this helps to develop concrete implementations.

2. GUM MEASUREMENT MODELLING

The heart of the GUM approach to data processing is a mathematical description of a measurement, called a measurement function or measurement model. In fairly general terms, a model can be expressed as

$$Y = f(X_1, X_2, \cdots, X_l) \ , \tag{1}$$

where Y is the measurand and the inputs $X_1, X_2, \cdots, X_l$ are external factors that influence the outcome of a measurement.[2] The measurement model may be considered as a recipe for evaluating the measurand. If values for all the inputs, $X_1, X_2, \cdots, X_l$, were exactly known, then the actual value of Y would be evaluated by $f(\cdot)$.

In the notation adopted here, capital letters designate quantities. Exact quantity values are never available, so approximations (estimates) must be used. Lower case letters (e.g., $x_1, x_2, \cdots, x_l$ and y) represent values that approximate the corresponding quantities. So, for example, a measurement estimates a measurand, Y, and the result obtained, y, will be reported together with information about the accuracy of y as an estimate of Y.

Although some measurements are simple in principle, the GUM uncertainty calculations often become

[1] Another paper presented at this meeting discusses the requirements for digital representation of traceability in more detail [2].

[2] Some of these terms may represent other measured quantities. For example, one might measure electrical resistance by first measuring potential difference V and current I and then finding the resistance as their ratio $R = V/I$. There will also be terms representing nuisance factors that perturb the measurement, such as Johnson noise in a resistor.

complicated—even unwieldy. It is necessary to characterise the physical and numerical aspects of a measurement in order to assess how susceptible the process is to perturbation. This is the nature of traceability and the need for reliable information about accuracy at the end of a traceability chain.

A GUM calculation assesses the sensitivity of a measurement to each input,

$$c_i = \frac{\partial Y}{\partial X_i} \; , \tag{2}$$

and weights this by the typical magnitude of likely error in the input value, denoted $u(x_i)$ and called a standard uncertainty. This obtains a component of uncertainty,

$$u_i(y) = c_i \, u(x_i) \; , \tag{3}$$

where the subscript 'i' refers to the input quantity X_i. When reporting a final result, the various components of uncertainty will be combined in particular way (see equation (7) below). However, this is only necessary at the end of the traceability chain where an inference about the measurand will be made. Along the chain, sets of components of uncertainty should be passed between stages.

To express the nature of a traceable measurement properly, we must extend the usual GUM notation. Quite generally, a full measurement function $f(\cdot)$ can be decomposed into an arbitrary number of intermediate steps or stages, $h = 1, \cdots, m$, each described by a function

$$Y_h = f_h(\Lambda_h) \; . \tag{4}$$

The set of inputs to the h^{th} stage, Λ_h, may include previous stage outputs, $Y_1, \cdots, Y_{h-1}$ and any of the model inputs $X_1, \cdots X_l$. The last stage yields the measurand, $Y = Y_m$.

In this notation, the component of uncertainty in a stage output y_h due to uncertainty in the i^{th} model input value is

$$u_i(y_h) = \sum_{z_k \in \Lambda_h} \frac{\partial Y_h}{\partial Z_k} u_i(z_k) \; , \tag{5}$$

where Z_k is a dummy variable for a direct input to the stage function and z_k is the corresponding estimate. This equation is simply the chain rule for partial differentiation applied to equation (3). Note that the number of elements in Λ_h is the number of direct arguments to the stage function.

A simple, but not uncommon example of a single stage is when a quantity is compared at two locations and, or, times. The stage evaluates the difference between intermediate outputs. If two previous stage outputs, Y_q and Y_r say, are subtracted at stage h, then equation (5) becomes

$$u_i(y_h) = u_i(y_q) - u_i(y_r) \; . \tag{6}$$

Clearly, the contribution to uncertainty in the difference due to any common influence i (a systematic influence) may be reduced (or even cancel completely, if $u_i(y_q) = u_i(y_r)$).

A complete set of components of uncertainty, $\{u_1(y_h), u_2(y_h), \cdots, u_l(y_h)\}$, at stage h can be obtained by evaluating (5) for $i = 1, 2, \cdots, l$.[3] We emphasize the importance of subscripts, because terms in the mathematical model must be identified in the data model.

3. THE DATA MODEL

A useful abstraction is created by encapsulating a value and a corresponding set of components of uncertainty in a data structure called an uncertain number. Uncertain numbers represent quantities (i.e., capitalised terms) in the mathematical model.

A logical model of uncertain numbers for real-valued data is shown as a UML class diagram in Figure 1.[4] An `UncertainReal` object encapsulates a value and associated components of uncertainty. This class satisfies the common requirements for data, but there are two specialisations: an `Elementary` object represents an input to the measurement model (one of the X_i), and an `Intermediate` object represents an intermediate stage output (one of the Y_h). Objects of these subclasses have a unique identifiers, which refer to a specific object and play the role of subscripts in the mathematical notation.

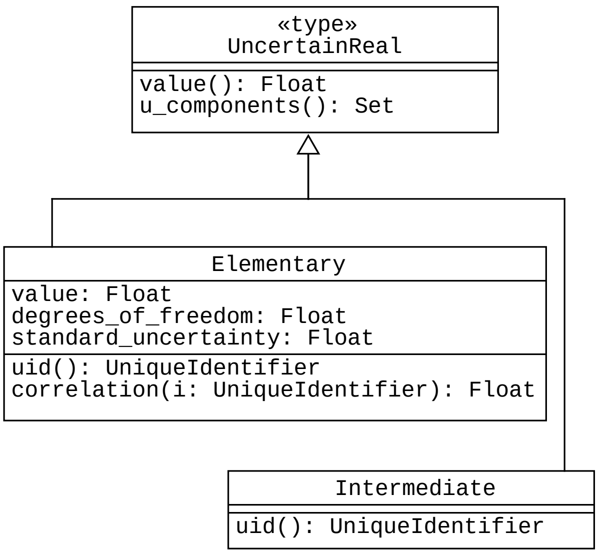

Fig. 1: There are two specialisations of the `UncertainReal` class: `Elementary` and `Intermediate`. An `Elementary` object represents a model input and an `Intermediate` object represents a stage output. The `uid` operation produces a unique reference to an uncertain-number object, which plays the role of a subscript (i or h) in the mathematical notation.

[3] Note, when $j = k$, x_j and z_k are the same and so $u_j(z_j)$ represents $u(x_j)$—the standard uncertainty of the input estimate x_j.

[4] The Unified Modelling Language (UML) is a general-purpose modelling language used to visualize the design of a system.

`Elementary` objects are constructed with a value (estimate), a standard uncertainty and a number of degrees of freedom.[5] An input (one of the X_i) has just one component of uncertainty, which equals the standard uncertainty (see footnote 3). A correlation coefficient can be declared between two `Elementary` objects. These coefficients are used to evaluate the final stage uncertainty (see §4 below).

A `Set` of `ComponentOfUncertainty` objects is returned by `u_components()`. This is needed to evaluate equation (5) from one stage to the next, before the final stage, and to evaluate the combined uncertainty and degrees of freedom at the final stage. Each element in this set consists of a value and a reference to the corresponding input (elementary uncertain number), as shown in Figure 2.

```
ComponentOfUncertainty
------------------------------
component_value: Float
uid: UniqueIdentifier
------------------------------
```

Fig. 2: A `ComponentOfUncertainty` encapsulates two elements: the numeric value of a component of uncertainty and a digital identifier corresponding to 'i' for model input X_i.

4. REQUIREMENTS ON THE DATA MODEL

The model described in the previous section has the essential ingredients for a GUM uncertainty analysis. At the final stage, a combined standard uncertainty will be evaluated. The GUM calculation is

$$u(y) = \left[\sum_{i=1}^{l} \sum_{j=1}^{l} u_i(y)\, r(x_i, x_j)\, u_j(y) \right]^{1/2} , \qquad (7)$$

where $r(x_i, x_j)$ is the correlation coefficient between the estimates of X_i and X_j. Component of uncertainty values are obtained from elements of the set returned by `u_components()`, as well as unique identifiers for each `Elementary` object. A value of $r(x_i, x_j)$ is returned by `Elementary::correlation(i)`.

A parameter, called the effective degrees of freedom, is needed if any input quantities were estimated with finite degrees of freedom. The effective degrees of freedom, ν_{y}, is obtained from the Welch-Satterthwaite equation [1, (G.2a)]

$$\frac{u^4(y)}{\nu_y} = \sum_{i=1}^{l} \frac{u_i^4(y)}{\nu_i} . \qquad (8)$$

Again, `u_components()` provides the components of uncertainty needed. The degrees of freedom are provided by the `degrees_of_freedom` attribute of each input.

[5] The degrees of freedom may be infinity.

The combined standard uncertainty and the effective degrees of freedom are used to evaluate what is called the expanded uncertainty, which is qualified by a particular level of confidence, typically $95\,\%$ (see [1, Appendix G]).

4.1. Archiving records

Because of the distributed nature of traceability chains and the need to retain metrological data for many years, measurement data must endure over space and time. The uniqueness of digital identifiers must be guaranteed anywhere and at any time after they have been created.

The ability to store data is needed to implement measurement traceability chains. To provide a secure and enduring record of an uncertain number, the value and associated set of components of uncertainty must be stored, together with all the elementary uncertain numbers referenced in the component-of-uncertainty set. This allows results to be restored later and combined with other data. Only `Elementary` or `Intermediate` objects are stored.

5. APPLICATIONS OF THE MODEL

5.1. Reporting calibrations

According to the International Vocabulary of Measurement, metrological traceability is implemented by relating a measurement result back to a *reference through a documented unbroken chain of calibrations, each contributing to the measurement uncertainty* [3, §2.41].

The stages of a measurement model may be considered to correspond to the different calibration stages that establish traceability. At each stage, a report is produced by one group of people (a laboratory) and sent to a different group responsible for the next stage. This process presently requires skilled operators to interpret data, but digital systems could exchange data using uncertain numbers.

It is very common, nowadays, to report uncertainty as a single number (representing an uncertainty interval), rather than a set of components of uncertainty. This practice has surely arisen from the convenience it affords, because it is not actually prescribed in the GUM. Only for international measurement comparisons (discussed in §5.3) are components of uncertainty currently reported as a matter of routine (actually a requirement). Our data model satisfies the reporting requirements of measurement comparisons. However, it could also be used to replicate single number uncertainty reporting to people, while maintaining a more detailed digital representation. In doing so, the familiarity of current practice could be retained without sacrificing *internally consistency* in data processing [1, §04].

5.2. Automatic uncertainty calculation

When a mathematical expression is evaluated by a digital system, the expression is decomposed into a sequence of simple expressions corresponding to predefined operations.[6] It is possible to think of a staged measurement model in this way too. The mathematical expression of a model can be decomposed into basic functions, like simple arithmetic, trigonometric functions, and other standard mathematical functions. A digital system can then simultaneously evaluate the values with associated sets of components of uncertainty. This is a powerful way for dealing with complicated measurement procedures [4, 5].

An example of this is a recent study that applied uncertain-number software to a four-axis goniometric system for measuring optical reflectance [6]. The measurement model of this system has many configuration terms that are not known exactly and must be considered to account for final uncertainties. By using uncertain numbers, the authors were able to study the system performance closely under different configuration settings. They were able to gain a better understanding of the inherent correlations between various measurement errors and significantly improve the accuracy of certain measurements.

5.3. Comparison reporting and analysis

Reporting requirements for international measurement comparisons carried out under the International Committee for Weights and Measures (CIPM) Mutual Recognition Arrangement are demanding [7]. Comparison protocols stipulate that participants shall provide detailed uncertainty budgets together with measured values. In effect, this is asking for uncertain numbers to be reported.

A recent study looked at using an uncertain-number data model for measurement comparisons. A fictitious scenario was created where participants reported results as uncertain numbers and uncertain-number software was used for subsequent data processing [8]. Based on actual comparison data, results from a CIPM key comparison and a subsequent Regional Metrology Organisation (RMO) key comparison were processed and then linked to obtain degrees of equivalence for every participant. Although in principle the data processing involved is straightforward, in practice it becomes complicated. Common error terms give rise to correlations in the data that must be carefully handled, so a direct GUM approach becomes impractical. However, the study showed that uncertain-number data model and software considerably simplified the analysis and comparison linking, and provided insights into the results than would not otherwise have been available.

6. FINAL REMARKS

The data model presented here is fully GUM-compliant yet quite simple. It implements the GUM notion of internal consistency. Deployment of the model should not involve too much work. An uncertainty analysis must be carried out and adequately documented to satisfy traceability requirements, so this information is available already and could be included in the exchange of data. The significant advantage offered is that correlation between stage results due to common factors can be properly accounted for. These effects can be propagated along chains and included in the end-user's handling of a result.

[6] For example, computations on a pocket calculator are executed as a sequence of basic operations.

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