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Measuring, Estimating, and Deciding under Uncertainty

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HIGHLIGHTS

- Bayesian statistics provides the sole basis of recent developments in metrology.
- The original GUM now turns out to be a special case of a general methodology to quantify uncertainty.
- As a consequence the GUM is being revised in order to align it with its supplements.
- The GUM provided a basis for calculating characteristic values of measurements.
- In the course of a routine revision, ISO 11929 will be made consistent with the revised GUM.

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ABSTRACT

The problem of uncertainty as a general consequence of incomplete information and the approach to quantify uncertainty in metrology is addressed. Then, this paper discusses some of the controversial aspects of the statistical foundation of the concepts of uncertainty in measurements. The basics of the ISO Guide to the Expression of Uncertainty in Measurement as well as of characteristic limits according to ISO 11929 are described and the needs for a revision of the latter standard are explained.

1. Uncertainty and measurement

Uncertainty is a general characteristic of human existence. It originates from ignorance. The ignorance, that one does not know what the dice will show, whether it will be a girl or a boy, whether a wing beat of a butterfly is responsible for today's weather, when a nucleus will decay, what the future will be, what the truth is, which quantities influence the results of an experiment, whether there is causal connection between two quantities, whether a system is deterministic, stochastic or chaotic, or whether chance is ruling the world.

Uncertainties are important characteristics of human reasoning, decision making and action and, in the end, they are a consequence of limited and incomplete information. Humans always have to decide and to act under uncertainty, i.e. on the basis of incomplete information.

In the case of ignorance one can only rely on probabilities. Uncertainty can be quantified by probabilities. James Clerk Maxwell said in this context "The true logic for this world is the calculus of probabilities, which takes account of the magnitude of the probability which is, or ought to be, in a reasonable man's mind" (Maxwell, 1850). Success decides about the truth.

A complete description of the uncertainty can be obtained by deriving a probability density function (PDF) over the space of possibilities. Probability theory and probability calculus provide the tools to establish and propagate probabilities. Just a few principles are sufficient for a given problem to derive from the available information the desired PDF. Fundamental is the Principle of Indifference, also called Principle of Insufficient Reason (Laplace, 1812). Given $n > 1$ distinguishable, mutually exclusive and collectively exhaustive events, the Principle of Indifference states that without further information each event should be assigned a probability equal to $1/n$. The Principle of Indifference is closely related with the Principle of Maximum Entropy (PME) (Jaynes, 1982) and the Bayes Theorem (Bayes, 1763).

In metrology, these principles are used to quantify uncertainty in measurement. In the 1990ties the quantification of measurement uncertainties was standardized by the ISO Guide to the Expression of Uncertainty in Measurement (GUM) (ISO, 1993) and the standard series DIN 1319 (DIN, 1996, 1999). A Bayesian theory of measurement uncertainties (Weise and Wöger, 1993) provided a

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theoretical basis for the GUM. This basis makes uses of the Bayes Theorem and the Product Rule to establish and propagate the desired PDFs. After initial problems of acceptance and manifold discussions the GUM was newly published [JCGM, 2008a] and extended [JCGM, 2008b, 2011] by the Joint Committee on Guides in Metrology and today represents the internationally accepted methodology for the quantification of measurement uncertainties.

Uncertainty manifests itself in metrology as follows. By a measurement one obtains an uncertain estimate y (measurement result) of the unknown and unknowable true quantity value $\tilde{y}$ of a measurand Y. So, the conditional probability $f_Y(\tilde{y}|y)$, i.e. the probability that the true value of the measurand Y is $\tilde{y}$ given the measurement result y, provides the complete description of the uncertainty associated with the measurement result y. $f_Y(\tilde{y}|y)$ is the PDF of a random variable serving as an estimator of Y; as a PDF it is normalized: $\int_{-\infty}^{\infty} f_Y(\tilde{y}|y)\ \mathrm{d}\tilde{y} = 1$. Instead of the PDF $f_Y(\tilde{y}|y)$ which completely describes the uncertainty, the uncertainty can also be described by a coverage interval $[y^{<}, y^{>}]$ which contains the true value of the measurand with a preselected probability $(1-\gamma)$ or by the best estimate and its associated standard uncertainty. With the PDF $f_Y(\tilde{y}|y)$ the best estimate $\hat{y}$ of the true value $\tilde{y}$ is the expectation $\hat{y} = \mathrm{E}(f_Y(\tilde{y}|y)) = \int_{-\infty}^{+\infty} \tilde{y}\cdot f_Y(\tilde{y}|y)\,\mathrm{d}\tilde{y}$; the variance $u^2(\hat{y}) = \mathrm{Var}(f_Y(\tilde{y}|y)) = \int_{-\infty}^{+\infty} (\tilde{y} - \hat{y})^2 \cdot f_Y(\tilde{y}|y)\,\mathrm{d}\tilde{y}$ gives the standard uncertainty $u(\hat{y})$ associated with the best estimate $\hat{y}$.

The PDF depends on the available information. The GUM-not so clearly-and the GUM Supplement 1 explicitly make use of the PME to derive various PDFs depending on the available information. If there is more information available than y only, e.g. any other available prior information $\Im$, the PDF completely describing the desired probability is $f_Y(\tilde{y}|y, \Im) = C\cdot f_Y(\tilde{y}|y)\cdot f_Y(\tilde{y}|\Im)$. Then, the best estimate of the true value $\tilde{y}$ is $\hat{y} = \mathrm{E}(f_Y(\tilde{y}|y, \Im))$ and its associated standard uncertainty $u^2(\hat{y}) = \mathrm{Var}(f_Y(\tilde{y}|y, \Im))$.

2. Probabilities and statistics

There is a persistent problem, namely that people using the GUM are still living in two different worlds: the worlds of Bayesian statistics and of conventional or frequentistic statistics. Though many results obtained by the two statistics are practically equal, the statistics themselves must not be confused with each other. The term probability does not have the same meaning in the two worlds of statistics. The conventional or frequentist view is that probability is the stochastic limit of relative frequencies. The Bayesian view is that probability is a measure of the degree of belief an individual has in an uncertain proposition. This meaning of probability in Bayesian statistics is the same as in the statement that “the probability to get a six, when tossing a 6-sided dice, is 1/6”. If asked “What is the probability of tossing a six?”, a frequentist would answer “I do not know; I did not yet toss the dice.”

Bayesians follow the tenet that the mathematical theory of probability is applicable to the degree to which a person believes a proposition. Bayesians also hold that Bayes Theorem can be used as the basis for a rule for updating beliefs in the light of new information – such updating is known as Bayesian inference; see below. In this sense, Bayesian statistics is an application of the probability calculus and a probability interpretation of the term probable.

In his posthumously published “Essay towards solving a problem in the doctrine of chances”, Thomas Bayes (* 1702, † 1761) invented the “Bayesian estimation”, i.e. calculating the probability of the validity of a proposition on the basis of a prior estimate of its probability and new relevant evidence (Bayes, 1763). Bayesian estimation is the natural way of human learning: incorporating new experience into the available set of prior assumptions. This is also applied in a Bayesian theory of measurement uncertainties (Weise and Wöger, 1993).

The GUM Suppl. 1 makes the clear statement that the GUM can only work on the basis of Bayesian statistics. Frequentistic statistics cannot take into account type B uncertainties. Further it only allows establishing the conditional probability $f_Y(y|\tilde{y})$ but not $f_Y(\tilde{y}|y)$.

3. Bayesian measurement uncertainties

The Bayesian theory of measurement uncertainties (Weise and Wöger, 1993), which provides a basis of the GUM approach, factorizes the desired PDF $f_Y(\tilde{y}|y, \Im)$

$$f_Y(\tilde{y}|y, \Im) = C\cdot f_Y(\tilde{y}|y)\cdot f_Y(\tilde{y}|\Im) \tag{1}$$

and derives $f_Y(\tilde{y}|y)$ by PME (Jaynes, 1982)

$$S = -\int f_Y(\tilde{y}|y)\cdot \ln\left(f_Y(\tilde{y}|y)\right) \mathrm{d}y = \max \tag{2}$$

and assumes as the only prior information that the measurand Y is non-negative.

If only y and $u(y)$ are known, they are the best estimate and its associated standard uncertainty. Thus, they give for the application of the PME the constraints, $y = \mathrm{E}(f_Y(\tilde{y}|y))$and $u^2(y) = \mathrm{Var}(f_Y(\tilde{y}|y))$. The PME leads with these constraints to the searched PDF$f(\tilde{y}|y)$ by means of variational methods and Lagrangian multiplicators and yields the solution $f_Y(\tilde{y}|y) = \exp(-(\tilde{y} - y)^2/(2\cdot u^2(\tilde{y})))$ and thus:

$$f_Y(\tilde{y}|y, \Im) = C\cdot f_Y(\tilde{y}|\Im)\cdot \exp\left(-(\tilde{y} - y)^2/(2\cdot u^2(y))\right) \tag{3}$$

The Gaussian distribution in Eq. (3) is neither an approximation nor a probability distribution from repeated or counting measurements.

If by turning the argument one assumes that only a true value $\tilde{y}$ and its associated standard uncertainty $\tilde{u}(\tilde{y})$ are known one obtains the constraints $\tilde{y} = \mathrm{E}(f_Y(y|\tilde{y}))$ and $\tilde{u}^2(\tilde{y}) = \mathrm{Var}(f_Y(y|\tilde{y}))$ which yield with the PME $S = -\int f_Y(y|\tilde{y})\cdot \ln(f_Y(y|\tilde{y}))\,\mathrm{d}y = \max$ the solution

$$f_Y(y|\tilde{y}) = \exp\left(-(\tilde{y} - y)^2/(2\cdot \tilde{u}^2(\tilde{y}))\right). \tag{4}$$

Again, this is neither an approximation nor a probability distribution from repeated or counting measurements.

The GUM and ISO 11929:2010 are minimalistic for the purpose of general applicability and therefore assume that only y and $u(y)$ are known. This leads to the Gaussian PDF $f(\tilde{y}|y)$ in Eq. (3). The PDF describing the prior knowledge is also minimalistic, namely it is only assumed that the measurand is non-negative. The knowledge $\tilde{y} \geq 0$is then taken into account by a Heaviside function $H(y)$ as PDF

$$f_Y(\tilde{y}|\Im) = H(y) = \begin{cases} \text{const} & (\tilde{y} \geq 0) \\ 0 & (\tilde{y} < 0) \end{cases}. \tag{5}$$

It must be emphasized that the user is free to take it into account more information, if it is available. Then, one has to follow the GUM Suppl. 1 approach and to use the tools provided by the PME, the Product Rule, and the Bayes Theorem for establishing, updating and propagating distributions.

4. The GUM concept of uncertainty in measurement

The GUM distinguishes two ways by which measurement