Information based probability distribution function (pdf) for a quantity

W. Wöger, PTB Braunschweig

Wolfgang.Woeger@ptb.de

The modern approach to the evaluation of measurement data as recommended in the Guide to the Expression of Uncertainty in Measurement (GUM) is based on the mathematical formulation of the simple idea that relevant information of any kind about the measurand generates an according state of knowledge about the measurand. The state of knowledge after measurement never is complete since the given information does not fix the value of the measurand exactly. Rather, there always is an uncertainty in knowing the measurand. Mathematically, the state of knowledge is represented by a distribution of information-based probabilities defined over all possible values of the measurand. Here, the probability of the value of the measurand to coincide (within an infinitesimal increment) with a chosen possible value is understood as degree of rational expectation for this event to be true. The rational expectation (probability) corresponds to the total given scientifically gained information about the measurand. The information in metrology usually consists of statistical data as well as of non-statistical data like, for instance, the limits enclosing a systematic deviation. The interpretation of probability in this approach cannot be unified with the conventional frequency based interpretation of probability. It is much more general and flexible reflecting Einstein's statement that science is nothing else than common sense reasoning in a refined way. Applying the Principle of Maximum Information Entropy (PME) and Bayes' Theorem one can find the probability distribution function (pdf) for the measurand corresponding to the given total but incomplete information.

It must be understood that a pdf reflects the assessment of the measurand on the basis of given information about the measurand and, thus, never can be interpreted as a frequency distribution of observed values. Rather, beside of information about systematic effects the statistical behaviour of indicated values constitutes additional information that will be incorporated in the pdf for the measurand. In contrast to frequency distributions of indicated values the pdf for the measurand, thus, is known in form and parameters. If ξ denotes the possible values and X the unknown value of the measurand the expectation value

$$x = \mathrm{E}X = \int \xi f_X(\xi | I) \mathrm{d}\xi$$

of the pdf $f_X(\xi | I)$ is the best estimate of the value of the measurand (result of measurement). The notation of the pdf explicitly takes account of the fact that each and every pdf is conditioned on the information I in hand about quantity X. The variance

$$u^2(x) = \mathrm{Var}(X) = \int (\xi - x)^2 f_X(\xi | I)\mathrm{d}\xi$$

of the pdf is the square of the standard uncertainty associated with the result of measurement. The standard uncertainty, thus, is a parameter of the pdf. It refers to the uncertainty in knowing the meausrand and does not reflect a probability statement about *X* as is the case for the socalled expanded uncertainty. The integrals in the two expressions above may be rather complicated. In such case a computer must be used. Adequate numerical methods will be addressed by Maurice Cox and Bernd Siebert in this seminar.

Although not explicitly stated in the GUM, the concept of pdf underlies all the recommendations in that document. The concept mainly is due to the successful work of Bernoulli, Bayes and Laplace. The described approach to data evaluation replaces the conventional frequency based error analysis that for long time was applied in metrology. Error analysis for obvious reasons is unable to handle systematic deviations on the same footing as random deviations which fact in the past inevitably led to inconsistencies and to uncertainty statements that in practice often were of unreasonable magnitude. All deficiencies of error analysis are avoided by the described Bayesian approach. In the often unrealistic case that the only source of uncertainty consists of pure statistical information the two approaches in practice numerically yield the same results.

In this contribution it will be discussed how to assign a pdf to an unknown quantity in case of more or less global information (PME). Also, the case of more detailed statistical information in form of measurement series under repeatability conditions will briefly be addressed (Bayes' theorem). Examples will be provided.

Global information about a quantity *X* is assumed to consist of known estimates γ_j of functions $G_j(X)$. The estimates must be contained in the pdf for *X* such that $\mathrm{E}G_j(X) = \gamma_j$. Of the many pdfs compatible with the given information one quite naturally will choose that unique pdf that incorporates minimal information content otherwise. A measure of the missing information implied by a pdf after C. E. Shannon (1948) is the information entropy

$$S = -\int_{\Omega} f_X(\xi)\ln f_X(\xi)\mathrm{d}\xi \,.$$

Accordingly, the PME – formulated by E. T. Jaynes, 1957 – consists of maximizing this functional, subject to the given constraints $\mathrm{E}G_j(X) = \gamma_j$.

In case of information about the form of the frequency distribution underlying sampled indicated values, pdfs for the unknown parameters of the frequency distribution can be established using Bayes' theorem. The latter is a consequence of the basic multiplication rule for conditional probabilities in probability theory. Given an original assessment (prior pdf) of a parameter, the theorem tells in which way a new assessment (posterior pdf) of that parameter emerges from the observation of values sampled from the frequency distribution. The formal rule for this learning process briefly is *posterior µ likelihood ¥ prior*. The prior may be a pdf obtained by applying the PME to global information that is given without statistical data. A typical example is the problem of recalibration.