Uncertainty: Part 2

Estimation of Measurement Uncertainty

Q How can measurement uncertainty be estimated?

A In the previous article in this series, we pointed out that uncertainty has two components, precision and bias, and examined the relationship between precision and measurement uncertainty. In this article, we briefly describe estimating the precision component of measurement uncertainty.

The previous article mentioned GUM Type A and Type B estimates of measurement uncertainty.[1] Type A estimates are statistical estimates based on analysis of routine testing of control samples or on designed experiments. Type B estimates are based on the theory of propagation of error and on assumed distributions for various potential sources of error.

Type A estimates are recommended over Type B estimates whenever possible because estimates based on data collected from well-designed quality control systems or well-designed experiments tend to be more realistic than estimates that are not grounded in data. There are, however, cases in which Type A estimates may need to be augmented using Type B methods. An example would be a case in which a sample extract must be diluted to bring it into the working range of the measurement method. Since there is volumetric and/or weighing error in the process of dilution, the uncertainty associated with measurement of an undiluted sample, estimated by a Type A approach, cannot simply be scaled up by the intended dilution factor. The error in the dilution factor enters into the calculation as a multiplicative error, which is more complex than an additive error. The standard guide for reporting uncertainty of test results and use of the term measurement uncertainty in ASTM test methods (E2655), is a very useful guide to understanding these concepts.

The type of precision identified with measurement uncertainty is intermediate precision. It is the precision of measurements, using a particular test method performed at a particular laboratory over time, of a control material representative of routine samples. The practice for estimating and monitoring the uncertainty of test results of a test method using control chart techniques (E2554) describes how this type of precision can be estimated based on data from a control sample program. Another method of estimating intermediate precision is to use designed experiments following the approach known as measurement system analysis, which is described in ASTM standard E2782. An MSA study to estimate intermediate precision will include all potentially important factors in the study design, for instance, time, instrument, and operator.

The International Organization for Standardization (ISO) definition of measurement uncertainty clearly implies that for each measurement we must construct a probability distribution on possible values of the measurand (the property being measured), conditional on the measurement, in order to determine "the values that could reasonably be attributed to the measurand." This is not to say that the true value of the measurand is random but rather that the uncertainty about the true value should be characterized using a probability distribution.

Construction of an interval for plausible values implicitly requires a model (conditional probability distribution) for the true value of the property conditional on the measurement. On the other hand, what we are able to construct directly from laboratory studies using designed experiments and/or analysis of quality control data are models (conditional probability distributions) for the measured value conditional on the true value and on auxiliary information about the measurement. How do we bridge the gap between these two types of models?

The answer is to use Bayes Rule to construct what is known as a posterior distribution for the measurand conditional on the measurement and auxiliary information. The posterior distribution is not a statistical description of the characteristics of the testing process but rather of the uncertainty about the true value of a property measured in a particular sample. GUM Type B estimates of measurement uncertainty explicitly use Bayes Rule. GUM Type A (statistical) estimates can use it as well and use it more effectively, since the estimates will be based on real data. Several examples of this can be found in Technical Note 1900 from the National Institute of Standards and Technology.[2]

In the simplest case, measurement errors are believed to follow a normal (Gaussian) distribution, precision is independent of property level, the test method is unbiased, no unusual steps are required in testing (like sample dilution) and any value of the measurand within the working range of the test method is believed to be equally likely. In this case, the uncertainty for a test result may be approximately represented by using a normal distribution with expected value equal to the observed measurement and standard deviation equal to the standard deviation of intermediate precision. Uncertainty intervals are routinely calculated on the basis of this model.

However, in many cases all possible values of the measurand are known to be not equally likely. For instance, the concentrations of impurities in a manufacturing process tend to be very low because that is how the process is operated. Lower concentrations are much more likely than higher concentrations. The same is typically true for environmental samples. For this situation, the simple normal model for measurement uncertainty does not hold. However, in order to maintain "fairness" in commercial transactions or to better detect a process upset, one may wish to adopt the equally likely assumption. Such a priori assumptions about the likelihood of values of the measurand are represented through a probability distribution known as the prior distribution.

In many cases of measurement, precision is an increasing function of the level of the measurand. This is a well-known phenomenon in both analytical chemistry and mechanical testing. A power law, including constant coefficient of variation as a special case, between measurand level and precision of measurement is a common relationship. To cover this situation, control samples should cover a range of values of the measurand for either a control sample program or an MSA study. However, at present, neither E2554 nor E2782 covers estimation of level/precision relationships.

When the measurand level and precision of measurement are not independent, the situation is complex. For unknown samples, the true property value is not known. Only the measurement, the measured value and auxiliary information, can be observed. But, how well the measured value estimates the measurand value is directly dependent on the measurement uncertainty, which is a function of the unknown measurand value. These complications are solvable using more advanced statistical methods, in partiular Bayesian methods (based on Bayes Rule). These methods are extremely useful and are beginning to be used more widely inmeasurement uncertainty. However, they are often complex and are not yet addressed by ASTM standards. This will take time to change but is a needed development. For now, in any but the simplest case, it would be wise to seek the help of a statistician.

The next article in this series will discuss the role of bias and its estimation in measurement uncertainty.

REFERENCES

1. "Evaluation of Measurement Data – Guide to the Expression of Uncertainty in Measurement," Joint Committee for Guides in Metrology, Geneva, Switzerland, 100: 2008.
2. Possolo, Antonio, "NIST Technical Note 1900: Simple Guide for Evaluating and Expressing the Uncertainty of NIST Measurement Results," National Institute of Standards and Technology, U.S. Department of Commerce, 2015.

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