IJIRR

International Journal of Information Research and Review
Vol. 02, Issue, 12, pp. 1442-1446 December, 2015

Research Article

MONTE CARLO SIMULATION IN UNCERTAINTY ESTIMATION

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ARTICLE INFO

Article History:

Received 12th, September 2015
Received in revised form
16th, October 2015
Accepted 09th, November 2015
Published online 30th, December 2015

Keywords:

Uncertainty,
GUM Method,
Monte Carlo,
Simulation, Hardness.

ABSTRACT

The general method which has been widely used for computation of Uncertainty of measurement is law of propagation method as discussed in Guide for Uncertainty of Measurement (GUM). Numbers of other new methods, with the time, have been evolved for the assessment of Uncertainty of measurement. Among those methods, Monte Carlo Method, now has been given the most emphasis and has been recommended by JCGM wide its supplement for Uncertainty of measurement. This paper is an attempt to discuss briefly, the procedure and role of Monte Carlo Method technique in Uncertainty of measurement.

INTRODUCTION

The objective of a measurement is to establish the value of the measurand, that is, the value of particular quantity to be measured. A measurement thus begins with a suitable specification of the measurand, the process of measurement, and the measurement method. The concept of uncertainty is a perceptible trait in the history of measurement. The concept of *uncertainty* as a quantifiable trait is relatively new in the history of measurement, although error and analysis of error have long been a part of the practice of metrology, it is now broadly renowned that, when all of the identified or alleged components of error have been evaluated and the suitable corrections have been applied, there still leftover an uncertainty about the correctness of the stated result, that is, a doubt about how well the result of the measurement represents the value of the quantity being measured.

Uncertainty

Definition

The word "uncertainty" means doubt, and thus in its broadest sense "uncertainty of measurement" means doubt about the validity of the result of a measurement, because of the lack of different words for this *general concept* of uncertainty and the specific quantities that provide *quantitative measures* of the concept.

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For every measurement - even the most careful - there is always a margin of doubt. The uncertainty of measurement result denotes the lack of exact information of the value of the measurand. Still, after correction for recognized systematic effects, the result of measurement is only an approximation the value of the measurand because there are some random effects and imperfect correction of the result of measurement arise uncertainty. Some of these random components that comprises uncertainty of measurement may be evaluated from the statistical distribution of the results of series of measurements and can be characterized by experimental standard deviations and other components are evaluated from assumed probability distributions based on experience or other information and also can be characterized by standard deviations.

Possible Sources of Uncertainty

- Incomplete definition of the measurand;
- Imperfect realization of the definition of the measurand;
- Non representative sampling — the sample measured may not represent the defined measurand;
- Inadequate knowledge of the effects of environmental conditions on the measurement or imperfect measurement of environmental conditions;
- Personal bias in reading analogue instruments;
- Finite instrument resolution or discrimination threshold;
- Inexact values of measurement standards and reference materials;

- Inexact values of constants and other parameters obtained from external sources and used in the data-reduction algorithm;
- Approximations and assumptions incorporated in the measurement method and procedure;
- Variations in repeated observations of the measurand under apparently identical conditions.
- These sources are not necessarily independent, and some of sources (a) to (i) may contribute to source (j). Of course, an unrecognized systematic effect cannot be taken into account in the evaluation of the uncertainty of the result of a measurement but contributes to its error.

LPU Method for Uncertainty evaluation

The LPU (GUM) method is not magic. Its application will not produce accurate estimates of measurement uncertainty from bad tests or poor research. What the GUM does provide is a consistent method for estimating measurement uncertainties. These words from that document summarize the situation well: Although this Guide provides a framework for assessing uncertainty, it cannot substitute for critical thinking, intellectual honesty and professional skill. The evaluation of uncertainty is neither a routine task nor a purely mathematical one; it depends on detailed knowledge of the nature of the measurand and of the measurement. The quality and utility of the uncertainty quoted for the result of a measurement therefore ultimately depend on the understanding, critical analysis, and integrity of those who contribute to the assignment of its value. The area of a square piece of material is calculated from two input quantities, length and width. These quantities may be affected by influence quantities such as temperature and the resolution of the measuring instrument

Steps involved in LPU Method:

- Express mathematically the relationship between the measurand Y and the input quantities X_i on which Y depends: $Y = f(X_1, X_2, ..., X_N)$. The function f should contain every quantity, including all corrections and correction factors that can contribute a significant component of uncertainty to the result of the measurement.
- Determine x_i, the estimated value of input quantity X_i, either on the basis of the statistical analysis of series of observations or by other means.
- Evaluate the *standard uncertainty* $U(x_i)$ of each input estimate x_i. For an input estimate obtained from the statistical analysis of series of observations.
- Evaluate the covariance associated with any input estimates that are correlated.
- Calculate the result of the measurement, that is, the estimate y of the measurand Y, from the functional relationship f using for the input quantities X_i the estimates x_i obtained in step 2.
- Determine the *combined standard uncertainty* $U_c(y)$ of the measurement result y from the standard uncertainties and covariance associated with the input estimates. If the measurement determines simultaneously more than one output quantity, calculate their covariance.
- If it is necessary to give an *expanded uncertainty* U, whose purpose is to provide an interval $y - U$ to $y + U$ that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand Y, multiply the combined standard uncertainty $Uc(y)$ by a *coverage factor* k, typically in the range 2 to 3, to obtain $U = kU_c(y)$. Select k on the basis of the level of confidence required of the interval.
- Report the result of the measurement y together with its combined standard uncertainty $U_c(y)$ or expanded uncertainty

Limitation of LPU approach

- The model used for calculating the measurand must have insignificant non-linearity. When the model presents strong elements of non-linearity, the approximation made by truncation of the first term in the Taylor series used by the GUM approach may not be enough to correctly estimate the uncertainty output.
- Validity of the central limit theorem is another limitation of GUM approach. Central limit theorem states that the convolution of a large number of distributions has a resulting normal distribution. Thus, it is assumed that the probability distribution of the output is approximately normal and can be represented by a t-distribution. In some real cases, this resulting distribution may have an asymmetric behavior or does not tend to a normal distribution, invalidating the approach of the central limit theorem.
- In addition, the GUM approach may not be valid when one or more of the input sources are much larger than the others, or when the distributions of the input quantities are not symmetric
- GUM methodology may also not be appropriate when the order of magnitude of the estimate of the output quantity and the associated standard uncertainty are approximately the same.

History of Monte Carlo method

Before the Monte Carlo method was developed, simulations tested a previously understood deterministic problem and statistical sampling was used to estimate uncertainties in the simulations. Monte Carlo simulations invert this approach, solving deterministic problems using a probabilistic analog. An early variant of the Monte Carlo method can be seen in the Buffon's needle experiment, in which π can be estimated by dropping needles on a floor made of parallel and equidistant strips. In the 1930s, Enrico Fermi first experimented with the Monte Carlo method while studying neutron diffusion, but did not publish anything on it. In 1946, physicists at Los Alamos Scientific Laboratory were investigating radiation shielding and the distance that neutrons would likely travel through various materials.

Despite having most of the necessary data, such as the average distance a neutron would travel in a substance before it collided with an atomic nucleus, and how much energy the neutron was likely to give off following a collision, the Los Alamos physicists were unable to solve the problem using conventional, deterministic mathematical methods. Stanislaw Ulam had the idea of using random experiments. Uses of Monte Carlo methods require large amounts of random numbers, and it was their use that spurred the development of pseudorandom number generators, which were far quicker to use than the tables of random numbers that had been previously used for statistical sampling.

Monte Carlo simulation: a simulation is a fictitious representation of reality, a Monte Carlo method is a technique that can be used to solve a mathematical or statistical problem, and a Monte Carlo simulation uses repeated sampling to determine the properties of some phenomenon (or behavior). Examples:

- Simulation: Drawing one pseudo-random uniform variable from the interval [0,1] can be used to simulate the tossing of a coin: If the value is less than or equal to 0.50 designate the outcome as heads, but if the value is greater than 0.50 designate the outcome as tails. This is a simulation, but not a Monte Carlo simulation.
- Monte Carlo method: Pouring out a box of coins on a table, and then computing the ratio of coins that land heads versus tails is a Monte Carlo method of determining the behavior of repeated coin tosses, but it is not a simulation.
- Monte Carlo simulation: Drawing a large number of pseudo-random uniform variables from the interval [0,1], and assigning values less than or equal to 0.50 as heads and greater than 0.50 as tails, is a *Monte Carlo simulation* of the behavior of repeatedly tossing a coin.

Monte Carlo Simulation

A Monte Carlo method is a computational algorithm that relies on repeated random sampling to compute its results. Because of their reliance on repeated computation and random or pseudo-random numbers, Monte Carlo methods are most suited to calculation by a computer. Monte Carlo methods tend to be used when it is infeasible or impossible to compute an exact result with a deterministic algorithm. The Monte Carlo method as discussed by the GUM Supplement 1 involves the propagation of the distributions of the input sources of uncertainty by using the model to provide the distribution of the output, whereas according to GUM, the uncertainties are to be propagated according to their distributions.

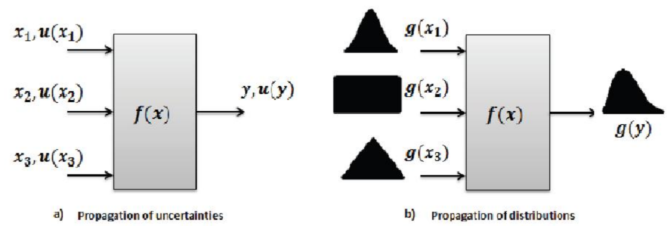


Figure 1. Law of Propagation of Uncertainty (LPU) and Monte Carlo Method (MCM)

Illustrations of the methodologies of a) propagation of uncertainties, where x_1, x_2 and x_3 are input quantities, $u(x_1)$, $u(x_2)$ and $u(x_3)$ are their respective uncertainties and y and u(y) are the measurand and its uncertainty, respectively; and b) propagation of distributions, where $g(x_1)$, $g(x_2)$ and $g(x_3)$ are the distribution functions of the input quantities and g(y) is the distribution function of the measurand

MEASUREMENT PROCEDURE OF UNCERTAINITY

Procedure in MS EXCEL

- Using the readings of force (F) & diameters (d) calculate average & standard deviation(σ) values respectively.
- DOF for force and diameter is (n-1).
- Calculate the t-value.
- Now calculate uncertainty of repeatability using formula $(T*\sigma)/\sqrt{n}$ for the input quantities.
- Standard uncertainty of load cell and microscope involved in testing procedure is provided by NPL.
- Thus uncertainties involved in all the input quantities are obtained (U_1, U_2,U_3,U_4…)
- Calculate the combined standard uncertainty (U). Formula used-

$$U = \sqrt{(U_1^2 + U_2^2 + U_3^2 + U_4^2 \dots)}$$

- Calculate effective degree of freedom without considering the standard uncertainty of load cell & microscope. Formula used-

$$U^4/ (U_1^4/n\text{-}1 + U_2^4/n\text{-}1 + \dots)$$

- Calculate value of δ using formula-

$$\delta=10^l/2 \;;$$

l= integral value equal to order of uncertainty

e.g. - $37*10^{-2}$, l=-2

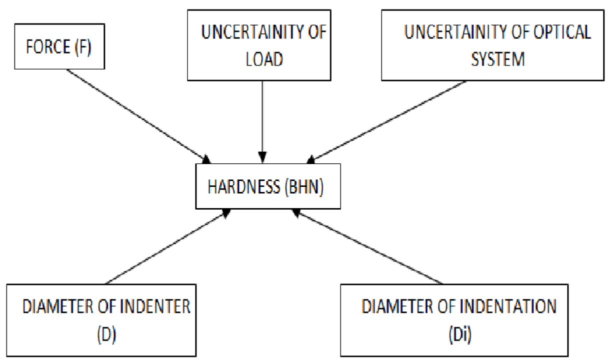
Procedure for simulation using MCS

- Using the mean and standard deviation values of the input quantities like force and diameter we will generate a large numbers of readings using Data analysis in MS excel.
- Calculate the value of hardness for respective readings using the Brinell hardness formula.
- Calculate the mean value of hardness.
- Generate the histogram in MS excel
- Calculate the sensitivity coefficient of force by differentiating the hardness with respect to force i.e. dH/dF. (C_1)
- Similarly calculate sensitivity coefficient of diameter using dH/dD. (C_2)
- Calculate the sensitivity coefficient of all the uncertainties involved using C_1 & C_2.
- Calculate the combined standard uncertainty using the same formula.
- Calculate the effective degree of freedom.
- Calculate the final standard uncertainty in MCS

CALCULATION OF UNCERTAINITY

Definition of problem

Assessment of MCS and calculation of uncertainty in the Brinell hardness test.



FORMULA USED:

BHN = 2F/∏D (D $-\sqrt{(D^2 - Di^2)}$)

F: Applied load**, kg**
D: Diameter of the ball indenter, **mm**
Di: Mean diameter of indentation, **mm**

INPUT TABLE

- **For 1st block:**

Table 1. Brinell hardness test readings for 1st block

Force (kgf)	187.5	187.5	187.5	187.5	187.5
Diameter(mm)	2.5	2.5	2.5	2.5	2.5

- **For 2nd block:**

Table 2. Brinell hardness readings for 2nd block

Force (kgf)	3000	3000	3000	3000	3000
Diameter(mm)	10	10	10	10	10

Uncertainty of Load cell at 95% confidence level: $\pm$ 0.2 kgf
Uncertainty of Microscope at 95% confidence level: $\pm$ 0.01 mm

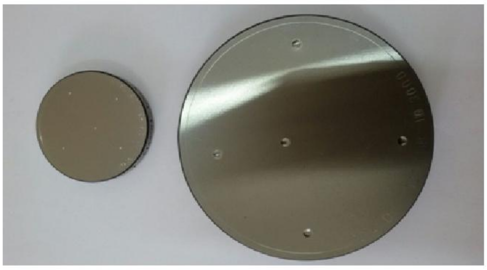


Figure 3. Hardness tested blocks, Block 1st (2.5/187.5) (left), Block 2nd (10/3000) (right). {Ref: NPL}

OBSERVATION TABLE

- **For 1st block:**

Table 3. Uncertainty table for 1st block

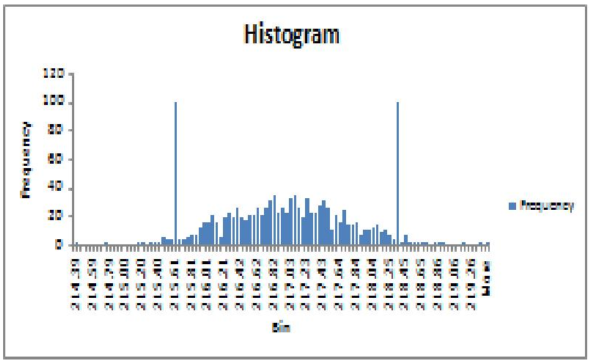
Parameters	Standard Uncertainty	Average	Standard Deviation	Distribution
Force (F)	0.09375	187.5	0.293941	Normal
Load Cell	0.1%	----	----	----
Indenter Dia. (D)	0.000025	2.5	0.00000588	Normal
Indentation Dia.(Di)	0.000194	1.0248	0.0005864	Normal
Microscope	0.00005	----	----	----

Combined Standard Uncertainty: =
(0.00002^2+0.1^2+0.0001941^2+0.000049^2)^0.5
Effective Degree of Freedom: 634383891217.80700000
Final Uncertainty: 0.100000202

Calculation for MCS

Sensitivity Co-efficient of Force (F): 1.159678
Sensitivity Co-efficient of Diameter: 8.36605
Sensitivity Co-efficient of indentation diameter (d): 443.8083
Sensitivity Co-efficient of Force x St. Uncertainty of Force (F) = 0.108720
Sensitivity Co-efficient of Diameter x St. Uncertainty of diameter (D) = 0.000209
Sensitivity Co-efficient of indentation dia. x Uncertainty of Diameter (d) = 0.086099
Standard uncertainty (U) = 0.138683298
Coverage Factor at 95% confidence level = **2**
Expanded uncertainty= 0.277366596
Y (average value of hardness from random trials) = 216.96

HISTOGRAM



- **For 2nd block**

Table 4. Uncertainty table for 2nd block

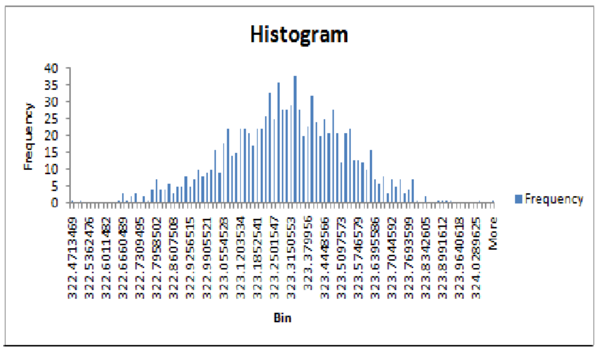
Parameters	Standard Uncertainty	Average	Standard Deviation	Distribution
Force (F)	1.5	3000	0.316228	Normal
Load Cell	0.1%	----	----	----
Indenter Dia. (D)	0.000025	10	0.015811	Normal
Indentation Dia.(Di)	0.000116495	3.3834	0.001158555	Normal
Microscope	0.00005	----	----	----

Combined Standard Uncertainty: =
(0.005^2+0.1^2+0.000116495^2+0.00005^2) ^0.5
Effective Degree of Freedom: 4911126774829.37000000
Final Uncertainty: 0.10012499
Delta:

Calculation for MCS

Sensitivity Co-efficient of Force (F): 0.006754
Sensitivity Co-efficient of Diameter: 2.026067
Sensitivity Co-efficient of indentation diameter (d): 197.0859
Sensitivity Co-efficient of Force x St. Uncertainty of Force (F) = 0.010130336
Sensitivity Co-efficient of Diameter x St. Uncertainty of diameter (D) = 0.00005065168
Sensitivity Co-efficient of indentation dia. x Uncertainty of Diameter (d) = 0.022959552
Standard uncertainty (U) = 0.025095165
Coverage Factor at 95% confidence level = **2**
Expanded uncertainty= 0.05019033
Y (average value of hardness from random trials) = 323.2891

HISTOGRAM



RESULTS AND DISCUSSION

Comparison of values of uncertainty for both blocks

- **For 1st block**

	Experimental Data	Data using MCS
Standard Uncertainty	0.13	0.138683298
Expanded Uncertainty	0.27	0.277366596

- **For 2nd block**

	Experimental Data	Data using MCS
Standard Uncertainty	0.07	0.025095165
Expanded Uncertainty	0.23	0.05019033

The standard uncertainty and the expanded uncertainty obtained from the Monte Carlo Simulation method is less than or approximately equal to the respective values obtained from the fundamental method of uncertainty evaluation, this validates the calculation of uncertainty using MCS. MCS proved to be valuable & flexible computational tool in uncertainty measurement. In MCS it is relatively easy to handle multiple sources of uncertainty as here there are different factors influencing the uncertainty in measurement of hardness (force, indenter diameter, indentation diameter).

Random numbers are generated from the observed values of input quantities to determine if the index values go up or down. In MCS we propagate the distribution of each input quantity. The type of distribution is according to the number of observations taken and the data mentioned in the fundamental document. On the other hand in LPU we propagate the uncertainty involved in each input quantity. Due to this reason the uncertainty involved in measurement is reduced after Monte Carlo Simulation technique.

Thus the validation of MCS is approved and we can say that MCS supports the fundamentals of LPU. But this has to be made very clear that validation of MCS doesn't discard LPU. In fact LPU gives the fundamentals about uncertainty measurement and MCS takes the results to greater efficiency. Thus we can more closely analyze the risk involved in the measurement and the confidence level of consumer is increased to a greater level.

Conclusion

The present study discusses the uncertainty of measurement evolution for Brinell hardness blocks by the conventional techniques (LPU) and recently adopted by JCGM, Monte Carlo simulation. Hardness measurement is very important for characterizing any material and shows the ability of the material against any scratch or resistance to deformation. Hardness is in fact a destructive testing procedure and hence, the blocks used for measuring the properties of material are reference one. Uncertainty of measurement is very important in terms of confidence of the measurement procedure and helps the scientist/technocrats to prove their claims about the experimental measurements. Uncertainty of measurement evaluated broadly by law of propagation of uncertainty which is based on fundamental law of statics and assumes the uncertainty propagates while calculating the uncertainty of measurement of any measurement process. Monte Carlo Simulation techniques though have been evolved in late 1940s has been used for various industrial and management issues have been used for uncertainty of measurement evolution in early 2000s andin2008, adopted for uncertainty evolution. In the present study two blocks of different scales of brinell hardness (2.5/187.5, 10/3000) scales have been used as a artifact. The hardness blocks are calibrated according to the standard evolution procedure ISO. Using the primary standard of brinell hardness at NPL, India (which maintain the standard at primary level in country). The uncertainty of measurement is evaluated by LPU and found to be well within limits. Monte Carlo Simulation techniques have been used to evaluate the uncertainty of measurements of hardness blocks and suitable procedure adopted accordingly. The uncertainty computed by both the means is found within limits and MCS supports the claims of LPU. In addition, it is also to be said that MCS doesn't attempt to downside LPU as MCS is complementary to LPU and attempts to validate the results of LPU. In addition, it is now expected that the procedure adopted for present investigation to be extended throughout the different types of scales of hardness i.e. Rockwell, vicker, brinell as well as different scale of each type of scale like BHN 2.5/187.5, 5/750, 10/3000 etc. for future re-affirmation.

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