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"SASO Uncertainty Machine" - Advanced Pythonic ML Algorithm for Estimating Uncertainty in General Calibration Services at Saudi Standards, Metrology, and Quality Organization-SASO-KSA

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Abstract – **The missions of the National Metrology Calibration Centre (NMCC) at Saudi Standards, Metrology, and Quality Organization (SASO) as a national metrology institute are to maintain, disseminate, develop and realize the International SI units. One of the introduced services by the laboratories is the routine calibration that covers nearly all fields and sectors such as industrial, medical, environmental, etc.... This work aimed to digitized a web-based software application to evaluate the measurement uncertainty associated with a measurement's quantity for all kind of model functions (linear, non-linear, polynomial, logarithmic, etc..) that related to the calibration, testing, accreditation, verification and validation services. Pythonic machine learning algorithm was built based on the requirements of JGCM-100 to give the normal user a full information report about the experiment and measurement uncertainty during three main steps. The validation of the automated algorithm is carried out on five examples that are reported by JGCM standard with completely numeric matching. The article will provide open-source step by step algorithm as a part of digital transformation trend around the world.**

Keywords: SOSO, NMCC, Digitalization, Uncertainty, JGCM-100, Calibration, Testing, AI.

I. INTRODUCTION

The term "uncertainty" signifies doubt, "uncertainty of measurement" denotes doubt regarding the validity of a measurement result [1]. Due to the absence of distinct terms for both the general concept of uncertainty and the specific quantities, such as standard deviation, that quantitatively represent it . Measurement uncertainty typically involves multiple factors. Some of these factors can be assessed through the statistical analysis of a series of measurement results and are defined by experimental standard deviations. Other factors, which can also be defined by standard deviations, are evaluated using assumed probability distributions based on experience or other information. Uncertainty in general consists of two main parts [1], type A which is related to the statistical analysis of series of observations, type B is related to sources that affect the measurement process. Combined standard uncertainty is the standard uncertainty of a measurement result that is derived from the values of several other quantities. It is calculated as the positive square root of the sum of terms, with each term representing the variances or covariances of these other quantities. These terms are weighted according to how the measurement result changes with variations in these quantities. Finally, expanded uncertainty is a measure that defines a range around the result of a measurement, which is expected to cover a significant portion of the distribution. In order to estimate the uncertainty, it should be following the process (figure 1) and determine the sources of uncertainty Table 1. The Type A and Type B classification [1, 2] serves to differentiate between two distinct methods of assessing uncertainty components. This distinction does not imply any inherent differences in the nature of the components derived from each evaluation method. Both methods rely on probability distributions, and the resulting uncertainty components are quantified through variances or standard deviations [1, 2].

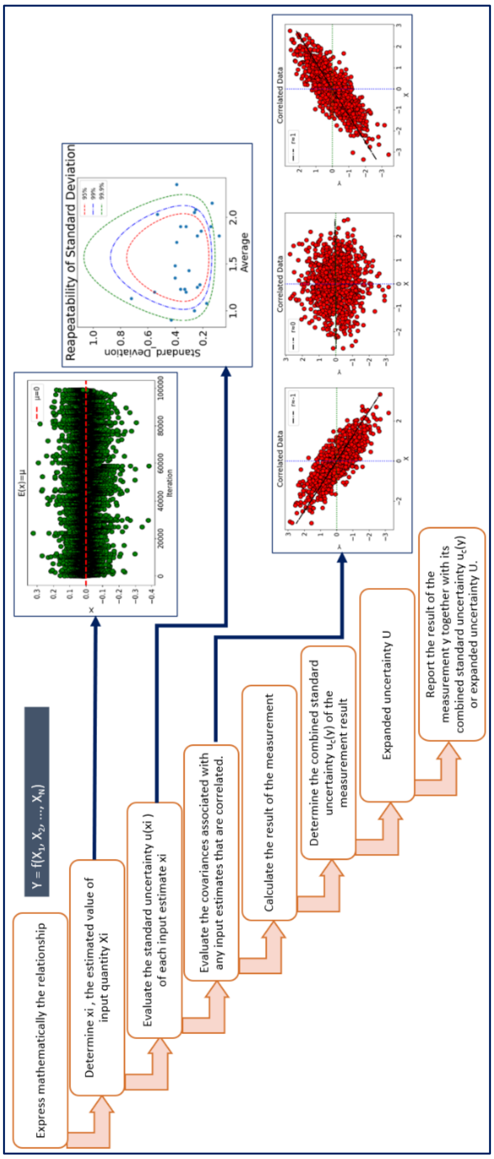


Fig 1. Summary of procedure for evaluating and expressing uncertainty

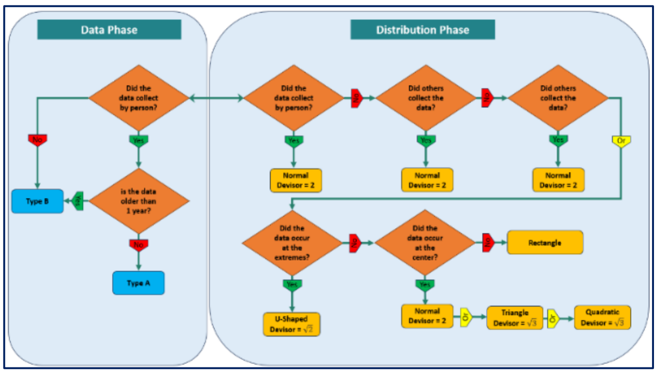


Fig 2. Classification of data and distributions

Table 1. The uncertainty sources that may including (but not limited to) experiment

Method	**Equipment/ Reference Material**	**Personnel**	**Environment**
• Model function • Preparation • Testing • Calibration • Analysis • Calculations • Conversions • Rounding	• Repeatability • Stability • Bias • Drift • Resolution • Certificates • Stability • Linearity • Hysteresis • Homogeneity • Technical Documents • Manufacture Manuals • Specifications • Accuracy • Precision	• Reproducibility • Reading analogue instruments	• Temperature • Humidity • Pressure • Gravity • Vibration • Noise • EMI • Illumination

In order to classify the sources into Type A or B which is driven from **C**lassification **A**lgorithm in **M**achine **L**earning (CAML), we can summarize the concepts as shown in figure 2. Some time is useful to investigate the behind the measurements error, it can be classified into tow main sources, the systematic and random error (figure 3.a). Drift and bias also considered errors (figure 3.b), both are related to the used equipment, with variable and constant behavior respectively [1, 2, 3, 4].

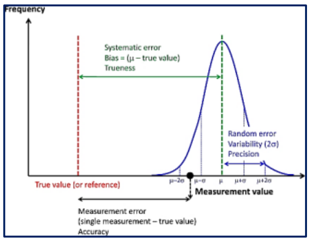


Fig 3.a. Systematic and random error concept

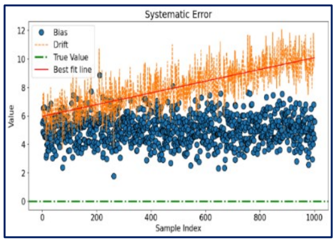


Fig 3.b. Drift and bias concept

II. SASO UNCERTAINTY MACHINE (SASO-UM)

(SASO-UM) is a web-based software tool designed to assess, evaluate and estimate the measurement uncertainty related to an output quantity as specified by a measurement model function. The code architecture is based on python programming code that used several libraries to complete ethe technical report to the users. The process starts with input the results and end with reporting the results, full techniques will be discussed in the following sections. The source code used under python and Jupiter note book environment [5]. Jupyter lab [5, 6] is used as an interactive environment with python, different sets of libraries used for building the algorithm. NumPy [7], which is short for Numerical Python, is a robust Python library that is widely utilized in scientific computing. It offers assistance for vast, multi-dimensional arrays and matrices, as well as an extensive selection of mathematical operations such as algebra and matrices that can be performed on these structures. Pandas [8] is a data manipulation tool that operates at a high level and is constructed on top of NumPy. It offers user-friendly data structures and analysis tools for managing tabular data in Python. Pandas has two primary classes, namely Series and Data Frame, for managing data. Additionally, it has robust capabilities for indexing, filtering, selecting, and transforming subsets of data. Matplotlib [9] is a data visualization library built on top of NumPy. It provides a variety of plotting functions to create complex visualizations and graphs in Python. Plotly [10] is a data visualization library that provides interactive and dynamic visualizations. It can be used with NumPy to create informative graphs in Python. SciPy (Science Python) [11] is a library that builds on NumPy to provide a wide range of scientific computing tools. It includes modules for optimization, integration, linear algebra, and more. SciPy can perform complex mathematical operations with ease and efficiency. Seaborn [12] is a data visualization library based on matplotlib. It provides a high-level interface for drawing attractive and informative statistical graphics. Statsmodels [13] is a Python module that provides classes and functions for the estimation of many different statistical models, as well as for conducting statistical tests, and statistical data exploration. An extensive list of result statistics is available for each estimator. Scikit-learn (Sklearn) [14] is the most useful and robust library for machine learning in Python. It provides a selection of efficient tools for machine learning and statistical modeling including *classification*, *regression*, clustering and dimensionality reduction via a consistence interface in Python.

III. MATHEMATICAL MODEL

1. MODEL FUNCTION

Consider an estimate of the measurand Y, denoted by y and an estimate of the input X_N, denoted by x_N

$$Y = f(X_{1,} X_{2,}, \dots \dots \dots . X_N) \quad 1$$

$$y = f(x_{1,} x_{2,}, \dots \dots \dots . x_N) \quad 2$$

The arithmetic mean or average

$$y = \bar{Y} = \frac{1}{n}\sum_{k=1}^{n} Y_k = \frac{1}{n}\sum_{k=1}^{n} f(X_{1,k}, X_{2,k}, \dots, X_{N,k}) \quad 3$$

The estimate of the expectation or expected value μ_x of a quantity x for n independent observations x_k

$$\bar{x} = \frac{1}{n}\sum_{k=1}^{n} x_k \quad 4$$

The experimental variance of the observations, which estimates the variance σ^2 of the probability distribution of x.

$$s^2(x_k) = \frac{1}{n-1}\sum_{j=1}^{n} (x_j - \bar{x})^2 \quad 5$$

The experimental variance of the mean is the best estimate of $\sigma^2(\bar{q}) = \sigma^2/n$

$$s^2(\bar{x}) = \frac{s^2(x_k)}{n} = \frac{1}{n(n-1)}\sum_{j=1}^{n} (x_j - \bar{x})^2 \quad 6$$

The standard uncertainty

$$u(\bar{x}) = s(\bar{x}) = \sqrt{s^2(\bar{x})} = \frac{s(x_k)}{\sqrt{n}} \quad 7$$

2. COMBINED STANDARD UNCERTAINTY

Combined standard uncertainty of the estimate y is denoted by $u_c(y)$, the combined standard uncertainty $u_c(y)$ is the positive square root of the combined variance $u_c^2(y)$

3. UNCORRELATED INPUT QUANTITIES

Combined uncertainty In term uncorrelation

$$u_c^2(y) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) \quad 8$$

The partial derivatives $\frac{\partial f}{\partial x_i}$ are called sensitivity coefficients

$$c_i = \frac{\partial f}{\partial x_i} = \left.\frac{\partial f}{\partial X_i}\right|_{x_1, x_2, \dots, x_N}, \; u_c^2(y) = \sum_{i=1}^{N} [c_i u(x_i)]^2 \quad 9$$

4. CORRELATED INPUT QUANTITIES

$$u_c^2(y) = \sum_{i=1}^{N} c_i^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} c_i c_j COV(x_i, x_j) \quad 10$$

The relation between correlation and covariance is

$$\rho(x_i, x_j) = \frac{COV(x_i, x_j)}{u(x_i)u(x_j)} = \frac{COV(x_i, x_j)}{\sigma_{x_i}\sigma_{x_j}} \quad 11$$

The covariance between components

$$COV(x_i, x_j) = \frac{1}{n(n-1)}\sum_{k=1}^{n}(x_{ik} - \mu_{x_i})(x_{jk} - \mu_{x_j}) \quad 12$$

Combined uncertainty in term correlation

$$u_c^2(y) = \sum_{i=1}^{N} c_i^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} c_i c_j u(x_i) u(x_j) \boldsymbol{\rho}(x_i, x_j) \quad 13$$

If the model function in form $Y = cX_1^{P_1} X_2^{P_2} \dots \dots X_N^{P_N}$, the equation 13 can be expressed as $\left[\frac{u_c(y)}{y}\right]^2 = \sum_{i=1}^{N} \left[P_i \frac{u(x_i)}{x_i}\right]^2$

5. EFFECTIVE DEGREE OF FREEDOM

A t-distribution (eq. 14) with an effective degrees of freedom ν_{eff} obtained from the Welch-Satterthwaite formula, $v_{eff}\; eq(15)$.

$$t = \frac{(\bar{x} - \mu)}{s(x)} = \frac{(\bar{x} - \mu)}{u(x)} \quad 14$$

$$v_{eff} = \frac{u_c^4(y)}{\sum_{i=1}^{N} \frac{u_i^4(i)}{v_i}} \quad 15$$

6. COVERAGE FACTOR AND LEVELS OF CONFIDENCE

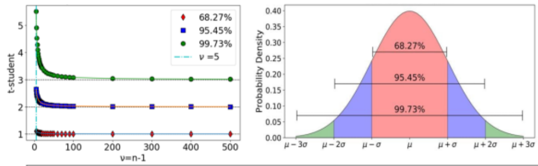
The relation between t-student and coverage factor k is

$$As\ \nu \to \infty \cdots t_p \approx \left(\sqrt{1 + \frac{2}{\nu}}\right) k_p \quad 16$$

In order to determind the specific value of coverage factor, SASO-UM able to detect the distribution of data if it was manualy entered or satisfied by user.All possiple distribution are introduced to SASO-UM algorithm but we will discuss in details the most common distributions in the uncertainty in general.

7. NORMAL DISTRIBUTION

For a quantity x is cosider a normal distribution with expectation μ_x and standard deviation σ, the value of k_p that produces an interval $\mu_x \pm k_p\sigma$ [1] is shown in figure 4.

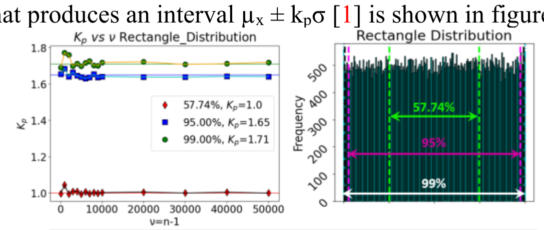


Fraction p in percent							
ν	50	68.27	90	95	95.45	99	99.73
∞	0.67	1.000	1.645	1.960	2.000	2.576	3.000

Figure 4. Confidence intervals and levels in normal distribution.

8. RECTANGLE DISTRIBUTION

If a quantity x is defined by a rectangle distribution, the expectation μ_x and standard deviation σ, the value of k_p that produces an interval $\mu_x \pm k_p\sigma$ [1] is shown in figure 5.



Fraction p in percent						
ν	50	57.74	90	95	99	100
∞	0.864156	1.000	1.555955	1.643018	1.71129	1.73 ≈ √3

Figure 5. Confidence intervals and levels in rectangle distribution.

Recall the estimator and expectation of moment about the mean, the mean can be estimated as

$$\mu = E[x] = \int_a^b x f(x)dx. \quad 17$$

Where a and b is the limits of rectanglar distribution and $f(x)$ is its function, $f(x) = \frac{1}{b-a}$.

$$\mu = \int_a^b x\frac{1}{b-a}dx = \frac{1}{b-a}\left.\frac{x^2}{2}\right|_a^b = \frac{b^2-a^2}{2(b-a)} = \frac{b+a}{2}. \quad 18$$

The variance is estimated as $\sigma^2 = E[x^2] - \mu^2$

$$E[x^2] = \int_a^b x^2\frac{1}{b-a}dx = \frac{1}{b-a}\left.\frac{x^3}{3}\right|_a^b = \frac{b^3-a^3}{3(b-a)} == \frac{b^2+ab+a^2}{3}$$

$$\sigma^2 = E(X^2) - \mu^2 = \frac{(b-a)^2}{12} \quad 19$$

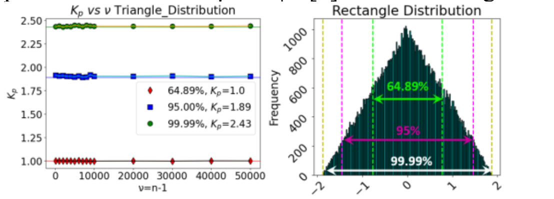
The standard deviation is estimated as

$$\sigma = \sqrt{\sigma^2} = \frac{b-a}{2\sqrt{3}} \quad 20$$

For symetrical distrtibution, $a = b, b - a = 2a = 2b$ and the standerd deviation becomes $\sigma = \frac{a}{\sqrt{3}}$

9. TRIANGLE DISTRIBUTION

If a quantity x is defined by a triangle distribution, the expectation μ_x and standard deviation σ, the value of k_p that produces an interval $\mu_x \pm k_p\sigma$ [1] is shown in figure 6.



Fraction p in percent						
ν	50	64.89	90	95	96.69	99.99
∞	0.719573	1.000	1.665737	1.894298	2.000	2.429255

Figure 6. Confidence intervals and levels in Triangle distribution.

The mean can be estimated as equation18. The variance and the standatd deviation are $\frac{(b-a)^2}{24}$ and $\frac{b-a}{2\sqrt{6}}$ respectively. For symetrical distribution, $a = b, b - a = 2a = 2b$ and the standerd deviation becomes $\frac{a}{\sqrt{6}}$

10. EXPANDED UNCERTAINTY

SASO-UM is exporting report contains three confidence levels and intervals, the expanded unceratinty is expressed as $Yy \pm ku_c(y)$ with confidence interval $y - ku_c(y) \leq y \leq y - ku_c(y)$ and confidence levels at 68%, 95% and 99%

IV. INPUT STAGE

The front of the application is a simple data entry form, as shown in Figure 7. It begins with the model function for the measurement process, which should be written in Pythonic mathematical syntax [1]. The variables included in the model function are counted to generate (Number of Model Function Variables) × 7 cells. Each row describes one variable, with 7 columns representing the following details: variable symbol, unit, mean, standard deviation (or standard uncertainty), type of distribution, source type, and degree of freedom. The distribution dropdown list includes the options: Normal, U-Shape, Rectangle, Triangle, Quadratic, Log-Normal, and Rayleigh. If the variables are correlated with each other (as per Equation 13), the "Generate Matrix" button is used. The user is able to generate a matrix of size n × (Number of Model Function Variables), where n is the number of measurements for those variables. An example is provided in the validation section.

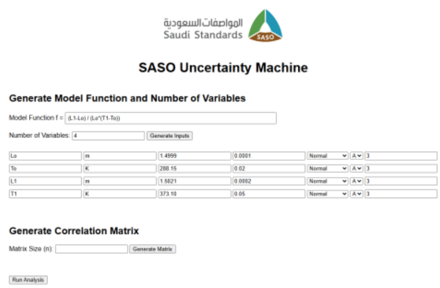


Figure 7. Front page of SASO-UM Application.

V. PROCESSING STAGE

The data are collected from the Input-Stage as a JSON file and posted to FastAPI (Application Programming Interface). The data are then directed to the Python script, as illustrated in the data pipeline in Figure 8.a. After completing the mathematical calculations and statistical analysis, the script exports four types of data, as shown in Figure 8.b.

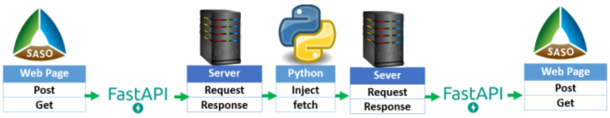


Figure 8-a. Data pipeline

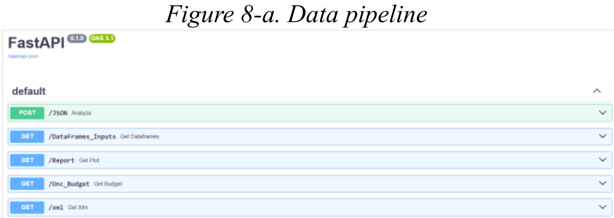


Figure 8-b. Post and Get data in FastAPI

VI. OUTPUT STAGE

In this section, we will discuss one of the four outputs mentioned earlier: the statistical report. The statistical report consists of seven tables and a plotted graph, providing a detailed explanation for the user about the internal workings of the ML algorithm. It starts with an introduction to the model function and variables and concludes with a table detailing the uncertainty budget.

The first table presents the sensitivity coefficients, including the symbol of the partial derivative, its derivative expression, and its computed value. The second table addresses uncertainty Type A, which follows the usual format of an uncertainty budget. The third table describes the model function, while the fourth table outlines uncertainty Type B. The fourth table will display zeros if the user inputs all data entry variables as Type A.

Table 6 combines the uncertainties, and the coverage value (K) is calculated based on the effective degrees of freedom at different confidence levels. The statistical report concludes by plotting the confidence interval as a normal distribution, centered on the mean, figure 9.

VII. SASO-UM VALIDATION

To judge the performance of the machine, it would be better to apply the same examples and numeric that was mentioned in JCGM 100 then compare the output results from API with JCGM-100 text and NIST Uncertainty Machine [15]

1. RELIABILITY OF STANDARD ERROR (UNCERTAINTY OF UNCERTAINTY)

The reliability of the standard error, often referred to as the "uncertainty of uncertainty," is a critical aspect of evaluating measurement processes. It reflects the confidence in the calculated uncertainties and ensures that the reported values are not only precise but also accurate representations of the underlying variability. The close alignment of these data points, as shown in Figures 10 and 11, highlights strong agreement across different methodologies. Additionally, the percentage values decrease with larger sample sizes, effectively illustrating that larger samples reduce uncertainty, leading to more reliable statistical measurements, as demonstrated in Equations 21 and 22.

$$\frac{\sigma[s(\bar{q})]}{[\sigma(\bar{q})]} = \frac{1}{\sqrt{2(n-1)}}\ (approximation) \qquad 21$$

$$\frac{\sigma[s(\bar{q})]}{[\sigma(\bar{q})]} = \frac{\sqrt{V\left(\frac{s}{\sqrt{n}}\right)}}{E\left(\frac{s}{\sqrt{n}}\right)} \qquad 22$$

Sensitivity Coefficients

	Sensitivity_Coeff	Expresion	Value	StD
Target	∂f/∂Lo	−1/(Lo*(T1−To))−(L1−Lo)/(Lo**2*(T1−To))	-0.00785979	0.0001
Target	∂f/∂To	(L1−Lo)/(Lo*(T1−To)**2)	2.03251e-07	0.02
Target	∂f/∂L1	1/(Lo*(T1−To))	0.00784828	0.0002
Target	∂f/∂T1	−(L1−Lo)/(Lo*(T1−To)**2)	-2.03251e-07	0.05

Uncertainty Type A

	Unc. Sources	Type	Unit	Distribution	Devisor	Degree of Freedom	Standard Unc. u_i	Sensitivity Coeff. c_i	c_i*u_i
Target	Lo	A	m	Normal	1	3	0.0001	-7.85979e-3	-7.8598e-7
Target	To	A	K	Normal	1	3	0.02	2.03251e-7	4.0650e-9
Target	L1	A	m	Normal	1	3	0.0002	7.84828e-3	1.5697e-6
Target	T1	A	K	Normal	1	3	0.05	-2.03251e-7	-1.0163e-8

Model Function

	Mean	Standard Uncertainty	Model_Function	Effective_dof
Target	1.7266208957779672e-05	1.75547792597546e-06	1.7266208957779672e-05 ± 1.7555e-06	10

Uncertainty Type B

	Unc. Sources	Type	Unit	Distribution	Devisor	Degree of Freedom	Standard Unc. u_i	Sensitivity Coeff. c_i	c_i*u_i
Target	0	0	0	0	0	0	0	0	0

Combined Uncertainty

	Mean	Standard Uncertainty_Type_A	Standard Uncertainty_Type_B	Combined Uncertainty	Expanded Uncertainty
Target	1.7266208957779672e-05	1.75547792597546e-06	0.0	1.75547792597546e-06	3.51095585195092e-06

Coverage Factor

	68%	90%	95.45%	99%
Target	1.0464226104979557	1.8124611228107335	2.2281388519649385	3.169272667175838

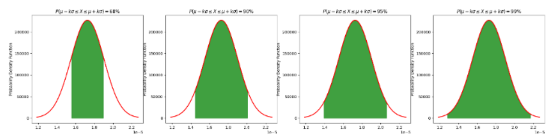


Figure 9. Statistical Report

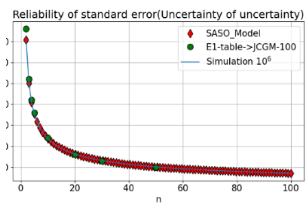


Figure 10. Reliability vs n

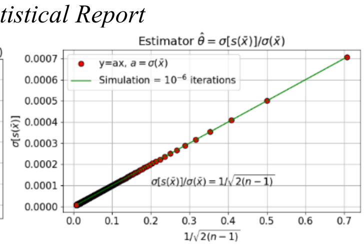


Figure 11. Reliability vs $\frac{1}{\sqrt{2(n-1)}}$

2. SIMULTANEOUS RESISTANCE AND REACTANCE MEASUREMENT

In Example H.2 of the GUM, the measurement model for the resistance of an element of an electrical circuit is $R = \frac{V}{I}\cos\emptyset$.The inputs data and output statistical report are described in detailed in figures 12. The example here is includes correlated parameter, so we generate 5 x 3 matrix (three variables with five observations as given by GUM)

Sensitivity Coefficients

	Sensitivity_Coeff	Expresion	Value	StD	ci*ui	mul_ciui*	corr	corr_fact
Target	af/av	cos(phi)/i	25.5515	0.0032	0.08176480000000001	-0.005046436376488001	-0.3553112198175119	0.0017930554646614163
Target	af/ai	− v * cos(phi)/i * * 2	-6496.73	9.5e-06	-0.061718935	0.010176542027208751	-0.6451112176892568	-0.006565001419038536
Target	af/aphi	− v * sin(phi)/i	-219.847	0.00075	-0.16488525	-0.013481809489200003	0.8576242108399617	-0.011562326223869858

Uncertainty Type A

	Unc. Sources	Type	Unit	Distribution	Devisor	Degree of Freedom	Standard Unc. u_i	Sensitivity Coeff. c_i	$c_i * u_i$
Target	v	A	Volt	Normal	1	4	0.0032	2.55515e+1	0.081765
Target	i	A	Amper	Normal	1	4	9.5e-06	-6.49673e+3	-0.061719
Target	phi	A	Rad	Normal	1	4	0.00075	-2.19847e+2	-0.16489

Model Function

	Mean	Standard Uncertainty	Model_Function	Effective_dof
Target	127.73216992810208	0.07080473690116203	127.73216992810208 ± 7.0805e-02	10

Uncertainty Type B

	Unc. Sources	Type	Unit	Distribution	Devisor	Degree of Freedom	Standard Unc. u_i	Sensitivity Coeff. c_i	$c_i * u_i$
Target	0	0	0	0	0	0	0	0	0

Combined Uncertainty

	Mean	Standard Uncertainty_Type_A	Standard Uncertainty_Type_B	Combined Uncertainty	Expanded Uncertainty
Target	127.73216992810208	0.07080473690116203	0.0	0.07080473690116203	0.14160947380232405

Coverage Factor

	68%	90%	95.45%	99%
Target	1.0464226104979557	1.8124611228107335	2.2281388519649385	3.169272667175838

Figure 12. Statistical Report of H.2

The comparison between the GUM, SASO and NIST machines yielded values of $50000838\ nm \pm 32\ nm$, $50000838\ \pm 31.71\ nm$ and $50000838\ \pm 31.7\ nm$ respectively.

3. DENSITY MEASUREMENT

In the following example, the experiment was carried out at NMCC SASO using regular xls file. The model function is

$$\rho_L = \frac{\{\rho_T[1+\beta(T_T-T_0)] - \rho_{a2}\}(\alpha O_2 + \Gamma_L/g)}{\alpha O_2 - \alpha O_3 + \frac{\Gamma_L}{g} + m_s - V_s\rho_T[1+\beta_S(T_s-T_0)]} + \rho_{a2}$$

The density measurements by xls file were 0.702182 gm/cm^3 with expanded uncertainty 7.49 E-05, SASO uncertainty machine gives as the following figure 13.

Model Function

	Mean	Standard Uncertainty	Model_Function	Effective_dof
Target	0.7021816775668897	7.438740513328605e-05	0.7021816775668897 ± 7.4387e-05	15

Figure 13. Density measurements by SASO-UM

CONCLUSION

A web-based application has been developed to interact with JCGM-100:2008. The SASO team has automated the standards to ensure simplicity of use, helping all users determine, evaluate, and build their own uncertainty budgets with ease. The architecture of the SASO machine is based on a decision tree algorithm, trained continuously for 112 days to achieve a robust model with high accuracy. The application was built using the FastAPI framework, like the one used by BIPM KCDB [16]. The machine has been validated using examples from JCGM-100 to compare the obtained results against the standard and the NIST machine. As the next step soon, the XML extension will be linked with the DCC, marking an important milestone in digital transformation.

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