

SENSITIVITY ANALYSIS IN METROLOGY: STUDY AND COMPARISON ON DIFFERENT INDICES FOR MEASUREMENT UNCERTAINTY

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Sensitivity analysis is an important part of metrology, particularly for the evaluation of measurement uncertainties. It enables the metrologist to have a better knowledge of the measurement procedure and to improve it. A tool for sensitivity analysis is developed in the Guide for the evaluation of Uncertainty in Measurement (GUM) [1]. Supplement 1 to the GUM [2] that deals with Monte Carlo Methods (MCM) provides a similar sensitivity index known as “One At a Time” (OAT). Other sensitivity indices have been developed, but have not yet been used in metrology so far. In this paper, we put forward four indices and we compare them by means of metrological applications. We particularly focus on the Sobol indices [3], based on the evaluation of conditional variances. In order to compare the performance of these indices, we have chosen two examples, different from a mathematical point of view. The first example is the mass calibration example, mentioned in Supplement 1 to the GUM ([2], §9.3). It highlights the relevance of Sobol index to estimate interaction effects. The second example is based on Ishigami function, a non-monotonic function, ([3], §2.9.3). It leads to the conclusion that when the model is non-monotonic, indices based on partial derivatives and SRRC give wrong results, according to the importance of each input quantity.

1. Introduction to Sensitivity Analysis

Sensitivity analysis is a wide topic that has different interpretations regarding the scientific community (Statistics, numerical analysis...). In the uncertainty framework, sensitivity analysis is considered as Factor’s prioritization. The aim is then to identify the input quantities X_i that impact the most the variance of the output quantity Y from a quantitative point of view. It enables the metrologist to have a better knowledge of the measurement procedure and to improve it. Scientific literature and guides for uncertainty provide different indices S_i that are interesting to study in the metrologist context to identify the most relevant ones.

2. Sensitivity Analysis Indices

2.1. Partial Derivative Approach - GUM

According to the GUM approach, the sensitivity indices are based on the partial derivatives that have been calculated when applying the law of propagation of uncertainty (LPU).

$$S_i = \frac{\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i)}{u^2(y)} \quad (1)$$

These indices are the contributory uncertainties of the input quantities to the variance of the measurand in the linear case with independent input quantities.

2.2. “One At a Time” Index – GUM S1

The GUM-S1 (Appendix B) only suggests a “One At a Time” method to estimate sensitivity indices for a Monte Carlo method. The principle consists in holding all input quantities but one fixed at their best estimate while performing MCM. This provides the PDF for the output quantity having just that input quantity as a variable.

It can be seen as a generalization of the partial derivative approach adapted to Monte Carlo Method, where:

- $c_i = \frac{u_i(y)}{u(x_i)}$ is the sensitivity coefficient with $u_i^2(y)$ is the variance of the measurand when all input quantities but X_i are fixed.
- $c_i^2 u^2(x_i)$ is the contribution to the variance
- $S_i = \frac{u_i^2(y)}{u^2(y)}$ is the ratio in the uncertainty budget

These indices are very intuitive. They are computed next to the propagation step and imply N more trials for Monte Carlo simulations for each sensitivity index to estimate.

2.3. Rank Correlation

In the case of a monotonic but nonlinear model, the Standardized Rank Regression Coefficient can be used as a sensitivity index:

$$SRRC(r_x; r_y) = \frac{\sum_{i=1}^n (r_{xi} - \bar{r}_x)(r_{yi} - \bar{r}_y)}{\sqrt{\sum_{i=1}^n (r_{xi} - \bar{r}_x)^2 \sum_{i=1}^n (r_{yi} - \bar{r}_y)^2}} \quad (2)$$

where r_x and r_y are respectively the rank vectors of the data X and Y .

We used the normalized indices in order to assess the relative contribution of X_i :

$$S_i = \frac{SRRC_i^2}{\sum_i SRRC_i^2} \quad (3)$$

These coefficients are easy to compute within Monte Carlo method and provide sensitivity indices simultaneously as the propagation step.

2.4. Variance Based Method - Sobol Indices

2.4.1. Definitions

Sobol [4] indices rely on a decomposition of the variance of the output quantity into terms of increasing dimensionality. These terms are the variances of the conditional expectation of Y (conditionally to X_i), suitable measures of the importance of X_i .

$$V(Y) = V(E[Y|X_i]) + E[V(Y|X_i)] \quad (4)$$

$$V_i = V(E[Y|X_i]), \quad V_{ij} = V(E[Y|X_i, X_j]) - V_i - V_j,$$

$$\dots, \quad V_{1\dots p} = V(Y) - \sum_{i=1}^p V_i - V_j - V_k$$

First order Sobol indices measure the main effects of the variables X_i :

$$S_i = \frac{V(E[Y|X_i])}{V(Y)} \quad (5)$$

Second order Sobol indices measure the interaction effects of the quantities X_i and X_j :

$$S_{ij} = \frac{V_{ij}}{V(Y)} \quad (6)$$

One important property is that the sum of all the indices is equal to one.

2.4.2. Estimation

The estimation of Sobol indices is based on two M -sample of the input quantities $X_i^{(1)}$ and $X_i^{(2)}$, where M is the number of Monte Carlo trials. For instance, first order Sobol indices are estimated according to:

$$\hat{S}_i = \frac{1}{M} \sum_{k=1}^M f\left(X_{k,1}^{(1)}, \dots, X_{k,p}^{(1)}\right) f\left(X_{k,1}^{(2)}, \dots, X_{k,i-1}^{(2)}, X_{k,i}^{(1)}, X_{k,i+1}^{(2)}, \dots, X_{k,p}^{(2)}\right) \quad (7)$$

Such an estimation has been implemented on both R and Matlab and the dispersion of the estimations has been controlled with bootstrap methods and also with standard deviations on the indices.

3. Examples

3.1. Mass Calibration

We consider the calibration of a weight W as described in GUM S1 [2]:

$$m_w = (mrc - dmrc) \left(1 + (a - 1200000) \left(\frac{1}{rhow} - \frac{1}{rhor} \right) \right) \quad (8)$$

The input quantities are defined as follows:

- a Gaussian distribution with 100 000 mean and 0.05 standard deviation is assigned to mrc (X_1 , mg)
- a Gaussian distribution with 1.234 mean and 0.02 standard deviation is assigned to $dmrc$ (X_2 , mg)
- a uniform distribution between $1.1 \cdot 10^6$ and $1.3 \cdot 10^6$ is assigned to a (X_3 , mg/m^3)
- a uniform distribution between $7 \cdot 10^9$ and $9 \cdot 10^9$ is assigned to $rhow$ (X_4 , mg/m^3)
- a uniform distribution between $7.95 \cdot 10^9$ and $8.05 \cdot 10^9$ is assigned to $rhor$ (X_5 , mg/m^3)

Table 1. Results of sensitivity indices for mass calibration

Variable	LPU 1st order	LPU 2nd order	OAT - GUM S1	Ranks	Sobol
X_1	0.862	0.445	0.437	0.862	0.439
X_2	0.138	0.071	0.070	0.135	0.068
X_3	0.000	0.000	0.000	0.003	0.000
X_4	0.000	0.000	0.000	0	0.000
X_5	0.000	0.000	0.000	0	0.000
Interaction					
X_3 - X_4	-	0.483	-	-	0.489
Interaction					
X_3 - X_5	-	0.001	-	-	0.004

Indices based on the ranks, first order partial derivatives and OAT do not allow estimate the interaction effects. Thereby they lead to an underestimation of the importance of the variables X_3 and X_4 in the uncertainty budget.

3.2. Ishigami Function

This function is a very well known example used in the literature; see [3] to illustrate the importance of the choice of the suitable sensitivity indices.

$$Y = \sin(X_1) + 7(\sin(X_2))^2 + 0.1X_3^4 \sin(X_1) \quad (9)$$

A uniform distribution between $-\pi/10$ and $\pi/10$ is assigned to X_1 , X_2 and X_3 . The calculation of Sobol indices has been implemented with R and Matlab and the quality of the estimation has been controlled with bootstrap methods.

Table 2. Results of sensitivity indices for Ishigami function

Variable	LPU 1st order	OAT	Ranks	Sobol - Matlab	Sobol - R
X_1	1.000	0.448	1	0.312	0.315
X_2	0.000	0.552	0	0.442	0.443
X_3	0.000	0.000	0	0.000	0.000

Interaction X_1 - X_3 : $S_{13} = 0.245$ only available within the variance based decomposition of Sobol. In addition, due to the non-linear and non-monotonic

model, Ranks and LPU 1st order indices do not provide the correct contributions of the input quantities.

4. Conclusion

When performing a MC Method, under the assumptions of linearity or monotony, one should prefer easy to handle indices, OAT and ranks correlation indices. When applying the Sobol's theory, no assumptions are made on the mathematical model of measurement regarding linearity or monotony. It offers then the ideal theoretical background to the problematic of sensitivity analysis in the sense of Factor's prioritization. It allows the computation of interaction effects simultaneously as the propagation of uncertainty. However the computational execution time of the model is a major concern when using complex codes and could be a strong limit to the estimation of the Sobol indices.

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