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Contribution to the sample mean plot for graphical and numerical sensitivity analysis

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ABSTRACT

The contribution to the sample mean plot, originally proposed by Sinclair, is revived and further developed as practical tool for global sensitivity analysis. The potentials of this simple and versatile graphical tool are discussed. Beyond the qualitative assessment provided by this approach, a statistical test is proposed for sensitivity analysis. A case study that simulates the transport of radionuclides through the geosphere from an underground disposal vault containing nuclear waste is considered as a benchmark. The new approach is tested against a very efficient sensitivity analysis method based on state dependent parameter meta-modelling.

1. Introduction

The explicit acknowledgement of uncertainties when trying to understand, predict and control the behaviour of natural and industrial systems is now gaining acceptance and becoming affordable in practice thanks to the tremendous advances in computing capabilities. In the standard probabilistic framework, the uncertain model inputs $X=(X_1,X_2,\dots,X_k)$ and the resulting model outputs $Y=(Y_1,Y_2,\dots,Y_r)$ are treated as random variables characterised by probability distribution functions [1]. Random or quasi-random sampling strategies are adopted in order to select the model inputs and multiple model evaluations (i.e. Monte Carlo simulation) are used for the propagation of this uncertainty. Subsequently, a detailed analysis of the mapping can be carried out using the input samples and related model realisations.

Sensitivity analysis (SA) is the study of how uncertainty in the output of the model can be apportioned to different sources of uncertainty in the model inputs [2]. Ideally uncertainty and sensitivity analysis should be run in tandem (iterative strategy). Graphical methods are important tools to support, guide and interpret the results provided by sensitivity and uncertainty analysis. While bars, tornado graphs or radar charts can be particularly useful to communicate importance measures, box-and-whisker plots are more suitable for the representation of uncertainty analysis results. Valuable information can also be presented in condensed form by the so-called cobweb plots [3], which are able to represent graphically multi-dimensional distributions with a two-dimensional plot. Flexible conditioning capabilities facilitate an extensive insight into particular regions of the mapping and a careful analysis of cobweb plots facilitates the characterisation of dependence and conditional dependence between inputs and outputs. However, for the visualisation of the input–output mapping, the simplest and most widely used plots are the so-called scatterplots. For a given model input X_i and a single-valued model output Y, a scatterplot corresponds to a projection in the (X_i,Y) plane of the sample points defining the (X,Y) hyper-surface. Among the possible extensions, model inputs can be plotted against each other with an intensity ramp corresponding to the values of the model response (matrix of scatterplots), and different colours corresponding to different subsets can be used on a single graph (overlaid scatterplots).

Using the classical version of the scatterplot, although a visual inspection can be seen as an empirical and somehow subjective appraisal of pattern randomness, scatterplots provide rich information on mapping, which the other global SA techniques tend to condense into a few sensitivity indices. It is possible to visualise the values taken by the model response Y across the range of X_i. When a pattern can be observed in the scatterplot, the stronger the pattern, the more important the influence of the corresponding input on the model output. Some techniques referred to as grid-based methods can be used to assess the randomness of the distribution of points across the range divided into bins. Various statistical tests have been developed in order to

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assess common means (CMNs), common distributions or locations (CLs) [4], common medians (CMDs) or statistical independence (SI) (see [5–7] for recent reviews and comparisons). However, as emphasised by [7], it is possible that the violation of statistical test assumptions could be leading to misrankings of input importance. In addition, there is no universal rule for the determination of an appropriate division of the range (i.e definition of the grid).

In the Probabilistic System Assessment Group framework, a research group established by the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency (NEA), Sinclair [8] investigated changes in the mean and in the variance of various output quantities resulting from finite changes in the inputs' uncertainties (e.g., shifts or shrinks of their distributions). An approach was proposed in order to estimate the derivative of the expectation of the analysed model response with respect to the parametrised change of shape. In order to circumvent the difficulties related to discontinuities in the model inputs probability distribution functions, the author suggests to fit a smooth curve to the marginal dependence of the mean of the output on the selected inputs. Although it is not necessary to portray this relation graphically for the adopted approach, the contribution to the sample mean (CSM) plot was recognised as a general tool for SA.

Even before Sinclair, the same type of curves were used by social economists as measures of inequality [9]. In that field, they are known as *Lorenz curves*, associated to the concept of *concentration curve*, and frequently used to compare the situation in different countries or to assess the evolution of the concentration of wealth over time in a given country. In this paper, the CSM plot is revived in the context of SA of computer models. Rather than aggregated data from official statistics, random samples characterising the input–output mapping of mathematical models are analysed. In Section 3, the scope and potential of this generalised approach are discussed; the outcomes are illustrated using the application example presented in Section 2. In Section 4, a permutation-based statistical test is proposed in order to determine whether the behaviour characterised by the CSM plot significantly departs from randomness. Results from numerical experiments are reported and discussed in Section 5; finally, conclusions are drawn in Section 6.

2. Description of the test case

In order to illustrate the potential of the plot proposed by Sinclair [8] and evaluate the reliability of the proposed approach, we consider a model reproducing the behaviour of a radioactive high-level waste repository and the disposed contaminant. The so-called Level E model was used as a benchmark for SA methods [10,11]. In this section, the main features of the model will be described and asymptotic Monte Carlo estimates characterising the behaviour of the model will be reported.

2.1. Level E model for a radioactive high-level waste repository

The model predicts the radiological dose to humans over geological time scales due to the underground migration of radionuclides from a nuclear waste disposal site. The scenario considered in the model tracks the one-dimensional migration of four radionuclides (^{129}I and the chain $^{237}\text{Np}\rightarrow{}^{233}\text{U}\rightarrow{}^{229}\text{Th}$) through two geosphere layers characterised by different hydrogeological properties. The processes being considered in the model are radioactive decay, dispersion, advection and chemical reaction between the migrating nuclides and the porous medium. The repository is represented as a point source. The simulation model includes 12 uncertain inputs, which are listed in Table 1 together with a set of parameters which are assumed constant.

2.2. Characterisation of the model behaviour

The quantity of interest considered in this study is the annual radiological dose due to the four radionuclides. As emphasised in

Table 1
List of model inputs for the Level E.

Notation	Definition	Distribution	Range	Units
T	Containment time	Uniform	$[100, 1000]$	y
k_I	Leach rate for iodine	Log-uniform	$[10^{-3}, 10^{-2}]$	mol/y
k_C	Leach rate for Np chain nuclides	Log-uniform	$[10^{-6}, 10^{-5}]$	mol/y
$V^{(1)}$	Water velocity in geosphere's 1st layer	Log-uniform	$[10^{-3}, 10^{-1}]$	m/y
$L^{(1)}$	Length of geosphere's 1st layer	Uniform	$[100, 500]$	m
$R_I^{(1)}$	Retention factor for I (1st layer)	Uniform	$[1, 5]$	–
$R_C^{(1)}$	Factor to compute retention coefficients for Np chain nuclides (1st layer)	Uniform	$[3, 30]$	–
$V^{(2)}$	Water velocity in geosphere's 2nd layer	Log-uniform	$[10^{-2}, 10^{-1}]$	m/y
$L^{(2)}$	Length of geosphere's 2nd layer	Uniform	$[50, 200]$	m
$R_I^{(2)}$	Retention factor for I (2nd layer)	Uniform	$[1, 5]$	–
$R_C^{(2)}$	Factor to compute retention coefficients for Np chain nuclides (2nd layer)	Uniform	$[3, 30]$	–
W	Stream flow rate	Log-uniform	$[10^5, 10^7]$	m^3/y
C_I^0	Initial inventory for ^{129}I	Constant	100	mol
C_{Np}^0	Initial inventory for ^{237}Np	Constant	1000	mol
C_U^0	Initial inventory for ^{233}U	Constant	100	mol
C_{Th}^0	Initial inventory for ^{229}Th	Constant	1000	mol
w	Water ingestion rate	Constant	0.73	m^3/y
β_I	Ingestion-dose factor for ^{129}I	Constant	56	Sv/mol
β_{Np}	Ingestion-dose factor for ^{237}Np	Constant	6.8×10^3	Sv/mol
β_U	Ingestion-dose factor for ^{233}U	Constant	5.9×10^3	Sv/mol
β_{Th}	Ingestion-dose factor for ^{229}Th	Constant	1.8×10^6	Sv/mol