Title: Introduction: Sensitivity Analysis

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# Introduction: Sensitivity Analysis

#### **Abstract**

Sensitivity analysis provides users of mathematical and simulation models with tools to appreciate the dependency of the model output from model input, and to investigate how important is each model input in determining its output. All application areas are concerned, from theoretical physics to engineering and socio-economics. This introductory paper provides the sensitivity analysis aims and objectives in order to explain the composition of the overall "Sensitivity Analysis" chapter of the Springer Handbook. It also describes the basic principles of sensitivity analysis, some classification grids to understand the application ranges of each method, a useful software package and the notations used in the chapter papers. This section also offers a succinct description of

sensitivity auditing, a new discipline that tests the entire inferential chain including model development, implicit assumptions and normative issues, and which is recommended when the inference provided by the model needs to feed into a regulatory or policy process. For the "Sensitivity Analysis" chapter, in addition to this introduction, nine papers have been written by around twenty scientists coming from universities, research institutes and industries. They cover the most widely used methods for this subject: the deterministic methods as the local sensitivity analysis, the experimental design strategies, the sampling-based and variance-based methods developed from the 1980s and the new importance measures and metamodel-based techniques established and studied since the 2000s. In each paper, toy examples or industrial applications illustrate their relevance and usefulness.

Keywords: Computer Experiments, Uncertainty Analysis, Sensitivity Analysis, Sensitivity Auditing, Risk Assessment, Impact Assessment

#### Introduction

In many fields such as environmental risk assessment, behavior of agronomic systems, structural reliability or operational safety, mathematical models are used for simulation, when experiments are too expensive or impracticable, and for prediction. These computer models are used to make simulations as well as predictions or sensitivity studies. Complex computer models calculate several output values (scalars or functions) that can depend on a high number of input parameters and physical variables. Some of these input parameters and variables may be unknown, unspecified, or defined with a large imprecision range. Inputs include engineering or operating variables, variables that describe field conditions, and variables that include unknown or partially known model

parameters. In this context, the investigation of computer code experiments remains an important challenge.

This computer code exploration process is the main purpose of the Sensitivity Analysis (SA) process. SA allows the study of how uncertainty in the output of a model can be apportioned to different sources of uncertainty in the model input [47]. It may be used to determine the input variables that contribute the most to an output behavior, and the non-influential inputs, or to ascertain some interaction effects within the model. The SA process refers to the computation and analysis of the so-called sensitivity or importance indices of the input variables with respect to a given quantity of interest in the model output. Importance measures of each uncertain input variable on the response variability provide a deeper understanding of the modeling in order to reduce the response uncertainties in the most effective way [47], [25], [18]. For instance, put more efforts on knowledge of influential inputs will reduce their uncertainties. The underlying goals for SA are model calibration, model validation and assisting with the decision making process. This chapter then addresses engineers, researchers and students who wish to apply SA techniques in any scientific field (physics, engineering, socio-economics, environmental studies, astronomy, etc.).

Several textbooks and specialist works [47], [49], [2], [9], [10], [8] have covered most of the classic SA methods and objectives. In parallel, a scientific conference called SAMO ("Sensitivity Analysis on Model Output") has been organized every three years since 1995 and extensively covers SA related subjects. Works presented at the different SAMO conferences can be found in their proceedings and several special issues published in international journals (mainly in "Reliability Engineering and System Safety").

The main goal of this chapter is to provide an overview of classic and advanced SA methods, as none of the referenced works have reported all the concepts and methods in one single document. Researchers and engineers will find this document to be an up-to-date report on SA as it currently stands, although this scientific field remains very active in terms of new developments. The present chapter is only a snapshot in time and only covers well-established methods.

The next section of this paper provides the SA basic principles. It has been argued [50] that sensitivity analysis, mandated by existing guidelines as a good practice to use in conjunction with mathematical modeling, is insufficient to ensure quality in the treatment of scientific uncertainty for policy purposes. For this reason, in the third section, a process for the sensitivity auditing of models in a policy context is discussed, by providing seven rules that extend the use of SA. Next, the SA methods contained in the chapter are described using a classication grid, together with specialized software packages. The main mathematical notations of the chapter papers are also given. The concluding section lists some important recent research works that could not be covered in the present chapter.

#### Basic principles of sensitivity analysis

The first historical approach to SA is known as the local approach. The impact of small input perturbations on the model output is studied. These small perturbations occur around nominal values (the mean of a random variable, for instance). This deterministic approach consists of calculating or estimating the partial derivatives of the model at a specific point of the input variable space [56]. The use of adjoint-based methods allows models with a large number of input variables to be processed. Such approaches are particularly well-suited to resolving uncertainty analysis, SA and data assimilation problems in environmental systems such as those in climatology, oceanography, hydrogeology, etc. [2], [39], [3].

To overcome the limitations of local methods (linearity and normality assumptions, local variations), another class of methods has been developed in a statistical framework. In contrast to local SA, which studies how small variations in inputs around a given value change the value of the output, global sensitivity analysis ("global" in opposition to the local analysis) does not distinguish any initial set of model input values, but considers the numerical model in the entire domain of possible input parameter variations [47]. Thus, the global SA is an instrument used to study a mathematical model as a whole rather than one of its solution around parameters specific values.

Numerical model users and modelers have shown high interest in these global tools that take full advantage of the development of computer materials and numerical methods (see Helton [17] and de Rocquigny et al [8] for industrial and environmental applications). Saltelli et al [48] emphasized the need to specify clearly the objectives of a study before making an SA. These objectives may include:

- The factors prioritization setting, which aims at identifying the most important factors. The most important factor is the one that, if fixed, would lead to the greatest reduction in the uncertainty of the output;
- The factors fixing setting, which aims at reducing the number of uncertain inputs by fixing unimportant factors. Unimportant factors are the ones that, if fixed to any value, would not lead to a significant reduction of the output uncertainty. This is often a preliminary step before the calibration of model inputs using some available information (real output observations, constraints, etc.);
- The variance cutting setting, which can be a part of a risk assessment study.

  Its aim is to reduce the output uncertainty from its initial value to a lower pre-established threshold value;
- The factors mapping setting, which aims at identifying the important inputs in a specific domain of the output values.

While in the deterministic framework, the model is analyzed at specific values for inputs, and the space of uncertain inputs may be explored in statistical approaches. In the simplest formulation of the probabilistic framework, the inputs are considered as random variables  $\mathbf{X} = (X_1, \dots, X_d) \in \mathbb{R}^d$ . The random vector  $\mathbf{X}$  has a known joint distribution, which reflects the uncertainty of the inputs. The computer code (also called "model") is denoted  $G(\cdot)$ , and for a scalar output  $Y \in \mathbb{R}$ , the model formula writes

$$Y = G(\mathbf{X}) . (1)$$

Model function G can represent a system of differential equations, a program code, or any other correspondence between X and Y values that can be calculated for a finite period of time. Therefore, the model output Y is also a random variable whose distribution is unknown (increasing the knowledge of it is the goal of the uncertainty propagation process). SA statistical methods consist of techniques stemming from the design of experiments theory (in the case of a large number of inputs), the Monte Carlo techniques (to obtain precise sensitivity results) and modern statistical learning methods (for complex CPU time-consuming numerical models).

## Sensitivity auditing

It may happen that a sensitivity analysis of a model-based study is meant to underpin an inference, and to certify its robustness, in a context where the inference feeds into a policy or decision making process. In these cases the framing of the analysis itself, its institutional context, and the motivations of its author may become a matter of great importance, and a pure SA - with its emphasis on parametric uncertainty - may be seen as insufficient. The emphasis on the framing may derive inter-alia from the relevance of the policy study to different constituencies that are characterized by different norms and values, and hence by a different story about 'what the problem is' and foremost

about 'who is telling the story'. Most often the framing includes more or less implicit assumptions, which could be political (e.g. which group needs to be protected) all the way to technical (e.g. which variable can be treated as a constant).

These concerns about how the story is told and who tells it are all the more urgent in a climate as today's where science's own quality assurance criteria are under scrutiny [20] and the explosion of the blogosphere invites more open debates on the scientific basis of policy decisions [36]. The Economist, a weekly magazine, has entered the fray by commenting on the poor state of current scientific practices and devoting its cover to "How Science goes wrong". It adds that, 'The false trails laid down by shoddy research are an unforgivable barrier to understanding' (The Economist [54], p. 11). Among the possible causes of such a predicament is a process of hybridization [27] of fact and values, and of public and private institutions and actors. Thus the classical division of roles among science, providing tested fact, and policy, providing legitimized norms, becomes arduous to maintain.

As an additional difficulty, according to Grundmann [16], 'One might suspect that the more knowledge is produced in hybrid arrangements, the more the protagonists will insist on the integrity, even veracity of their findings'.

In order to take these concerns into due consideration the instruments of SA have been extended to provide an assessment of the entire knowledge and model generating process. This approach has been called sensitivity auditing. It takes inspiration from NUSAP, a method used to qualify the worth of quantitative information with the generation of 'Pedigrees' of numbers [15],[57]. Likewise, sensitivity auditing has been developed to provide pedigrees of models and model-based inferences [50], [44], [45].

Sensitivity auditing has been especially designed for an adversarial context, where not only the nature of the evidence, but also the degree of certainty and uncer-

tainty associated to the evidence, will be the subject of partisan interests. Sensitivity auditing is structured along a set of seven rules/imperatives:

- 1. Check against the rhetorical use of mathematical modeling. Question addressed: is the model being used to elucidate or to obfuscate?;
- 2. Adopt an 'assumption hunting' attitude. Question addressed: what was 'assumed out'? What are the tacit, pre-analytical, possibly normative assumptions underlying the analysis?;
- 3. Detect Garbage In Garbage Out (GIGO). Issue addressed: artificial deflation of uncertainty operated in order to achieve a desired inference at a desired level of confidence. Also works also in reverse with artificial inflation of uncertainties, e.g. to deter regulation;
- 4. Find sensitive assumptions before they find you. Issue addressed: anticipate criticism by doing careful homework via sensitivity and uncertainty analyses before publishing results.
- 5. Aim for transparency. Issue addressed: stakeholders should be able to make sense of, and possibly replicate, the results of the analysis;
- 6. Do the right sums, which is more important than 'Do the sums right'. Issue addressed: is the viewpoint of a relevant stakeholder being neglected? Who decided that there was a problem and what the problem was?
- 7. Focus the analysis on the key question answered by the model, exploring the entire space of the assumptions holistically. Issue addressed: don't perform perfunctory analyses that just 'scratch the surface' of the system's potential uncertainties.

The first rule looks at the instrumental use of mathematical modeling to advance one's agenda. This use is called rhetorical, or strategic, like the use of Latin by the elites and clergy before the Reformation. At times the use of models is driven a simple pursuit of profit; according to Stiglitz [52], this was the case for the modelers

'pricing' the derivatives at the root of the sub-prime mortgages crisis:

[...] Part of the agenda of computer models was to maximize the fraction of, say, a lousy sub-prime mortgage that could get an AAA rating, then an AA rating, and so forth, [...] This was called rating at the margin, and the solution was still more complexity, p. 161.

At times this use of models can be called 'ritual', in the sense that it offers a false sense of reassurance. An example is Fisher [11] (quoting Szenberg [53]):

Kenneth Arrow, one of the most notable Nobel Laureates in economics, has his own perspective on forecasting. During World War II, he served as a weather officer in the U.S. Army Air Corps and worked with a team charged with the particularly difficult task of producing month-ahead weather forecasts. As Arrow and his team reviewed these predictions, they confirmed statistically what you and I might just as easily have guessed: The Corps' weather forecasts were no more useful than random rolls of a die. Understandably, the forecasters asked to be relieved of this seemingly futile duty. Arrow's recollection of his superiors' response was priceless: "The commanding general is well aware that the forecasts are no good. However, he needs them for planning purposes" Szenberg [53].

The second rule about 'assumption hunting' is a reminder to look for what was assumed when the model was originally framed. Modes are full of *caeteris paribus* assumptions, meaning that e.g. in economics the model can predict the result of a shock to a given set of equations assuming all the rest all other input variables and inputs remains equal, but in real life *caeteris* are never *paribus*, meaning by this that variables tend to be linked with one another, so that they can hardly change in isolation.

Furthermore at times the assumption made by modelers do not to withstand scrutiny. A good example of assumption hunting is from John Kay [23], where the

author takes issue with modeling used in transport policy. This author discovered that among the input values assumed (and hence fixed) in the model was 'average car occupancy rates, differentiated by time of day, in 2035'. The point is that such assumptions are very difficult to justify. This comment was published in the Financial Times (where John Kay is a columnist) showing that at present times controversies that could be called epistemological evade the confines of academia and populate the media.

Rule three is about artificially exaggerating or playing down uncertainties wherever convenient. The tobacco lobbies exaggerated the uncertainties about the health effects of smoking according to Oreskes and Conway [38], while advocates of the death penalty played down the uncertainties in the negative relations between capital punishment and crime rate [28]. Clearly the latter wanted the policy, in this case the death penalty, and were interested in showing that the supporting evidence was robust. In the former case the lobbies did not want regulation (e.g. bans on tobacco smoking in public places) and were hence interested in amplifying the uncertainty in the smoking-health effect causality relationship.

Rule four is about 'confessing' uncertainties before going public with the analysis. This rule is also one of the commandments of applied econometrics according to Kennedy [24]: 'Thou shall confess in the presence of sensitivity. Corollary: Thou shall anticipate criticism'. According to this rule a sensitivity analysis should be performed before the result of a modeling study are published. There are many good reasons for doing this, one being that a carefully performed sensitivity analysis often uncovers plain coding mistakes or model inadequacies. The other is that most often than not the analysis reveal uncertainties that are larger than those anticipated by the model developers. Econometrician Edward Leamer in discussing this [28] argues that 'One reason these methods are rarely used is their honesty seems destructive'. In Saltelli and

dHombres [43], the negative consequences of doing a sensitivity analysis a-posteriori are discussed. The case is the first review of the cost of offsetting climate change done by Nicholas Stern of the London School of Economics (the so called Stern Review) which was criticized by William Nordhaus, of the University of Yale, on the basis of large sensitivity of the estimates upon the discount factors employed by Stern. Sterns own sensitivity analysis, published as an annex to the review, revealed according to the authors in [28] that while the discount factors were not the only important factors determining the cost estimate, the estimates were indeed very uncertain.

Rule five is about presenting the results of the modeling study in a transparent fashion. Both rules originate from the practice of impact assessment, where a modeling study presented without a proper SA, or as originating from a model which is in fact a black box, may end up being rejected by stakeholders [43]. Both rules four and five suggest that reproducibility may be a condition for transparency and that this latter may be a condition for legitimacy. This debate on Sciences transparency is very much alive in the US, in the dialectic relationship between the US Environmental Protection Agency (EPA) and the US Congress (especially the Republican Party) which objects to EPAs regulations on the basis that these are based on 'secret science'.

Rule six, about doing the right sum, is not far from the 'assumptions hunting' rule; it is just more general. It deals with the fact that often an analyst is set to work on an analysis arbitrarily framed to the advantage of a party. Sometime this comes via the choice of the discipline selected to do the analysis. Thus an environmental impact problem may be framed through the lenses of economics, and presented as a cost benefit or risk analysis, while the issue has little to do with costs or benefits or risks and a lot to do with profits, controls, and norms. An example is in Marris et al [35] on the issue of GMOs, mostly presented in the public discourse as a food safety issue while the spectrum of concerns of GMO opponents - including lay citizens - appears broader.

According to Winner [58] (p. 138-163), ecologists should not be led into the trap of arguing about the 'safety' of a technology after the technology has been introduced. They should instead question the broader power, policy and profit implications of that introduction and its desirability.

Rule seven is about avoiding perfunctory sensitivity analyses. As discussed in Saltelli and Annoni [42], an SA where each uncertain input is moved at a time while leaving all other inputs fixed is perfunctory. A true SA should make an honest effort at activating all uncertainties simultaneously, leaving the model free to display its full nonlinear and possibly non-additive behaviour. A similar point is made in Sam L. Savage's book 'The flaw of averages' [51].

In conclusion, these rules are meant to help an analyst to anticipate criticism. In drafting these rules the authors in [50], [44], [45] have tried to put themselves in the shoes of a modeler also based on their own experience and tried to imagine a model-based inference feeding into an impact assessment. What questions and objections may be received by the modeler? Here is a possible list:

- "You treated X as a constant when we know it is uncertain by at least 30%"
- "It would be sufficient for a 5% error in X to make your statement about Z fragile"
- "Your model is but one of the plausible models you neglected model uncertainty"
- "You have instrumentally maximized your level of confidence in the results"
- "Your model is a black box why should I trust your results?"
- "You have artificially inflated the uncertainty"
- "Your framing is not socially robust"
- "You are answering the wrong question"

The reader may easily check that a careful go through the sensitivity auditing checklist should provide ammunition to anticipate objections of this nature.

Sensitivity auditing can then be seen as a user guide to criticize the model-based studies and SA is a part of this guide. In the rest of this chapter, SA will be only discussed. In the following section, the SA methods contained in the chapter are described and positioned with respect to each other.

#### Methods contained in the chapter

Three families of methods are described in this chapter, based on which is the objective of the analysis:

- 1. First, screening techniques aim to a qualitative ranking of input factors at minimal cost in the number of model evaluations. Paper 2 (see Variational Methods, written by Maëlle Nodet and Arthur Vidard) introduces the local SA based on variational methods, while Paper 3 (see Design of Experiments for Screening, written by Sue Lewis and David Woods) explains the use of the design of experiments techniques, including some designs specifically developed in the context of computer experiments;
- 2. Second, sampling based methods are described. Paper 4 (see Sampling-based Procedures for Uncertainty and Sensitivity Analysis, written by Jon Helton, Cédric Salaberry and Curtis Storlie) shows how, from an initial sample of input and output values, quantitative sensitivity indices can be obtained by various methods (correlation, multiple linear regression, statistical tests, etc.). In Paper 5 (see Variance-based Sensitivity Analysis: Theory and Estimation Algorithms, written by Clémentine Prieur and Stefano Tarantola), the definitions of the variance-based importance measures (the so-called Sobol' indices) and the algorithms to calculate them will be

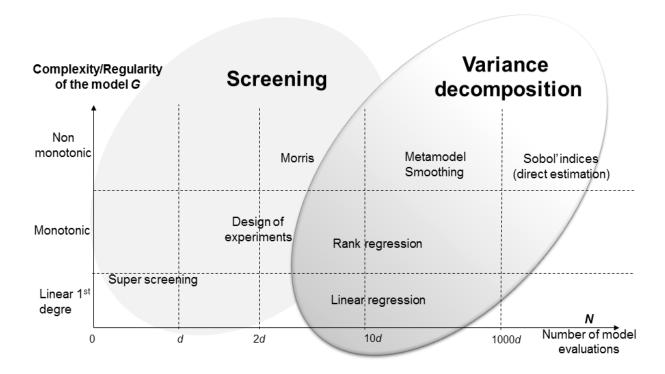
detailed. In Paper 6 (see Derivative based Global Sensitivity Measures, written by Sergeï Kucherenko and Bertrand Iooss), the global SA based on derivatives sample (the DGSM indices) are explained, while in Paper 7 (see Moment Independence Importance Measures and a Common Rationale, written by Emmanuele Borgonovo and Bertrand Iooss), the moment independent and reliability importance measures are described.

3. Third, in depth exploration of model behavior with respect to inputs variation can be carried out. Paper 8 (see Metamodel-based Sensitivity Analysis: Polynomial Chaos and Gaussian Process, written by Loïc Le Gratiet, Bruno Sudret and Stefano Marelli) includes recent advances made in the modeling of computer experiments. In fact, a metamodel is used as a surrogate model of the computer model with any SA techniques, when the computer model is too CPU time-consuming to allow a sufficient number of model calculations. Special attention is paid to two of the most popular metamodels: the polynomial chaos expansion and the Gaussian process model, for which the Sobol' indices can be efficiently obtained. Finally, Paper 9 (see Sensitivity Analysis of Spatial and/or Temporal Phenomena, written by Amandine Marrel, Nathalie Saint Geours and Matthias De Lozzo) extends the SA tools in the context of temporal and/or spatial phenomena.

This chapter is concluded by a discussion in Paper 10 (see Measuring the Importance of Variables in Composite Indicators, written by William Becker, Paolo Paruolo, Michaela Saisana and Andrea Saltelli) of the use of SA in analyzing composite indicators.

All the SA techniques explained in this chapter present a trade-off between the number of model computations required and the assumed model complexity. Figure 1 proposes a coarse classification of the method families described before. This figure shows how to place a method depending on its required number of computations and its underlying hypothesis on the complexity of the G model. For example "Non-

monotonic" means that the method can be applied to non monotonic models, as of course to monotonic and linear ones. A distinction is made between screening techniques (identification of non-influential variables among a large number of variables) and more precise variance-based quantitative methods.

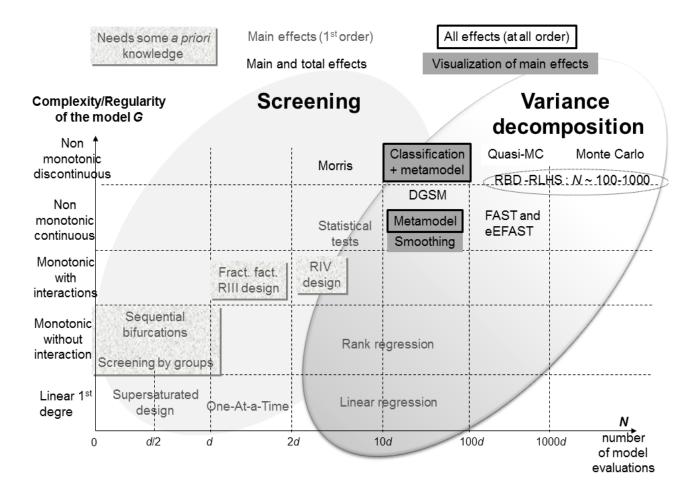


**Fig. 1.** Classification of SA methods in terms of required number of model evaluations and model complexity.

With the same axes than the previous figure, Figure 2 proposes a more accurate classification of the classic global SA methods, most of them being explained in the chapter papers. Note that this classification is not exhaustive and does not take into account potential improvements made to various methods. Overall, this classification tool has several levels of reading:

 positioning methods based on their cost in terms of the number of model calls (which linearly depends in the number of inputs for most of the methods, except for RBD and RLHS),

- positioning methods based on assumptions about model complexity and regularity,
- distinguishing the type of information provided by each method,
- identifying methods which require some prior knowledge about the model behavior.



**Fig. 2.** Classification of SA methods in terms of required number of model evaluations and model complexity.

Each of these techniques corresponds to different categories of problems met in practice. One should use the simplest method that is adapted to the study's objectives, the number of numerical model evaluations that can be performed, and the prior knowledge on the model's regularity. Each sensitivity analysis should include a validation step, which helps to understand if another method should be applied, if the number if model evaluations should be increased, and so on. Based on the characteristics of the different methods, some authors [8], [21] have proposed decision trees to help the practitioner to choose the most appropriate method for their problem and model.

#### **Specialized R software packages**

From a practical point of view, the application of SA methods by researchers, engineers, end-users and students is conditioned by the availability of an easy-to-use software. Several software include some SA methods (see the Software chapter of the Springer Handbook) but only a few are specialized on the SA issues. In this section, the sensitivity package of the R environment is presented [40]. Its development has started since 2006 and the several contributions that this package has received have made it particularly complete. It includes most of the methods presented in the papers of this chapter.

The R software is a powerful tool for knowledge diffusion in the statistical community. The open source and availability have made R the software of choice for many statisticians in education and industry. The characteristics of R are the following:

- R is easy to run and install on main operating systems. It can be efficiently used
  with an old computer, with a single workstation and with one of the most recent
  supercomputer;
- R is a programming language which is interpreted and object-oriented, and which contains vector operators and matrix computation;
- The main drawbacks of R are its virtual memory limits and non-optimized computation times. To overcome these problems, compiled languages as fortran or C are much more efficient, and can be introduced as compiled codes inside R algorithms requiring huge computation time.
- R contains a lot of built-in statistical functions;

- R is extremely well-documented with built-in help system;
- R encourages the collaboration, the discussion forums and the creation of new
  packages by researchers and students. Thousands of packages are made available
  on the CRAN website (http://cran.r-project.org/).

All these benefits highlight the interest to develop specific softwares in R and many packages have been developed on SA. For instance, the FME package contains basic SA and local SA methods (see Variational Methods).

For global SA, The sensitivity package includes a collection of functions for factor screening, sensitivity indices estimation and reliability sensitivity analysis of model outputs. It implements:

- A few screening techniques as the sequential bifurcations and the Morris method (see Design of Experiments for Screening). Note that the R package planor allows to build fractional factorial design (see Design of Experiments for Screening);
- The main sampling-based procedures as linear regression coefficients, partial correlations, rank transformation (see Sampling-based Procedures for Uncertainty and Sensitivity Analysis). Note that the R package CompModSA implements various nonparametric regression procedures for SA (see Sampling-based Procedures for Uncertainty and Sensitivity Analysis and Measuring the Importance of Variables in Composite Indicators);
- The variance-based sensitivity indices (Sobol' indices), by various schemes of the so-called pick-freeze method, the Extended-FAST method and the replicated orthogonal array-based Latin hypercube sample (see Variance-based Sensitivity Analysis: Theory and Estimation Algorithms). The R package fast is fully devoted to the FAST method;
- The Poincaré constants for the Derivative-based Global Sensitivity Measures (DGSM) (see Derivative based Global Sensitivity Measures);

- The sensitivity indices based on Csiszar f-divergence and Hilbert-Schmidt Independence Criterion of Da Veiga [5] (see Moment Independence Importance Measures and a Common Rationale);
- The reliability sensitivity analysis by the Perturbation Law-based Indices (PLI) (see Moment Independence Importance Measures and a Common Rationale);
- The estimation of the Sobol' indices with a Gaussian process metamodel (see Metamodel-based Sensitivity Analysis: Polynomial Chaos and Gaussian Process). the Gaussian process metamodel comes from the R package DiceKriging.

  Note that the R package GPC allows to estimate the Sobol' indices by building a polynomial chaos metamodel (see Metamodel-based Sensitivity Analysis: Polynomial Chaos and Gaussian Process);
- Sobol' indices for multidimensional outputs: Aggregated Sobol' indices and functional (1D) Sobol' indices (see Sensitivity Analysis of Spatial and/or Temporal Phenomena). Note that the R package multisensi is fully devoted to this subject while the R package safi implements new SA methods of models with functional inputs;
- The Distributed Evaluation of Local Sensitivity Analysis (DELSA) described in Rakovec et al [41].

The sensitivity package has been designed to work either models written in R than external models such as heavy computational codes. This is achieved with the input argument model present in all functions of this package. The argument model is expected to be either a function or a predictor (i.e. an object with a predict function such as lm). The model in invoked once for the whole design of experiment. The argument model can be left to NULL. This is referred to as the decoupled approach and used with external computational codes that rarely run on the statistician's computer.

Examples of use of all the sensitivity functions can be found using the R built-in help system.

### Main notations of the chapter

The different papers of this chapter use the same mathematical notations, which are summarized below:

 $G(\cdot)$  Numerical model

N, n Sample sizes

d Dimension of an input vector

p Dimension of an output vector

 $\mathbf{x} = (x_1, \dots, x_d)$  Deterministic input vector

 $\mathbf{X} = (X_1, \dots, X_d)$  Random input vector

 $x_i, X_i$  Deterministic and random input variable

 $\mathbf{x}_{\sim i} = \mathbf{x}_{-i} = \mathbf{x}_{\bar{i}} = (X_1, \dots, X_{i-1}, X_{i+1}, \dots, X_d)$ 

 $y, Y \in \mathbb{R}$  Deterministic and random output variable when p = 1

 $f_X(\cdot)$  Density function of a real random variable X

 $F_X(\cdot)$  Distribution function of X

 $\mu_X, \, \sigma_X$  Mean and standard deviation of X

 $x_{\alpha} = q_{\alpha}(X)$   $\alpha$ -quantile of X

V = Var(Y) Total variance of the model output Y

A Subset of indices in the set  $\{1, \ldots, d\}$ 

 $V_A$  Partial variance

 $S_A, S_A^{\text{tot}}$  First order and total Sobol indices of A

#### **Conclusion**

This introductory paper has presented the SA aims and objectives, the SA and sensitivity auditing basic principles, the different methods explained in the chapter papers by positioning them in a classification grid, useful R software packages and the notations used in the chapter papers. All these papers cover the most known methods for the SA subject: the deterministic methods as the local sensitivity analysis, the experimental design strategies, the sampling-based and variance-based methods developed from the 1980s and the new importance measures and metamodel-based techniques established and studied since the 2000s.

However, with such a rich subject, choices had to be made for the different chapter papers and some important omissions are present. For instance, the robust Bayesian analysis [1], [19] is not discussed, while it is nevertheless a great ingredient in the study of the sensitivity of Bayesian answers to assumptions and uncertain calculation inputs.

Due to their very new or incomplete nature, several other SA issues are not discussed in this chapter. For instance, estimating total Sobol' indices at low cost remains a problem of primary importance in many applications (see Saltelli and Annoni [42] for a recent review on the subject). Second-order Sobol indices estimations have recently been considered by Fruth et al [14] (by way of total interaction indices) and Tissot and Prieur [55] (by way of replicated orthogonal-array LHS). The latter work offers a powerful estimation method because the number of model calls is independent of the number of inputs (as in the spirit of permutation-based technique [32], [31]). However, for high-dimensional models (several hundreds inputs), estimation biases and computational costs remain considerable; De Castro and Janon [7] have proposed to introduce modern statistical techniques based on variable selection in regression models.

Another mathematical difficulty is the consideration of the dependence between the inputs  $X_i$  (i=1...d). Non-independence between inputs in SA has been discussed

by many authors such as Saltelli and Tarantola [46], Jacques et al [22], Xu and Gertner [59], Da Veiga et al [6], Li et al [30], Kucherenko et al [26], Mara and Tarantola [33] and Chastaing et al [4]. Despite all these works, much confusion still exists in practical applications.

Note that most of the works in this chapter focus on SA relative to the overall variability of model output. In practice, one can be interested in other quantities of interest, such as the output entropy, the probability that the output exceeds a threshold and a quantile estimation [47], [13], [29]. This is an active area of research as shown in this chapter (see Moment Independence Importance Measures and a Common Rationale), but innovative and powerful ideas have recently been developed by Fort et al. [12] and Da Veiga [5].

Finally, in some situations, the computer code is not a deterministic simulator but a stochastic one. This means that two model calls with the same set of input variables lead to different output values. Typical stochastic computer codes are queuing models, agent-based models, and models involving partial differential equations applied to heterogeneous or Monte Carlo-based numerical models. For this type of code, Marrel et al [34] have proposed a first solution for dealing with Sobol' indices. Moutoussamy et al [37] have tackled the issue in the context of metamodel building. Developing relevant SA methods in this context will certainly be subject of future works.

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#### References

- 1. Berger J (1994) An overview of robust bayesian analysis (with discussion). Test 3:5–124
- 2. Cacuci D (2003) Sensitivity and uncertainty analysis Theory. Chapman & Hall/CRC

- 3. Castaings W, Dartus D, Le Dimet FX, Saulnier GM (2009) Sensitivity analysis and parameter estimation for distributed hydrological modeling: potential of variational methods. Hydrology and Earth System Sciences Discussions 13:503–517
- 4. Chastaing G, Gamboa F, Prieur C (2012) Generalized Hoeffding-Sobol decomposition for dependent variables Application to sensitivity analysis. Electronic Journal of Statistics 6:2420–2448
- Da Veiga S (2014) Global sensitivity analysis with dependence measures. Journal of Statistical Computation and Simulation 85:1283–1305
- Da Veiga S, Wahl F, Gamboa F (2009) Local polynomial estimation for sensitivity analysis on models with correlated inputs. Technometrics 51(4):452–463
- 7. De Castro Y, Janon A (2014) Randomized pick-freeze for sparse Sobol indices estimation in high dimension. Submitted
- 8. de Rocquigny E, Devictor N, Tarantola S (eds) (2008) Uncertainty in industrial practice. Wiley
- 9. Dean A, Lewis S (eds) (2006) Screening Methods for experimentation in industry, drug discovery and genetics. Springer
- Fang KT, Li R, Sudjianto A (2006) Design and modeling for computer experiments. Chapman & Hall/CRC
- 11. Fisher RW (2011) Remembering Carol Reed, Aesop's Fable, Kenneth Arrow and Thomas Dewey. In: Speech: An Economic Overview: What's Next, Federal Reserve Bank of Dallas, http://www.dallasfed.org/news/speeches/fisher/2011/fs110713.cfm
- 12. Fort J, Klein T, Rachdi N (2014) New sensitivity analysis subordinated to a contrast. Communications in Statistics Theory and Methods, In press
- Frey H, Patil S (2002) Identification and review of sensitivity analysis methods. Risk Analysis 22:553–578
- Fruth J, Roustant O, Kuhnt S (2014) Total interaction index: A variance-based sensitivity index for second-order interaction screening. Journal of Statistical Planning and Inference 147:212–223
- Funtowicz S, Ravetz J (1990) Uncertainty and Quality in Science for Policy. Kluwer Academic Publishers, The Netherlands
- Grundmann R (2009) The role of expertise in governance processes. Forest Policy and Economics 11:398–403
- 17. Helton J (1993) Uncertainty and sensitivity analysis techniques for use in performance assessment for radioactive waste disposal. Reliability Engineering and System Safety 42:327–367

- Helton J, Johnson J, Salaberry C, Storlie C (2006) Survey of sampling-based methods for uncertainty and sensitivity analysis. Reliability Engineering and System Safety 91:1175–1209
- 19. Insua D, Ruggeri F (eds) (2000) Robust Bayesian Analysis. Springer-Verlag, New York
- 20. Ioannidis JPA (2005) Why most published research findings are false. PLoS Medicine 2(8):696-701
- 21. Iooss B, Lemaître P (2015) A review on global sensitivity analysis methods. In: Meloni C, Dellino G (eds) Uncertainty management in Simulation-Optimization of Complex Systems: Algorithms and Applications, Springer
- 22. Jacques J, Lavergne C, Devictor N (2006) Sensitivity analysis in presence of model uncertainty and correlated inputs. Reliability Engineering and System Safety 91:1126–1134
- 23. Kay J (2011) A wise man knows one thing The limits of his knowledge. Financial Times 29 november
- 24. Kennedy P (2007) A Guide to Econometrics, 5th ed. Blackwell Publishing, Oxford
- 25. Kleijnen J (1997) Sensitivity analysis and related analyses: a review of some statistical techniques.

  Journal of Statistical Computation and Simulation 57:111–142
- 26. Kucherenko S, Tarantola S, Annoni P (2012) Estimation of global sensitivity indices for models with dependent variables. Computer Physics Communications 183:937–946
- 27. Latour B (1993) We Have Never Been Modern. Cambridge, Harvard UP
- 28. Leamer EE (2010) Tantalus on the road to asymptopia. Journal of Economic Perspectives 4(2):31–46
- Lemaître P, Sergienko E, Arnaud A, Bousquet N, Gamboa F, Iooss B (2015) Density modification based reliability sensitivity analysis. Journal of Statistical Computation and Simulation 85:1200– 1223
- 30. Li G, Rabitz H, Yelvington P, Oluwole O, Bacon F, Kolb C, Schoendorf J (2010) Global sensitivity analysis for systems with independent and/or correlated inputs. Journal of Physical Chemistry 114:6022–6032
- 31. Mara T (2009) Extension of the RBD-FAST method to the computation of global sensitivity indices. Reliability Engineering and System Safety 94:1274–1281
- 32. Mara T, Joseph O (2008) Comparison of some efficient methods to evaluate the main effect of computer model factors. Journal of Statistical Computation and Simulation 78:167–178
- Mara T, Tarantola S (2012) Variance-based sensitivity indices for models with dependent inputs.
   Reliability Engineering and System Safety 107:115–121

- 34. Marrel A, Iooss B, Veiga SD, Ribatet M (2012) Global sensitivity analysis of stochastic computer models with joint metamodels. Statistics and Computing 22:833–847
- 35. Marris C, Wynne B, P S, , Weldon S (2001) Final report of the PABE research project funded by the Commission of European Communities. Tech. Rep. Contract number: FAIR CT98-3844 (DG12 SSMI), Commission of European Communities
- 36. Monbiot G (2013) Beware the rise of the government scientists turned lobbyists. The Guardian 29 april
- 37. Moutoussamy V, Nanty S, Pauwels B (2015) Emulators for stochastic simulation codes. ESAIM: PROCEEDINGS AND SURVEYS 48:116–155
- 38. Oreskes N, Conway EM (2010) Merchants of Doubt: How a Handful of Scientists Obscured the Truth on Issues from Tobacco Smoke to Global Warming. Bloomsbury Press, New York
- 39. Park K, Xu L (2008) Data assimilation for atmospheric, oceanic and hydrologic applications.

  Springer
- 40. Pujol G, Iooss B, Janon A (2015) sensitivity package, version 1.11. R Foundation for Statistical Computing, URL http://www.cran.r-project.org/web/packages/sensitivity/
- 41. Rakovec O, Hill MC, Clark MP, Weerts AH, Teuling AJ, Uijlenhoet R (2014) Distributed Evaluation of Local Sensitivity Analysis (DELSA), with application to hydrologic models. Water Resources Research 50:1–18
- 42. Saltelli A, Annoni P (2010) How to avoid a perfunctory sensitivity analysis. Environmental Modelling and Software 25:1508–1517
- 43. Saltelli A, dHombres B (2010) Sensitivity analysis didn't help. A practitioners critique of the Stern review. Global Environmental Change 20(2):298–302
- 44. Saltelli A, Funtowicz S (2014) When all models are wrong: More stringent quality criteria are needed for models used at the science-policy interface. Issues in Science and Technology Winter:79–85
- 45. Saltelli A, Funtowicz S (2015) Evidence-based policy at the end of the Cartesian dream: The case of mathematical modelling. In: Guimares Pereira, Funtowicz S (eds) The end of the Cartesian dream. Beyond the technoscientific worldview, Routledge's series: Explorations in Sustainability and Governance, pp 147–162
- 46. Saltelli A, Tarantola S (2002) On the relative importance of input factors in mathematical models: Safety assessment for nuclear waste disposal. Journal of American Statistical Association 97:702—

- 47. Saltelli A, Chan K, Scott E (eds) (2000) Sensitivity analysis. Wiley Series in Probability and Statistics, Wiley
- 48. Saltelli A, Tarantola S, Campolongo F, Ratto M (2004) Sensitivity analysis in practice: A guide to assessing scientific models. Wiley
- Saltelli A, Ratto M, Andres T, Campolongo F, Cariboni J, Gatelli D, Salsana M, Tarantola S
   (2008) Global sensitivity analysis The primer. Wiley
- 50. Saltelli A, Pereira G, Van der Sluijs JP, Funtowicz S (2013) What do I make of your latinorum? Sensitivity auditing of mathematical modelling. Int J Foresight and Innovation Policy 9(2/3/4):213–234
- 51. Savage SL (2009) The Flaw of Averages: Why We Underestimate Risk in the Face of Uncertainty.
  Wiley
- 52. Stiglitz J (2010) Freefall, Free Markets and the Sinking of the Global Economy. Penguin, London
- 53. Szenberg (1992) Eminent Economists: Their Life Philosophies. Cambridge, England: Cambridge University Press
- 54. The Economist (2013) How science goes wrong. The Economist 19 october
- 55. Tissot JY, Prieur C (2015) A randomized Orthogonal Array-based procedure for the estimation of first- and second-order Sobol' indices. Journal of Statistical Computation and Simulation 85:1358–1381
- 56. Turanyi T (1990) Sensitivity analysis for complex kinetic system, tools and applications. Journal of Mathematical Chemistry 5:203–248
- 57. Van der Sluijs JP, Craye M, Funtowicz S, Kloprogge P, Ravetz J, Risbey J (2005) Combining quantitative and qualitative measures of uncertainty in model based environmental assessment: the NUSAP system. Risk Analysis 25(2):481–492
- 58. Winner L (1989) The Whale and the Reactor: a Search for Limits in an Age of High Technology.

  The University of Chicago Press, Chicago
- 59. Xu C, Gertner G (2007) Extending a global sensitivity analysis technique to models with correlated parameters. Computational Statistics and Data Analysis 51:5579–5590