

# SENSITIVITY ANALYSIS OF MODEL OUTPUT: VARIANCE-BASED METHODS MAKE THE DIFFERENCE

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## ABSTRACT

This paper is intended to review a number of variance-based methods used in Sensitivity Analysis (SA) to ascertain how much a model (numerical or otherwise) depends on each or some of its input parameters. A class of variance-based methods (correlation ratio or importance measure) that is capable of measuring only the main effect contribution of each input parameter on the output variance are described briefly. In addition, two methods (Sobol' and FAST) that are capable of computing the so-called "Total Sensitivity Indices" (TSI), which measures a parameter's main effect and all the interactions (of any order) involving that parameter, are described in details. An illustrated example demonstrates that the incorporation of total effect indices is the only way to perform a rigorous quantitative sensitivity analysis.

## 1 INTRODUCTION

Mathematical models are developed to approximate engineering, physical, environmental, social, and economic phenomena of various complexity. Model development consists of several logical steps, one of which should be the determination of parameters which are most influential on model output. A 'sensitivity analysis' of the input parameters can serve as a guide to any further use of the model.

In general, SA is conducted by:

- (i) defining the model and its input parameters and output variable(s),
- (ii) assigning probability density functions to each input parameter,
- (iii) generating an input matrix through an appropriate random sampling method, evaluating the output, and
- (iv) assessing the influences or relative importance

of each input parameters on the output variable.

Modellers conduct sensitivity analysis for a number of reasons including the needs to determine:

- (a) which input parameters contribute the most to output variability and, possibly, require additional research to strengthen the knowledge base, thereby reducing output uncertainty;
- (b) which parameters are insignificant and can be eliminated from the final model;
- (c) if and which (group of) parameters interact with each other;
- (d) if all observed effects can be physically explained, when error may be present in a model;
- (e) the optimal regions within the parameters space for use in a subsequent calibration study.

There are many different ways to perform sensitivity analyses in answering these questions but they may not yield identical results. In this paper we will be concentrating on item (a) above.

Many authors, when referring to the degree to which an input parameter affects the model output, use the terms 'sensitive', 'important', 'most influential', etc. The methods that will be discussed and used to perform SA in this paper are called 'Variance-based methods', in that the variability, or uncertainty, associated with an important input parameter is propagated through the model resulting in a large contribution to the overall output variability.

Methods such as "importance measure" (Iman and Hora 1990, Saltelli et al. 1993, Homma and Saltelli 1996), or "correlation ratio" (Krzyszczak 1990, McKay 1996), are capable of estimating the "main effect" contribution of each parameter to the output variance. However, whether a parameter is influential or not depends also on the interactions and influences of all the parameters. Derived from quite a

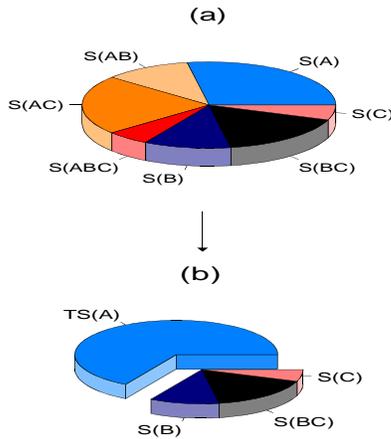


Figure 1: Graphical Representation of (a) Sensitivity Indices for the Three Parameters Case and (b) Total Sensitivity Indices of Parameter  $A$

different setting (see later), Fourier Amplitude Sensitivity Test (FAST) (Cukier et al. 1973, Saltelli and Bolado 1997, Saltelli et al. 1997) and Sobol' methods (1990a, 1993) not only can measure the “main effect” (or the so-called first order term) they can also compute the so-called “Total Sensitivity Indices” ( $TSI$ ). The Total Sensitivity Index of parameter  $i$ , denoted by  $TS(i)$ , is defined as the sum of all the sensitivity indices (including all the interaction effects) involving parameter  $i$  (Sobol' 1990a, Homma and Saltelli 1996). For example, suppose that we only have three input parameters ( $A$ ,  $B$  and  $C$ ) in our model. Figure 1 illustrates diagrammatically that the total effect of parameter  $A$ , for instance, on the output is,

$$TS(A) = S(A) + S(AB) + S(AC) + S(ABC),$$

where  $S(A)$  denotes the so-called first order sensitivity index for parameter  $A$ ,  $S(A_j)$  denotes the second order sensitivity index for the parameters  $A$  and  $j$  (for  $j \neq A$ ), i.e. the interaction between parameters  $A$  and  $j$  ( $\neq A$ ), and so on.

A set of input parameters can be grouped according to their  $TSI$  values, for example, parameters with  $TSI$  greater than 0.8 can be regarded as ‘very important’, between 0.5 and 0.8 ‘important’, between 0.5 and 0.3 ‘unimportant’, and less than 0.3 ‘irrelevant’. Figure 2 shows a graphical representation of grouping a set of parameters. The effectiveness of Sobol' and FAST methods is that  $TSI$  can be computed with just one Monte Carlo integral and one set of frequencies, respectively, per parameter.

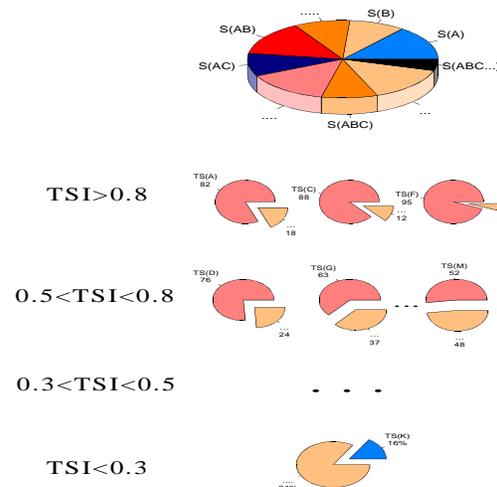


Figure 2: Graphical Representation of Grouping a Set of Input Parameters with the Total Sensitivity Indices

A brief review of “importance measure” or “correlation ratio”, Sobol' and FAST methods is given in Section 3. Then, in Section 5 we present an example to illustrate the methods described in Section 3 and in the final section we summarize our conclusions.

## 2- MODEL AND NOTATION

A mathematical model  $f(\cdot)$  is a construction by which an output or prediction  $y$  is determined from a set of  $n$  input parameters, namely  $y = f(\mathbf{x})$ . Throughout this chapter we assume a single output is observed but in a practical problem, multiple outputs could be encountered via a set of transfer functions, for instance a set of differential equations. Let us assume also that the vector of input parameters, denoted by  $\mathbf{x}$ , is a random vector, characterized by a joint probability density function  $p(\mathbf{x}) = p(x_1, x_2, \dots, x_n)$ , assumed to be known, even if the  $x_i$ 's are not actually random variables. In practice, the parameters are affected by several kinds of heterogeneous uncertainties which reflect our imperfect knowledge of the system. In these cases it may be convenient for the purpose of sensitivity analysis to treat them as random variables with assumed probability distributions. This implies that the output  $Y$  is also a random variable, as it is a function of the random vector  $\mathbf{X}$ , with its own probability density function (p.d.f.). (Here we use the convention, except where it is stated otherwise, that capital letters denote random variables and small letters correspond to the realizations.)

Summary statistics of the output,  $Y$ , can be computed from the  $r$ th moment which is given by

$$E(Y^r) = \int_{K^n} f^r(x_1, x_2, \dots, x_n) p(x_1, x_2, \dots, x_n) d\mathbf{x}, \quad (1)$$

where  $K^n$  is the  $n$ -dimensional space of the input parameters. The integral in (1) provides the basis of computing sensitivity measures of various kind. Note that the computation of (1) involves the evaluation of multidimensional integrals.

### 3- METHODS

The following sub-section gives a brief review of a class of variance-based methods which is capable of measuring only the main effect contribution of each input parameter on the output variance. Then, in the next two sub-sections, the Sobol' and FAST methods which are capable of computing sensitivity measure of a parameter, which takes into account the interaction between the parameter and the others parameters, are described.

#### 3.1- Correlation Ratios or Importance Measures

In this section we briefly describe a class of variance-based methods that is based on the estimation of the following quantity

$$\frac{Var_X[E(Y|X)]}{Var(Y)}, \quad (2)$$

where  $Y$  denotes the output variable,  $X$  denotes an input variable,  $E(Y|X)$  denotes the expectation of  $Y$  conditional on a fixed value of  $X$ , and the variance is taken over all possible values of  $X$ . McKay (1995) called the numerator of (2) *Variance Conditional Expectation (VCE)* and the ratio *Correlation Ratio* which is derived from the decomposition of  $Var(Y)$ , namely

$$Var(Y) = Var_{\mathbf{X}}[E(Y|\mathbf{x})] + E_{\mathbf{X}}(Var[Y|\mathbf{x}]), \quad (3)$$

where

$$Var_{\mathbf{X}}[E(Y|\mathbf{x})] = \int [E(Y|\mathbf{x}) - E(Y)]^2 p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x}, \quad E_{\mathbf{X}}(Var[Y|\mathbf{x}]) = \int \int [y - E(Y|\mathbf{x})]^2 p_{Y|\mathbf{x}}(y) dy p_{\mathbf{x}}(\mathbf{x}) d\mathbf{x},$$

and  $E(Y|\mathbf{x}) = \int y p_{Y|\mathbf{x}}(y) dy$ .

Kendall and Stuart (1979) described the use of (2) in the nonlinear relationship setting as a parallel to that of the usual correlation coefficient  $\rho$  for linear relationships between the output and the input parameters. The same method is described by Krzykacz (1990) who uses the correlation ratio without an explicit form for the conditional mean and called the

estimate, "empirical correlation ratio". By assuming the input parameters are independent of each other, Hora and Iman (1989) obtained the following relation

$$Var(Y) - E[Var(Y|x_i)] = U_i - [E(Y)]^2 \quad (4)$$

where

$$U_i = \int [E(Y|x_i)]^2 p_i(x_i) dx_i. \quad (5)$$

and used  $I_i = \sqrt{U_i - [E(Y)]^2}$  as the importance measures. The right hand side of (4) is simply *VCE*, as defined earlier. This measure was used in the analysis of fault trees assuming a linear polynomial approximation for the conditional expectation of  $Y$ . For numerical robustness reasons, Iman and Hora (1990) proposed the following as a measure of the importance of  $x_i$ ,  $Var_{X_i}[E(\log Y|X_i)]/Var[\log Y]$ , where  $Var_{X_i}$  denotes variance over all possible values of  $X_i$  and  $E[\log(Y)|X_i]$  is estimated using linear regression. Saltelli et al. (1993) discussed a modified version of the Hora and Iman (1989)' approach which relates to Krzykacz (1990). The idea of the correlation ratio can be extended to the partial correlation ratio, paralleling the partial correlation coefficient in linear models (see McKay 1995 for further details). Rank transformed versions of the correlation ratio or importance measures are discussed in McKay and Beckman (1994) and Homma and Saltelli (1996), respectively.

#### 3.2- Sobol' Indices

The main idea behind Sobol' approach for the computation of sensitivity indices is the decomposition of the function  $f(\mathbf{x})$  into summands of increasing dimensionality, namely

$$f(x_1, \dots, x_n) = f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{i=1}^n \sum_{j=i+1}^n f_{ij}(x_i, x_j) + \dots + f_{1,2,\dots,n}(x_1, \dots, x_n) \quad (6)$$

For (6) to hold  $f_0$  must be a constant, and the integrals of every summand over any of its own variables must be zero, i.e.

$$\int_0^1 f_{i_1, \dots, i_s}(x_{i_1}, \dots, x_{i_s}) dx_{i_k} = 0, \quad \text{if } 1 \leq k \leq s \quad (7)$$

A consequence of (6) and (7) is that all the summands in (6) are orthogonal, i.e. if  $(i_1, \dots, i_s) \neq (j_1, \dots, j_t)$ , then

$$\int_{K^n} f_{i_1, \dots, i_s} f_{j_1, \dots, j_t} d\mathbf{x} = 0. \quad (8)$$

Since at least one of the indices will not be repeated, the corresponding integral will vanish due to (7). Another consequence is that  $f_0 = \int_{K^n} f(\mathbf{x})d\mathbf{x}$ . Sobol' (1990a) showed that the decomposition (6) is unique and that all the terms in (6) can be evaluated via multidimensional integrals, namely  $f_i(x_i) = -f_0 + \int_0^1 \dots \int_0^1 f(\mathbf{x})d\mathbf{x}_{\sim i}$  and  $f_{ij}(x_i, x_j) = -f_0 - f_i(x_i) - f_j(x_j) + \int_0^1 \dots \int_0^1 f(\mathbf{x})d\mathbf{x}_{\sim \{ij\}}$  with the convention that  $\int_{K^n} d\mathbf{x}_{\sim i}$  and  $\int_{K^n} d\mathbf{x}_{\sim \{ij\}}$  denote integration over all parameters except  $x_i$ , and  $x_i$  and  $x_j$ , respectively. Here, " $\sim$ " means "complementary of". Analogous formulae can be obtained for the higher order terms.

The variance based sensitivity indices follow very naturally by this scheme; the total variance  $D$  of  $f(\mathbf{x})$  is defined to be

$$D = \int_{K^n} f^2(\mathbf{x})d\mathbf{x} - f_0^2 \tag{9}$$

while partial variances are computed from each of the terms in (6) namely

$$D_{i_1, \dots, i_s} = \int_0^1 \dots \int_0^1 f_{i_1, \dots, i_s}^2(x_1, \dots, x_s) dx_{i_1} \dots dx_{i_s} \tag{10}$$

where  $1 \leq i_1 < \dots < i_s \leq n$  and  $s = 1, \dots, n$ . By squaring and integrating (6) over  $K^n$ , and by (8) we have

$$D = \sum_{i=1}^n D_i + \sum_{i=1}^n \sum_{j=i+1}^n D_{ij} + \dots + D_{1,2,\dots,n}. \tag{11}$$

Hence, a sensitivity measure  $S(i_1, \dots, i_s)$  is defined as

$$S(i_1, \dots, i_s) = \frac{D_{i_1, \dots, i_s}}{D} \tag{12}$$

with the useful property that all the sensitive indices sum to 1, namely

$$\sum_{i=1}^n S(i) + \sum_{i=1}^n \sum_{j=i+1}^n S(i, j) + \dots + S(1, 2, \dots, n) = 1. \tag{13}$$

One attractive feature of Sobol' indices is that the integrals in (9) and in (10) can be computed with the same kind of Monte Carlo (MC) integral. Hence, the MC estimates of  $f_0$ ,  $D$  and  $D_i$  are given by the following formulae

$$\hat{f}_0 = \frac{1}{N} \sum_{m=1}^N f(\mathbf{x}_m); \tag{14}$$

$$\hat{D} = \frac{1}{N} \sum_{m=1}^N f^2(\mathbf{x}_m) - \hat{f}_0^2; \tag{15}$$

$$\hat{D}_i = \frac{1}{N} \sum_{m=1}^N f(\mathbf{x}_{\sim im}^{(1)}, x_{im}^{(1)})f(\mathbf{x}_{\sim im}^{(2)}, x_{im}^{(1)}) - \hat{f}_0^2. \tag{16}$$

In equations (14) - (16),  $N$  is the number of samples generated to obtain the MC estimates,  $\mathbf{x}_m$  is a sampled point in  $K^n$ , and  $\mathbf{x}_{\sim im} = (x_{1m}, \dots, x_{(i-1)m}, x_{(i+1)m}, \dots, x_{nm})$ .

The superscripts <sup>(1)</sup> and <sup>(2)</sup> in (16) indicate that we are using two sampling data matrices for  $\mathbf{x}$ . Both matrices have dimension  $(N, n)$ . Hence (16) says that in computing  $\hat{D}_i$  we multiply values of  $f$  corresponding to  $\mathbf{x}$  from matrix (1) by values of  $f$  computed using a different matrix (2), but with the  $i$ th column taken from matrix (1). Formulae similar to (16) can be derived for the partial variances of higher order (see Homma and Saltelli 1996). A drawback of the method is that a separate MC integral is needed to compute each term in (11), be it the first or higher order. Counting also the set of model evaluations that is needed to obtain  $\hat{f}_0$ , a total of  $2^n$  MC integrals are needed, far too many unless  $n$  is low.

Homma and Saltelli (1996) adapted the 'freezing unessential variables' approach (Sobol' 1993) to investigate the total influence of individual parameters. This is achieved by partitioning  $\mathbf{x}$  into  $\mathbf{x}_{\sim i}$  and  $x_i$ , where  $x_i$  is the parameter of interests. The Total Sensitivity Index for parameter  $x_i$  is given by

$$ST(i) = S(i) + S(i, \sim i) = 1 - S(\sim i), \tag{17}$$

where  $S(\sim i)$  is the sum of all the  $S(i_1, \dots, i_s)$  terms which do not include the index  $i$ , i.e. the total fractional variance complementary to parameter  $x_i$ . The integral that is needed for the computation of  $S(\sim i)$  is estimated by MC integral

$$\hat{D}_{\sim i} + \hat{f}_0^2 = \frac{1}{N} \sum_{m=1}^N f(\mathbf{x}_{\sim im}^{(1)}, x_{im}^{(1)})f(\mathbf{x}_{\sim im}^{(1)}, x_{im}^{(2)}),$$

where the superscripts <sup>(1)</sup> and <sup>(2)</sup> are defined as above. Hence,

$$\widehat{ST}(i) = 1 - \hat{D}_{\sim i} / \hat{D}$$

which is the estimated total contribution of parameter  $i$  to the total output variation. The number of Monte Carlo integrals needed is equal to the number of parameters plus one (for  $\hat{f}_0$ ). A rank transformation of this method is given in Saltelli and Sobol' (1995).

### 3.3- FAST Indices

The Fourier amplitude sensitivity test (FAST) is a procedure that has been developed for uncertainty and sensitivity analysis (Cukier et al. 1973; Shaibly and Shuler 1973; Cukier et al. 1975; Cukier et al. 1978). This procedure provides a way to estimate the expected value and variance of the output variable and the contribution of individual input parameters

to this variance. An advantage of FAST is that the evaluation of sensitivity estimates can be carried out independently for each parameter using just one simulation because all the terms in a Fourier expansion are mutually orthogonal.

The main idea of the FAST method is to convert the  $n$ -dimensional integral in (1) into one-dimensional integral in  $s$  by using the transformation  $x_i = G_i(\text{Sin}(\omega_i s))$  for  $i = 1, \dots, n$ . For properly chosen  $\omega_i$  and  $G_i$ , the expectation of  $Y$  can be approximated by

$$E(Y) \doteq \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s) ds. \quad (18)$$

where  $f(s) = f(G_1(\text{Sin}(\omega_1 s)), \dots, G_k(\text{Sin}(\omega_k s)))$ . Further, by using properties of Fourier series (see Saltelli et al. 1997), an approximation of the variance of  $Y$  is given by

$$\begin{aligned} \text{Var}(Y) &\doteq \frac{1}{2\pi} \int_{-\pi}^{\pi} f^2(s) ds - [E(Y)]^2 \\ &\approx \sum_{j=-\infty}^{\infty} (A_j^2 + B_j^2) - (A_0^2 + B_0^2) \\ &\approx 2 \sum_{j=1}^{\infty} (A_j^2 + B_j^2), \end{aligned} \quad (19)$$

where  $A_j$  and  $B_j$  are the Fourier coefficients and are defined as follows

$$A_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s) \text{Cos}(js) ds \quad (20)$$

and

$$B_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s) \text{Sin}(js) ds. \quad (21)$$

The expressions in (18) and (19) provide a mean to estimate the expected value and variance associated with  $Y$ .

Further, provided the  $\omega_i$  are integers and by evaluating the  $A_j$  and  $B_j$  for the fundamental frequency  $\omega_i$  and its higher harmonics — a periodic function with period  $2\pi/\omega_0$  has non-zero spectral components at the fundamental frequency  $\omega_0$  and at all its higher harmonics  $2\omega_0, 3\omega_0, \dots$  — denoted by  $p\omega_i$ , the contribution to total variance by  $X_i$  can be approximated by

$$\widehat{\text{Var}}_{\omega_i}(Y) = 2 \sum_{j=1}^{\infty} (A_{j\omega_i}^2 + B_{j\omega_i}^2). \quad (22)$$

Thus, the ratios  $\widehat{\text{Var}}_{\omega_i}(Y)/\text{Var}(Y)$ , denoted by  $S'(i)$ , provide a mean to rank individual variable importance on the basis of contribution to the variance of  $Y$ . Saltelli and Bolado (1997) showed that  $S'(i)$  is equivalent to the Sobol' sensitivity indices of the first order,  $S(i)$ .

Application of the FAST method involves

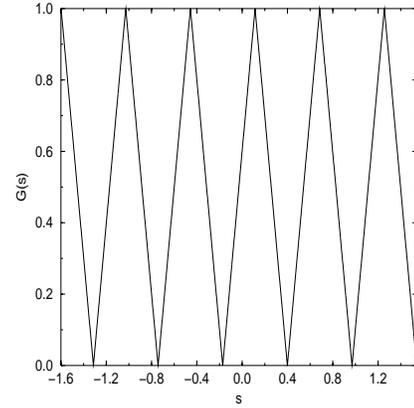


Figure 3: Plot of the Transformation given in Equation (23) with  $\omega_i = 11$  and  $\varphi_i = 0$

- (i) defining the  $\omega_i$  and  $G_i$ ,
- (ii) evaluating the original model at a sufficient number of points to allow numerical evaluation of the integrals in (20) and (21), and approximation of the sums in (19) and (22).

Discussions on the choice of  $\omega_i$  and item (ii) above are given in Saltelli et al. (1997). Here we will describe briefly a transformation,  $G_i$ , proposed by Saltelli et al. (1997), namely a curve defined by a set of parametric equations

$$x_i = \frac{1}{2} + \frac{1}{\pi} \arcsin(\sin(\omega_i s + \varphi_i)), \quad (23)$$

where  $s$  is a scalar variable varied over the range  $-\infty < s < +\infty$ ,  $\omega_i$  are a set of different (angular) frequencies associated with each parameter, and  $\varphi_i$  is a random phase shift chosen in  $[0, 2\pi)$ .

The curve specified by the transformation given in (23) is in fact a set of straight lines, oscillating over the range of  $s$  (see Figure 3). As  $s$  varies, all the parameters change simultaneously according to the transformation specified in (23), and systematically explore their range of uncertainty. The curve drives arbitrarily close to any point  $\mathbf{x}$  of the input domain *if and only if* a set of incommensurate frequencies is used. (A set of frequencies is said to be *incommensurate* if none of them may be obtained as a linear combination of the other frequencies with integer coefficients.) If this is the case then we say that the curve is space-filling (see Figure 4 for example).

The computation of the  $ST(i)$ 's is obtained by assigning different numerical values to the set of frequencies  $\omega_i$  for  $i = 1, 2, \dots, n$ . For instance, a certain value is assigned to the frequency  $\omega_i$  for parameter

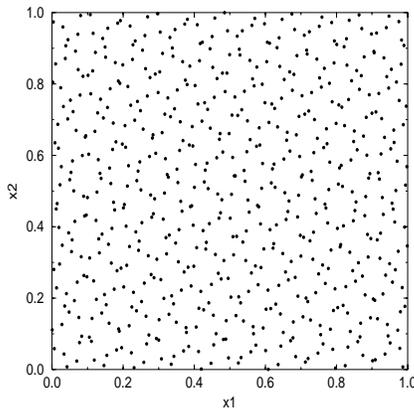


Figure 4: Scatter Plot of Sampling Points in a Two Parameters Case Based on the Straight Line Transformation given in Equation (23) with  $\{\omega_1, \omega_2\} = \{11, 21\}$

$i$  and a different set of values is assigned to all the other frequencies,  $\omega_{\sim i}$ , for the remaining parameters. Thus, by evaluating the spectrum at the frequencies  $\omega_{\sim i}$  and the related higher harmonics  $p\omega_{\sim i}$  we can estimate the partial variance  $D_{\sim i}$ . Furthermore, by summing all the spectral components we can estimate the total variance  $D$ . Then, it is easy to get  $ST(i)$  by (17). Usually, a high value is assigned to  $\omega_i$  and a low one to all the  $\omega_{\sim i}$ , for instance  $\omega_{\sim i}$ 's = 1. In this way the frequencies corresponding to  $D_i$  and  $D_{\sim i}$  are far from overlapping and  $D_{\sim i}$  can easily be estimated from the first few spectral components. A different set of model evaluations will be needed for the estimation of each  $ST(i)$ ,  $\forall i = 1, \dots, n$ . This is the price to pay in order to capture the total interaction terms. Yet, with the same set of model evaluations (i.e. at no extra computational cost) the analyst can compute both  $ST(i)$  and  $S(i)$  for each variable  $x_i$ . Further details and discussion of the new method, choice of frequencies, and optimization of the sampling procedure can be found in Saltelli et al. (1997) and Tarantola et al. (1997).

#### 4- COMPUTATIONAL ISSUES

The variance-based methods are classed as global SA in the sense that sensitivity assessment on the output to each input parameter is carried out by considering the combined variability of all the parameters simultaneously. A large array of randomly selected input parameter values, through some random sampling methods, such as simple random sampling, Monte Carlo, Latin Hypercube Sampling (LHS),  $LP_\tau$

sequences, etc., provides a mean for determining parameter sensitivity through a variety of procedures.

The random data matrix of the Sobol' method is usually generated using quasi-random numbers for computing the MC integrals. Quasi-random numbers are characterized by an enhanced convergence (Sobol' 1990b). Note that other sampling strategies such as the *LHS* (McKay et al. 1979), can be used to compute sensitivity indices but Homma and Saltelli (1995) found that  $LP_\tau$  sequences performed better than the others (see Homma and Saltelli 1995 for further details). As seen in Section 3.3, the FAST method has its own sampling scheme in that sampling points are generated from a search curve which filled the input parameters space. Estimation of the correlation ratio has been associated with *LHS* (McKay 1995, 1996). For the importance measure, a Monte Carlo technique is used to evaluate the integral in (5) if there is no analytical solution available. But this is computationally too expensive and impractical. Saltelli et al. (1993) adapted a computation scheme suggested by Ishigami and Homma (1989) to estimate (5) and if the random sample is that of  $LP_\tau$  then the resulting estimates are the same as the Sobol' first order sensitivity estimates.

#### 5- AN ILLUSTRATION

In this section we present an example to illustrate and to make a comparison amongst the variance-based techniques. An analytical function is used in this example, namely the Legendre polynomials of order  $d$ , is denoted by  $L_d(x)$  (see McKay 1996).

The model has two input parameters,  $x$  is a uniformly distributed random variable taking values over the range  $[-1, +1]$  and  $d$  is a discrete uniformly distributed random variable, assumed to take values from 1 to 5. The Legendre polynomials are orthogonal and integrate to zero over the interval  $[-1, +1]$ . This implies that the influence of  $d$  on the output is nil. The analytical values of the partial variances due to the variables  $d$  and  $x$  ( $D_d$  and  $D_x$ ) are given in Table 3 of McKay (1996). These analytical values are given as conditional expectations and variances, namely

$$Var[E(Y | \text{input})] = D_{\text{input}}.$$

And from (3), we have  $E(Var[Y | \text{input}]) = D_{\sim \text{input}} + D_{\text{input}, \sim \text{input}}$  and  $Var[Y] = D$ .

The corresponding analytical values of the sensitivity indices of the two input parameters are presented in a pie diagram (Figure 5). McKay (1996) commented that the variance-based measures of importance — which use the variance of the conditional expectation of the output,  $Var_X[E(Y|X=x)]$  —

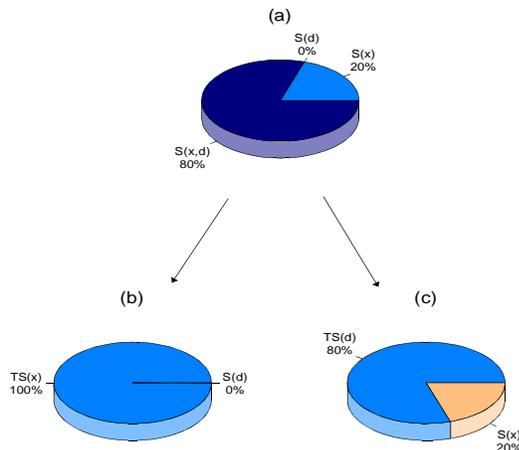


Figure 5: Graphical Representation of Sensitivity Indices of  $x$ , of  $d$ , and of  $x$  and  $d$

may not always be effective as indicators of importance, and hinted that additional notions of importance might be necessary for assessing uncertainty importance. As shown in Figure 5 the Total Sensitivity Indices offer such additional notions. Although on their own, both parameters  $d$  and  $x$  appear to be irrelevant to the output variable (the first order sensitivity indices being  $S(d) = 0$  and  $S(x) = 0.2$ ), the  $TSI$  for parameters  $d$  and  $x$  are 0.8 and 1.0, respectively. These values represent the total effect of the parameters  $d$  and  $x$  on the output variable, which account for 80% and 100%, respectively, of the total output variance. The reason for this behavior is that there is a large interaction between  $d$  and  $x$ . The effect of this interaction between  $d$  and  $x$  on the output is measured by  $S(d, x) = 1 - S(d) - S(x) = 1 - 0.0 - 0.2 = 0.8$ . Hence, this leads to the conclusion that both parameters influence the output variable, even though neither  $d$  nor  $x$  alone can explain the output variation. This example demonstrates the importance contribution that the  $TSI$  can make when a complete Sensitivity Analysis is required, and confirms the identity of McKay's correlation ratio with Sobol'/FAST first order indices.

In a simulation study carried out by Saltelli et al. (1997) to assess the robustness of Sobol' and FAST methods in estimating  $TSI$ , estimates of  $TSI$  were computed at six different sample sizes. They found that, on average, FAST yields better estimates than Sobol'. Also, in terms of robustness, FAST is better. The FAST estimates converge more rapidly to the analytical values, even at low sample sizes.

## 6 CONCLUSIONS

Non-linear, non-monotonic problems are often encountered in everyday model building. These problems call for a non-linear SA which is independent from assumptions about the model structure. Both FAST and Sobol' sensitivity measures can cope with non-linear and non-monotonic models. They can be considered as truly quantitative for global SA for numerical experiments. The word 'quantitative' here means that the parameters can be ranked in order of their relative importance in the model.

All the alternative global methods, variance-based or not, can offer, at best, a qualitative picture of the model sensitivity. The variance-based methods such as correlation-ratio or importance measures are model independent and can evaluate main effect contributions. FAST and Sobol' are completely automated and are able to compute the total effect indices which allows us to rank quantitatively the parameters in order of their influence (be it additive, non-linear or with interactions) on the output. As demonstrated in the example,  $TSI$ 's together with the first order indices should always be computed in order to investigate the predominance of lower or higher order terms, which is the only way to perform a rigorous quantitative sensitivity analysis.

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## REFERENCES

- Cukier, R. I., C. M. Fortuin, K. E. Shuler, A. G. Petschek, and J. H. Schaibly. 1973. Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I Theory. *The Journal of Chemical Physics* 59: 3873–3878.
- Cukier, R. I., J. H. Schaibly, and K. E. Shuler. 1978. Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. III. Analysis of the approximations. *The Journal of Chemical Physics* 63: 1140–1149.
- Cukier, R. I., H. B. Levine, and K. E. Shuler. 1978. Nonlinear Sensitivity Analysis of Multi-parameter Model Systems. *Journal of Computational Physics* 26: 1–42.
- Homma, T., and A. Saltelli. 1995. Sensitivity analysis of model output: performance of the Sobol' quasi random sequence generator for the integration of the modified Hora and Iman importance

- measure. *Journal of Nuclear Science and Technology* 32: 1164–1173.
- Homma, T., and A. Saltelli. 1996. Importance measures in global sensitivity analysis of nonlinear models. *Reliability Engineering and System Safety* 52: 1–17.
- Hora, S. C., and R. L. Iman. 1989. A comparison of maximum/bounding and Bayesian/Monte Carlo for fault tree uncertainty analysis. *Sandia National Laboratories report SAND85-2839*.
- Iman, R. L., and S. C. Hora. 1990. A robust measure of uncertainty importance for use in fault tree system analysis. *Risk Analysis* 10: 401–406.
- Ishigami, T., and T. Homma. 1990. An importance quantification technique in uncertainty analysis for computer models. In the *Proceedings of the ISUMA '90*, University of Maryland, USA, 398–403.
- Kendall, M. and A. Sturat. 1979. *The advanced theory of statistics*. 4th ed. New York: MacMillan Publishing Co.
- Krzykacz, B. 1990. Samos: a computer program for the derivation of empirical sensitivity measures of results from large computer models. *Technical Report GRS-A-1700*, Gesellschaft für Reaktorsicherheit (GRS) mbH, Garching, Germany.
- McKay, M. D. 1995. Evaluating prediction uncertainty. *Nuclear Regulatory Commission and Los Alamos National Laboratory Technical Report NUREG/CR-6311*.
- McKay, M. D. 1996. Variance-based methods for assessing uncertainty importance in NUREG-1150 analyses. Submitted.
- McKay, M. D., R. J. Beckman, and W. J. Conover. 1979. A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. *Technometrics* 21: 239–245.
- McKay, M. D., and R. J. Beckman. 1994. A procedure for assessing uncertainty in models. In *Proceedings of PSAM-II*, San Diego, CA: 20–25.
- Saltelli, A., S. Tarantola, and K. P.-S. Chan. 1997. A quantitative model independent method for global sensitivity analysis of model output. Submitted.
- Saltelli, A., and R. Bolado. 1997. Is there another way to compute Fourier Amplitude Sensitivity Test (FAST)? *Computational Statistics and Data Analysis* Accepted.
- Saltelli, A., and I. M. Sobol'. 1995. About the use of rank transformation in sensitivity analysis of model output. *Reliability Engineering and System Safety* 50: 225–239.
- Saltelli, A., T. Andres, and T. Homma. 1993. Sensitivity analysis of model output: an investigation of new techniques. *Computational Statistics and Data Analysis* 15: 211–238.
- Schaibly, J. H., and K. E. Shuler. 1973. Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. Part II, Applications. *The Journal of Chemical Physics* 59: 3879–3888.
- Sobol', I. M. 1990a. Sensitivity estimates for nonlinear mathematical models. *Matematicheskoe Modelirovanie* 2: 112–118 (in Russian).
- Sobol', I. M. 1990b. Quasi-Monte-Carlo methods. *Progress in Nuclear Energy* 24: 55–61.
- Sobol', I. M. 1993. Sensitivity Analysis for nonlinear mathematical models. *Mathematical Modeling & Computational Experiment* 1: 407–414.
- Tarantola, S., A. Saltelli, and K. Chan. 1997. Quantitative methods for global sensitivity analysis. Presented at the International Conference on Safety and Reliability, ESREL Lisbon, Portugal, 17–20 June 1997.

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