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Review of Sensitivity Analysis Methods and Experience for Geological Disposal of Radioactive waste and Spent Nuclear Fuel

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Content

1. Introduction

Performance Assessment (PA) is a main component to show the feasibility and safety of High Level Radioactive Waste (HLW) repositories. PA uses complex models, usually called system models, which integrate several submodels and simulate the behaviour of the system along large time periods. PA involves, among other activities, Uncertainty Analysis (UA) and Sensitivity Analysis (SA). UA consists in identifying relevant uncertainties (model uncertainties, scenario uncertainties and parameter uncertainties) affecting the behaviour of the system and propagating them correctly into the output space, in order to characterise appropriately the uncertainty in the output variables used to determine if the system is either safe enough or not.

SA helps PA users to study the impact of input uncertainties on output variables. Following Saltelli et al. (2000), the main purposes of a sensitivity analysis in the context of modelling, are:

1. To decide whether a model is accurate with respect to the process it models. If, for instance, the sensitivity analysis finds that a factor is very influent, while in reality it is not, then the model should be changed because it doesn't describe correctly the process.
2. To classify the factors starting from the most influent to the least influent.
   — The most influent factors are the ones that most contribute to the variation of the output; hence they might require additional research to improve their estimation.
   — On the contrary, the least influent factors (i.e. the ones that are less affecting the variation of the output) might eventually be removed from the model or considered as deterministic (and fixed to their mean value for instance).
3. To detect whether there exists some region in the input factors space where the output variation is maximum.
4. To determine the optimal regions of the input factors space to be used in a calibration study (i.e. to calibrate a model against field and laboratory data).
5. To detect the interaction between factors or groups of factors.

In the following, sensitivity analysis will be considered in the context of PA models which, from the point of view of mathematics, are models represented by a (possibly complex) function $f : IR^k \rightarrow IR$ which links the input of the model $X = (X_1, \ldots, X_k)$ to its output $Y = f(X)$. The function f is evaluated by a numerical code, which may be very time consuming (i.e. several hours of CPU time). The input of the model X is considered to be random and, without any loss of generality, the output Y is one-dimensional (scalar). In many cases, scalar outputs will evolve over time.

SA methods may be divided into three broad types: local methods, screening methods and global methods.
— Local methods focus on the study of the system model behaviour under very specific system conditions (the vicinity of an input space point) and are based on the partial derivatives of the output with respect to the inputs. Chapter 5 in Saltelli et al. (2000) is dedicated to those methods, and new advances based on the SVD method (Singular Value Decomposition) have been recently developed in Marchand (2007). As the local methods are concerned with first order sensitivities, when applied to non-linear problems, the results will be valid only for small variations (depending on the amplitude of the non-linearity of the model) around a specified value of the input. Other

references on this topic are Cacuci (2003), Turanyi (1990) and Rabitz et al. (1983). We will not discuss about these methods in this report.

— Screening methods focus on the functional relation between inputs and outputs disregarding input parameter distributions. They are used to identify a subset of inputs that controls most of the variability of the output.

— Global methods focus on how the whole input space (taking into account input distributions) maps into the output space.

The target of this work is to provide a summary of most useful methods to perform SA in the context of a PA and to provide some advise about their use. In this context, though local methods, screening methods and global methods provide relevant information about the system model, screening methods and global methods fit better within the structure of a PA, and that is the reason to focus all efforts on them. In order to illustrate the use and peculiarities of some specific techniques, a couple of simplified PA models will be used extensively along the whole text. When deemed necessary, well-known mathematical functions and examples from other areas of nuclear safety will be used. Additionally, some examples coming from applications developed within other tasks performed under PAMINA will also be used.

2. Notation

rv : random variable; iid : independent, identically distributed (for random variables)

X, Y : random variables;

$(X_1, X_2, ..., X_n)$: a random sample ;

$(X^{(1)}, X^{(2)}, ..., X^{(n)})$: a random ordered sample ;

$(X^{[1]}, X^{[2]}, ..., X^{[n]})$: a random re-ordered sample according to another variable;

$(x_1, x_2, ..., x_n)$: the corresponding realization of the random sample;

$(x^{(1)}, x^{(2)}, ..., x^{(n)})$: the corresponding ordered realization of the random sample;

$(x^{[1]}, x^{[2]}, ..., x^{[n]})$: the corresponding re-ordered sample according to another variable; $X = (X_1, ..., X_k)$: a random vector of size k (generally representing the input of the numerical model) ;

$x = (x_1, ..., x_k)$: a realization of a random vector of size k ;

$Y = f(X)$: the output of the numerical model $f : IR^k \rightarrow IR$

$y = f(x)$: the output of the numerical model for the sample

μ : mean of a random variable; E(X) : mathematical expectation of the rv X;

σ^2 : variance of a random variable; Var(X), $V(X)$: variance of the rv X;

$\bar{x}$: sample mean;

σ_x^2, s^2 : sample variance; σ_x, s : sample standard deviation;

3. Factors and interactions

In general, the model studied is a function of the input parameters, $Y = f(X)$. Each component of the vector $X = (X_1, ..., X_k)$ is called (input) parameter, main effect or (input) factor. The target of SA techniques is to identify which factors are important.

Nevertheless, as it was said in the introduction, the function $Y = f(X)$ may be very complex. The effect of a single factor may be very complex. A model may depend only on one factor but that dependence could have a very complex structure, which would make difficult the study of such a model. Additionally, models may have and may not have interactions. We say that two parameters or factors do not interact when the effect of increasing one of them a given quantity does not depend on the values that the other actually takes. If the effect of increasing one of the parameters does depend on the value of the second parameter, then both factors do interact. In order to understand this concept more easily, let us consider the following two models whose support is the square $[0,1]\times[0,1]$

$$y = 0.2x_1 + x_2 \tag{3.1}$$

and

$$y = 0.2x_1 + x_2 + 2x_1x_2. \tag{3.2}$$

Both are plotted in figures 3.1 and 3.2. As it can be seen, in the first model, the effect of increasing x_2 in one unit is increasing y in one unit, independently of the value of x_1, while in the second model the increase of the output is one unit when x_1 takes value 0 and three units when x_1 takes value 1. When performing SA studies, it is important to identify important factors and to estimate the single effect of each factor, but it is also very important to identify important interactions between factors. The interaction shown in this example is a second order interaction because involves only two input factors, but a model that contains k input factors may contain interactions up to order k. Section 5.3.1 contains the High Dimensional Model Representation (HDMR) of any integrable function, which introduces in a more formal (mathematical) way the concept of factor and interaction of any order.
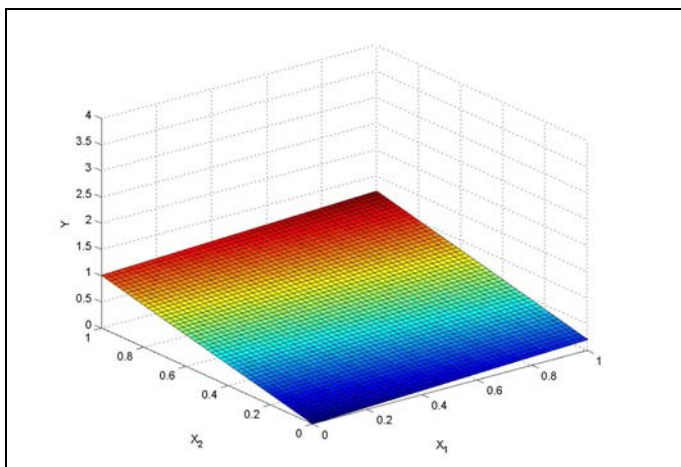
Figure 3.1.- Mathematical model with two input parameters with no interaction	**Figure 3.2.-** Mathematical model with two input parameters with interaction
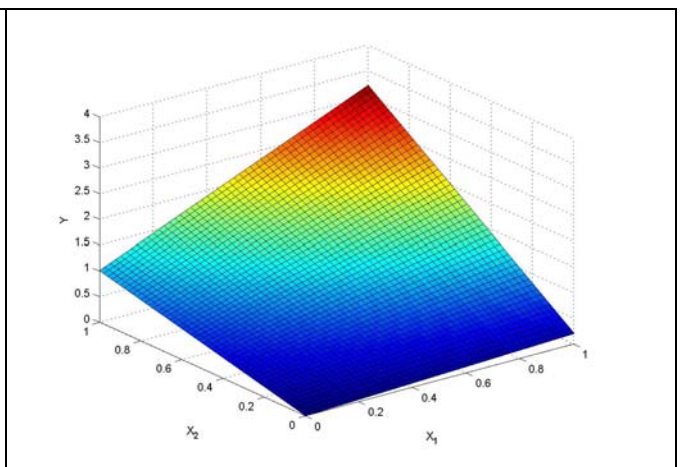
4. Screening methods

Screening methods proceed from the field of *design of experiments*, which was originally developed by statisticians working in the area of agriculture improvement and industrial processes, in both cases to optimise production. Typically they were applied to problems that involved from a few input factors to a few tens. Screening methods are widely used because whenever we deal with problems involving a large number of inputs it is quite reasonable to think that only a few of them are really influent. This

is known as the principle of parsimony or Occam's razor. Recently, its use has been promoted in the area of SA of computer codes, extending their application to models that have many input parameters.

In the next pages we develop the following screening methods: full factorial design, fractional factorial design, Morris' OAT design, and sequential bifurcation.

4.1.   *Full factorial designs*

In many studies developed to find the most important input factors or input parameters in a computer code, the approach used by researchers was the 'one at a time approach' (OAT). Usually, in this type of study, a reference point is considered, usually in the middle of the range of variation of the input factors involved, and one by one, the value of each parameter is changed, getting the value of the output variable of interest for each case. This way, the impact of each input factor may be estimated. Nevertheless, long ago, see Box and Draper (1987) and Box et al. (1978), this method was shown to be inefficient from two points of view, firstly because interactions are ignored and secondly because estimation errors are larger (this second issue is only important in the case of real experimentation, where experimental variability plays an important role, not being a matter of concern in the case of computer experiments).

The theory of two level factorial experiments (2^k designs) was developed in the late 1950's and early 1960's and was further improved with the introduction of fractions (2^{k-p} designs). Though it got its maturity in the late 1980's, it is still nowadays a fertile area of research in Statistics. In a 2^k design of experiments we consider that our computer model has k parameters and we are interested in studying its behaviour at two different levels. Those levels are called lower and upper level, or levels -1 and $+1$ respectively. In principle, those levels may be either quantitative or qualitative. In a numeric continuous parameter, levels -1 and $+1$ could represent the minimum and the maximum values in its range; in a qualitative parameter it could be, for example, the use of two different competing available submodels to simulate a given physicals or chemical phenomenon. Let us consider a computer model with only three parameters A, B and C. In order to study it, we will assume the following structure

$$y = \mu + \frac{a}{2} X_1 + \frac{b}{2} X_2 + \frac{c}{2} X_3 + \frac{(ab)}{2} X_1 X_2 +$$
$$+ \frac{(ac)}{2} X_1 X_3 + \frac{(bc)}{2} X_2 X_3 + \frac{(abc)}{2} X_1 X_2 X_3$$

(4.1.1)

where μ is the mean of the output variable and X_1, X_2 and X_3 represent respectively factors A, B and C and take values -1 when the factor is in its lower level and $+1$ when the factor is in its upper level. This model is completely general, its validity is restricted to the aforementioned values of the different parameters (-1 and +1) and has eight parameters: μ, a,…,(abc). The parameters in parentheses do not represent products; (ab) is the parameter associated to the interaction between factors A and B, not the product of a and b. Parameter (ab) accounts for the different impact of factor A depending on the level of factor B and vice versa. Consequently, we need at least eight runs of the computer code to be able to estimate all the parameters. The selection of the eight needed runs is done according to Table 4.1.1, crossing in all possible ways (8) the levels of the three factors. Columns headed by two or three letters are associated to the corresponding interactions and their elements (-1 or +1) are computed by

multiplying the corresponding values in the columns headed by A, B and C. The last column represents the results obtained when running the code, so y_{+1+1-1} is the value of the output variable obtained when running the code after setting factors A and B in their lower levels and factor C in its upper level. Figure 4.1.1 shows in a 3-D plot the points selected in a 2^3 full design.

Table 4.1.1.- 2^3 complete design

I	A	B	C	AB	AC	BC	ABC	Y
+1	-1	-1	-1	+1	+1	+1	-1	y_{-1-1-1}
+1	+1	-1	-1	-1	-1	+1	+1	y_{+1-1-1}
+1	-1	+1	-1	-1	+1	-1	+1	y_{-1+1-1}
+1	+1	+1	-1	+1	-1	-1	-1	y_{+1+1-1}
+1	-1	-1	+1	+1	-1	-1	+1	y_{-1-1+1}
+1	+1	-1	+1	-1	+1	-1	-1	y_{+1-1+1}
+1	-1	+1	+1	-1	-1	+1	-1	y_{-1+1+1}
+1	+1	+1	+1	+1	+1	+1	+1	y_{+1+1+1}

In order to estimate any parameter of the statistical model we will use the following scalar product

$$\hat{\theta}_i = \frac{1}{k/2} \mathbf{V}_i^{\mathrm{T}} \mathbf{Y} \qquad (4.1.2)$$

where $\mathbf{V_i}$ stands for the vector shown in Table 4.1.1 corresponding to factor or interaction i, $\mathbf{Y}$ stands for the vector of the output variable values and $\mathbf{T}$ stands for transpose vector. Applying equation 4.1.2 to estimate the impact on the output of moving from the lower to the upper level of factor C, we see that it is the average of the four output values that have their third subindex set to +1 less the average of the four output values that have their third subindex set to −1 (the average of the last four values less the average of the four first values). Equation 4.1.2 and table 4.1.1 allow us to know how to estimate the effect of factors and interactions. The mean is estimated, when needed, using the column of values under I and using k instead of $k/2$ in the denominator of equation 4.1.2.

Two methods are available to decide if the impact of a factor or of an interaction is relevant (statistically significant): The Mean Absolute Deviation (MAD), see Peña and Juan (1992), and the Analysis of Variance (ANOVA), see Box and Draper (1987). ANOVA is used when the number of factors and interactions in the statistical model is larger than the number of observations. Otherwise the MAD is used. Nevertheless, these tests are based on the fact that data come from experiments affected by random perturbations, which is not the case when working with computer models. The authors of this document consider that the results of such tests, when the data analysed have been obtained from computer codes, should be taken as indications, rather than as real statistical tests. This is due to the fact that the conditions under which those tests were developed are seriously violated (there is no experimental variability).
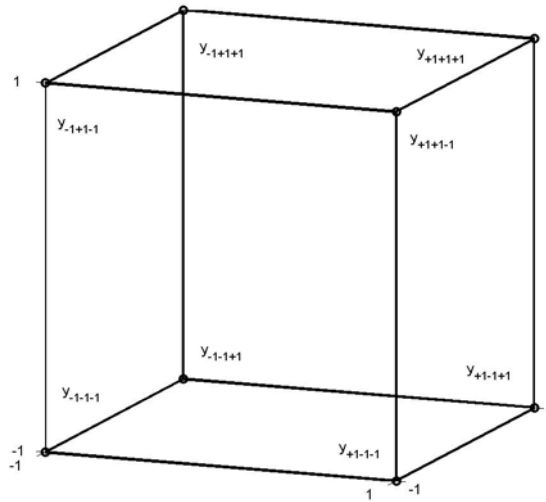
Figure 4.1.1.- Selection of design points in a 2^3 full factorial design

The main problem associated to 2^k experiments is the large number of computer runs demanded when the number of input factors increases. Just think that we will need 2^{10} runs to analyse a ten-factor model. The theory of fractional factorial two level designs was developed to cope with this problem.

4.2.   Fractional factorial design

A fraction of a design is a part of the runs considered in a complete 2^k design that fulfils some specific conditions. We also call it 2^{k-p} design. In this case we assume that most of the high order interactions are not relevant and we can dedicate the output variables to estimate the effect of factors and low order interactions, mainly second order interactions. For example, in Table 4.1.1 we could consider only the runs where ABC takes value +1. We represent this fact by

$$\mathbf{I = ABC} \tag{4.2.1}$$

because we have chosen the runs that have value +1 simultaneously in columns I and ABC, and we call it the generator of the fraction. This (half) fraction is shown in Table 4.2.1. Figure 4.2.1.a shows graphically what points are considered in the sample. This fraction is called half-fraction because half of the design points are kept.

Table 4.2.1.- 2^{3-1} design with generator **I=ABC.**

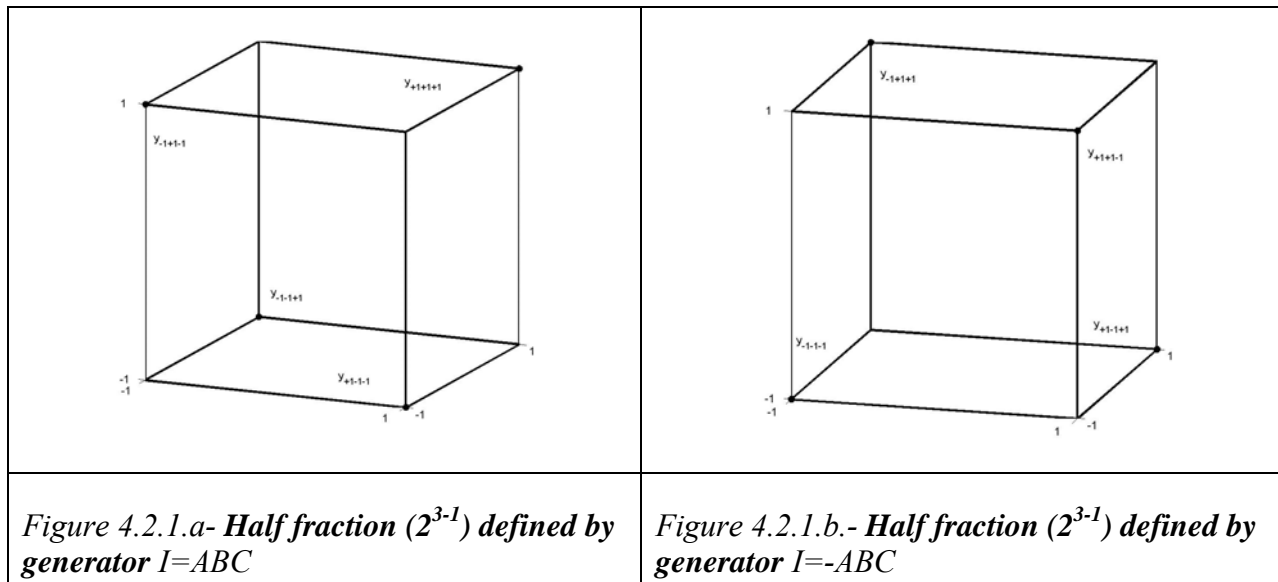| I	A	B	C	AB	AC	BC	ABC	Y
+1	+1	-1	-1	-1	-1	+1	+1	y_{+1-1-1}
+1	-1	+1	-1	-1	+1	-1	+1	y_{-1+1-1}
+1	-1	-1	+1	+1	-1	-1	+1	y_{-1-1+1}
+1	+1	+1	+1	+1	+1	+1	+1	y_{+1+1+1}

In Table 4.2.1 we can see that columns under A and BC are identical, and the same happens with B and AC, and with C and AB. This means that, when applying equation 4.1.2 to estimate the different factors in equation 4.1.1, the estimators, and hence the estimates, for A and BC will be equal, as will be for B and AC, and for C and AB. In these cases we say that those effects are aliased and we are not able to distinguish them from this design of experiments. Figure 4.2.1.b shows graphically the design points used when the half-fraction defined by the generator **I=-ABC** is considered.

Figure 4.2.1.a- **Half fraction (2^{3-1}) defined by generator** *I=ABC*	*Figure 4.2.1.b.-* **Half fraction (2^{3-1}) defined by generator** *I=-ABC*

The three main ideas on which the construction of these designs are based are:
— the sparsity of effects principle (when there are many inputs, the output is likely to depend significantly only on few main and low-order interaction effects)
— the projection property (they can be projected into larger designs in the subset of significant factors)
— sequential experimentation (two or more fractional design can be combined into a larger design, getting information about the system in a sequential manner, up to the point when no more relevant information is expected).

The main references on the sections concerning factorial designs are Box and Draper (1987), and Myers and Montgomery (2002). For specific utilisation in the SA context, see also Saltelli et al. (2008) or Saltelli et al. (2000). Additional important concepts not dealt with in the previous pages, as for example the resolution of a design, are further explained in these references.

4.2.1.   Example of application of a fractional factorial design

A fractional factorial design is used to identify, under given accident conditions in an advanced nuclear reactor, what factors affect more the increase of temperature in the hottest fuel bar (clad temperature), which is the output variable. Seven factors are considered in the study, which are coded as **A**, **B**, **C**, **D**, **E**, **F** and **G**. Conditional on the expensive cost of each run in terms of computational time (the computer code used is the Computational Fluid Dynamics -CFD- code CFX10, which takes approximately half a day per run), we decided to start the analysis with a saturated 2^{7-4} design (a saturated design is created by accommodating one new factor per column of interactions in an original full factorial design). This design allows studying the effect of seven parameters with only 8 runs. The order of the input parameters was not selected at random. In principle, the a priori most important parameters are in the first positions, while the a priori less important are in the last positions.

Table 4.2.1.1 provides the saturated design selected for this first experiment and the results obtained after running the code. For creating this design, we have taken a 2^3 design as a starting point for A, B and C, which will be saturated to produce a one-sixteenth replicate of a 2^7 design (it is called one-sixteenth because only one-sixteenth of the points in the 2^7 design are kept). This design is created by using column AB for accommodating factor D, column AC for E, BC for G and ABC for F, in such a way that the generators of this saturated fraction will be

$$\mathbf{I = ABD = ACE = BCG = ABCF} \quad . \tag{4.2.1.1}$$

By multiplying these generators in all possible ways, we get the complete set of generators that defines this 2^{7-4} design. The result is

$$\begin{aligned}
\mathbf{I} &= \mathbf{ABD = ACE = BCG = ABCF = BCDE =} \\
&= \mathbf{ACDG = CDF = ABEG = BEF = AFG =} \\
&= \mathbf{DEG = ADEF = BDFG = CEFG =} \\
&= \mathbf{ABCEFG}
\end{aligned} \tag{4.2.1.2}$$

The alias structure is computed by multiplying the full set of generators by the different main factors and interactions. In this first step we are far more interested in main factors than in interactions. In the following lines we show the alias structure of main factors, considering only interactions up to order 2

$$\hat{a} \rightarrow A + BD + CE + FG$$
$$\hat{b} \rightarrow B + AD + CG + EF$$
$$\hat{c} \rightarrow C + AE + BG + DF$$
$$\hat{d} \rightarrow D + AB + EG + CF \qquad (4.2.1.3)$$
$$\hat{e} \rightarrow E + AC + DG + BF$$
$$\hat{f} \rightarrow F + CD + BE + AG$$
$$\hat{g} \rightarrow G + BC + DE + AF$$

So, for example, when estimating the effect of factor E, the estimation will be contaminated by the effect of interactions AC, DG and BF, while when estimating factor A, its estimation will be contaminated by the effect of interactions BD, CE and FG.

Table 4.2.1.1.- 2^{7-4} saturated design corresponding to generators given in equation 4.2.1.1.

I	A	B	C	D=AB	E=AC	G=BC	F=ABC	Y
+1	-1	-1	-1	+1	+1	+1	-1	1768
+1	+1	-1	-1	-1	-1	+1	+1	1033
+1	-1	+1	-1	-1	+1	-1	+1	1715
+1	+1	+1	-1	+1	-1	-1	-1	1013
+1	-1	-1	+1	+1	-1	-1	+1	1826
+1	+1	-1	+1	-1	+1	-1	-1	1045
+1	-1	+1	+1	-1	-1	+1	-1	1781
+1	+1	+1	+1	+1	+1	+1	+1	1003

The estimates of the statistical model considered are

$$\hat{a} = -749 \qquad \#$$
$$\hat{b} = -40 \qquad *$$
$$\hat{c} = +31.5 \qquad *$$
$$\hat{d} = +9 \qquad\qquad (4.2.1.4)$$
$$\hat{e} = -30.5 \qquad *$$
$$\hat{f} = -7.5$$
$$\hat{g} = +3.5$$

The meaning of these results is that, when moving A from its lower level to its upper level, on average, Y decreases 749 K. In the case of B, Y decreases 40 K. The same change in C produces an average increase of 31.5 K in Y and so on. We can see that there are three sets of results, -749 (A), those whose absolute value is around 35 (B, C and E) and the rest (D, F and G). When applying the MAD method to determine which factors are relevant, we identify only A (#). Nevertheless, we should also pay attention to B, C and E, since changes of approximately 35 degrees in Y are certainly significant from a physical point of view. The problem we are facing now is how to proceed to get more information from our computer model. From equation 4.2.1.3 we know that these estimates are aliased with second and higher order interactions and we do not know which of them are responsible for the estimates obtained, or if all of them are equally responsible. In most of the models, factors are more important than second order interactions and these are more important than third order interactions and so on. So, in principle, these results are telling us that the most important factor, by far, is A, followed by B, C and E. Certainly, the inclusion of E among the most influent factors on Y is a surprise. We did not

expect this input parameter to be an important one. In order to detect if E is really important or if the estimate of its effect is due to interactions AC, DG or BF, and also to look for confirmation about the importance of the other three factors, we will take another saturated 2^{7-4} design. In order to make estimable all factors, with no alias with second order interactions, we will take the following generators

$$I = -ABD = -ACE = -BCG = ABCF \qquad (4.2.1.5)$$

The design points corresponding to this new fraction and the results obtained are shown in Table 4.2.1.2. Both fractions together will be used as a new joint design to continue the study. This means putting together all the information contained in Tables 4.2.1.1 and 4.2.1.2. A peculiarity of this new design is that, in addition to allowing estimating all main factors with no alias with second order interactions, it is a full 2^4 design in A, B, C and any of the other four factors excluding F. The full set of generators of this joint design is

$$\begin{aligned} I &= BCDE = ABEG = ABCF \\ &= CDEG = ADEF = CEFG = BDFG \end{aligned} \qquad (4.2.1.6)$$

where the three first are the original set of generators used to build up the design.

Table 4.2.1.2.- 2^{7-4} saturated design corresponding to generators given in equation 4.2.1.5.

I	A	B	C	D=-AB	E=-AC	G=-BC	F=ABC	Y
+1	-1	-1	-1	-1	-1	-1	-1	1768
+1	+1	-1	-1	+1	+1	-1	+1	1038
+1	-1	+1	-1	+1	-1	+1	+1	1701
+1	+1	+1	-1	-1	+1	+1	-1	1009
+1	-1	-1	+1	-1	+1	+1	+1	1824
+1	+1	-1	+1	+1	-1	+1	-1	1038
+1	-1	+1	+1	+1	+1	-1	-1	1783
+1	+1	+1	+1	-1	-1	-1	+1	1010

The results of this design are summarised in Table 4.2.1.3. In the first column we represent the factors, in the second one the sum of squares or part of the total variability of the output variable explained by each factor, in the third one the P-value of the associated F-test and in the fourth column the estimate of the effect of each factor. No interaction is shown in the table because all second order interactions are aliased with other second order interactions. The column under the heading P-value indicates if the factor produces a statistically significant effect (values under 0.05). The closer the P-value is to 1.0, the less important that factor is and the closer it is to 0, the more important it is. In an ANOVA table, the way to decide if a factor is statistically significant is to compare the variability it is able to explain with the residual variability.

Table 4.2.1.3.- Results, for A, B, C, D, E, F and G, of the design obtained by joining the two saturated designs in Tables 4.2.1.1 and 4.2.1.2.

Source	Sum of squares	P-value	Estimate	
A	2.23 E+06	0.00	*	-747.125
B	6601	0.01	*	-40.625
C	4389	0.03	*	33.125
D	14	0.88		-1.875
E	14	0.88		1.875
F	189	0.58		-6.875
G	105	0.68		5.125
Residual	4614			

From this table we can get two straightforward conclusions: 1) D, E, F and G are completely irrelevant factors, especially D and E and 2) comparing these results with the results in 4.2.1.4, since E has been shown to be irrelevant, some of the interactions AC, DG or BF could have some relevance, and could be responsible for the estimate obtained in 4.2.1.4. In principle, non-relevant factors only rarely could have important interactions, this fact bring us to consider DG a very unlikely interaction. Regarding BF, it could also be considered unlikely. So, the main candidate to be responsible for the non-expected result obtained in 4.2.1.4 is AC. This rationale brings us to consider as a likely statistical model to explain the sampled results obtained with our computer code a model with only A, B and C as main factors, plus all their interactions, formally a model exactly the same as in equation 4.1.1. Studying this model doesn't demand to get new computer runs. Table 4.2.1.4 is the ANOVA table of such a study.

Table 4.2.1.4.- Results, for A, B, C and all their interactions, of the design obtained by joining the two saturated designs in Tables 4.2.1.1 and 4.2.1.2.

A	2.23 E+06	0.00	*	-747.125
B	6601	0.00	*	-40.625
C	4389	0.00	*	33.125
AB	473	0.00	*	10.875
AC	4193	0.00	*	-32.375
BC	11	0.50		1.625
ABC	189	0.02	*	-6.875
Residual	171			

The results in Table 4.2.1.4 may be summarised as follows: 1) All main factors considered in this model (A, B and C) and their interactions are statistically significant, with the exception of BC, and 2) the residual variability is really tiny, only 171 (171+11 if we exclude BC and add the variability explained by this factor to the residual variability), which is less than 5% of the residual variability obtained with the previous model. This reduction in non-explained variability means that with only A, B and C and their interactions we are able to explain much more data variability. So, the statistical model selected in this study to explain the physical model data would be the one provided in equation 4.1.1 with the estimates provided in Table 4.2.1.4. This means that the main factor in this model is A, followed by B and C. The impact of B and C on the output Y is one order of magnitude smaller than A's. The interaction between A and C has shown to be almost as strong as main factors B and C. The only third order interaction is significant, though from a physical point of view it cannot be considered relevant given its impact on the output (its effect is less than one third the effect of any of the relevant second order interactions).

This example shows that fractional factorial experiments are very well suited to develop sequential experiments, where new design points are selected according to the information obtained in previous steps. Seven factors have been studied using only 16 computer runs, identifying three factors and two second order interactions as relevant. In our opinion, this strategy is adequate when the number of input factors is moderate, but it may become very difficult to implement when the number of input factors is large (several tens or larger). In those cases, more automatic and efficient methods should be used, as for example the methods that will be explained in sections 4.3 and 4.4.

4.3. Morris' one-at-a-time (OAT) design

Morris (1991) thought that, for any model output Y differentiable at least once with respect to each input, Y's partial derivative with respect to X_i at a given point **x** of Y's support is a measure of the influence of X_i on Y. This way, Morris considers that if the partial derivative is
1. 0 over all values of **x**. Then X_i's effect on Y is negligible.
2. a non-zero constant over all values of **x**. Then X_i's effect on Y is linear and additive.
3. a non-constant function of only X_i. Then X_i's effect on Y is non-linear.
4. a non-constant function of one or more X_j ($j \neq i$). Then X_i's effect on Y involves interactions with other input factors.

Morris considers that the target of a moderate-cost experimental design should be to provide information to classify input factors in three sets:
1. factors that have negligible effect on the output
2. factors that have linear effects without interactions
3. factors that have non-linear effects and/or interactions .

In order to get this target, the author proposes to normalise the input space to the unit k-dimensional hypercube ($[0,1] \times \ldots \times [0,1]$) and create a p-level grid in this hypercube (each input X_i is allowed to take values in the set $\{0, 1/(p-1), 2/(p-1), \ldots, 1\}$). The *elementary effect* of a given input factor X_i at a given point **x** within the unit hypercube is defined as

$$D_i(\boldsymbol{x}) = \frac{y(x_1, \ldots, x_{i-1}, x_i + \Delta, x_{i+1}, \ldots, x_k) - y(\boldsymbol{x})}{\Delta} \qquad (4.3.1)$$

where $x_i \leq 1-\Delta$ and Δ is a multiple of $1/(p-1)$. Under these circumstances, the number of elementary computable effects within the unit hypercube for each input factor is $p^{k-1}[p-\Delta(p-1)]$, which follows a given discrete probability density function. A large measure of central tendency (mean) of the distribution corresponding to input factor X_i means that this factor has an important influence on Y. A large measure of spread (standard deviation) shows that either interacts strongly with other factors or its impact on the output is not linear, or both. In next section we describe the sampling plan designed by Morris to estimate both measures in an efficient manner.

4.3.1. The implementation of the method

Morris proposed to create random sample paths along a grid like the one mentioned in last section to compute the distribution of elementary effects for each input factor. In order to get those random sampling paths, the following matrices and vectors are created

1. the (k+1)×k matrix **B**, which contains one zero followed by k ones in the first column, two zeros followed by k-1 ones
2. the k×k diagonal matrix $\mathbf{D}^*$ that takes values either –1 or +1 as diagonal elements with probability 0.5 each.
3. the (k+1)×k matrix $\mathbf{J}_{k+1,k}$ of ones (all its elements are 1), and the column matrix $\mathbf{J}_{k+1,1}$ (all its elements are 1)
4. the k×k random permutation matrix $\mathbf{P}^*$, whose columns contain all one
5. the random vector (k components, one per input factor) $\mathbf{x}^*$, whose components are taken at random from the set {0, 1/(p-1),2/(p-1),…,1-Δ}, each with equal probability.

Additionally, Morris suggests to restrict the application of the method to Δ=p/[2(p-1)], p taking an even value. This way, the matrix $\mathbf{B}^* = (\mathbf{J}_{k+1,1}\mathbf{x}^* + (\Delta/2)[(2\mathbf{B} - \mathbf{J}_{k+1,k})\mathbf{D}^* + \mathbf{J}_{k+1,k}])\mathbf{P}^*$ is created. This is a (k+1)×k matrix, which is called by Morris a random *orientation* of matrix B and defines k+1 points in the grid (each row of $\mathbf{B}^*$ is a point). Each point is created from the previous one adding a quantity +Δ or -Δ to only one of its components. This way, comparing the k+1th row with the first one, their components will be the ones of the first row plus or less Δ. These k+1 points are used to estimate one *elementary effect* per input factor; k in total.

Let us consider a specific case to see how a random orientation is created. Let us consider k=3, p=6 and Δ=p/[2(p-1)]=2/5. Under these circumstances

$$
\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{pmatrix}, \ \Delta\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{2}{5} & 0 & 0 \\ \frac{2}{5} & \frac{2}{5} & 0 \\ \frac{2}{5} & \frac{2}{5} & \frac{2}{5} \end{pmatrix}, \ \mathbf{D}^* = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \ \mathbf{J}_{4,3} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \ \mathbf{P}^* = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},
$$

(4.3.1.1)

and

$$
(1/2)[(2\mathbf{B} - \mathbf{J}_{k+1,k})\mathbf{D}^* + \mathbf{J}_{k+1,k}] = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix},
$$

(4.3.1.2)

As can be seen, each column of matrix $(1/2)[(2\mathbf{B} - \mathbf{J}_{k+1,k})\mathbf{D}^* + \mathbf{J}_{k+1,k}]$ is the same as the corresponding one of B or the same one substituting zeros by ones and vice versa. Observe that, while **B**, Δ**B** and $\mathbf{J}_{4,3}$ are fixed after setting k, p and Δ, $\mathbf{D}^*$ and $\mathbf{P}^*$ are the result of sampling and could take different values in different applications (for k=3, there are 8 -2^3- different possibilities for $\mathbf{D}^*$ each one with probability 1/8 and 6 possibilities -3!- for $\mathbf{P}^*$ each one with probability 1/6). Let us suppose that after sampling according to bullet 5, the vector $\mathbf{x}^{*T}$=(3/5,1/5,0) is obtained (**T** stands for transpose). Then $\mathbf{B}^*$ becomes

$$(\mathbf{J_{k+1,1}x^*} + (\Delta/2)[(2\mathbf{B} - \mathbf{J_{k+1,k}})\mathbf{D^*} + \mathbf{J_{k+1,k}}])\mathbf{P^*} = \left[\begin{pmatrix} \tfrac{3}{5} & \tfrac{1}{5} & 0 \\ \tfrac{3}{5} & \tfrac{1}{5} & 0 \\ \tfrac{3}{5} & \tfrac{1}{5} & 0 \\ \tfrac{3}{5} & \tfrac{1}{5} & 0 \end{pmatrix} + \begin{pmatrix} 0 & \tfrac{2}{5} & \tfrac{2}{5} \\ \tfrac{2}{5} & \tfrac{2}{5} & \tfrac{2}{5} \\ \tfrac{2}{5} & 0 & \tfrac{2}{5} \\ \tfrac{2}{5} & 0 & 0 \end{pmatrix} \right] \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \tfrac{3}{5} & \tfrac{3}{5} & \tfrac{2}{5} \\ 1 & \tfrac{3}{5} & \tfrac{2}{5} \\ 1 & \tfrac{1}{5} & \tfrac{2}{5} \\ 1 & \tfrac{1}{5} & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

. (4.3.1.3)

The first 4×3 matrix within brackets on the right hand side is the result of $\mathbf{J_{k+1,1}x^*}$. It provides the starting point for selecting a sample path in input space (*orientation*). The second 4×3 matrix within brackets on the right hand side is the result of $(\Delta/2)[(2\mathbf{B} - \mathbf{J_{k+1,k}})\mathbf{D^*} + \mathbf{J_{k+1,k}}]$, which sets what component of the vector in the input space we have to modify (adding or subtracting a quantity Δ=p/[2(p-1)]=2/5) to get the next sample point. Adding both first rows, we get the first point in the sample path: (3/5,3/5,0). Successive rows in the second matrix within brackets indicate that the second point is obtained by adding 2/5 to the first component of the first point, the third point is obtained by subtracting 2/5 to the second component of the second point and the last one is obtained by subtracting 2/5 to the third component of the third point. Multiplying by $\mathbf{P^*}$ a permutation of columns is obtained, which introduces symmetry in the treatment given to all components of the input parameter space (in this example the first and the second components are exchanged, remaining the third one unchanged). Finally, Matrix $\mathbf{B^*}$ becomes

$$\mathbf{B^*} = \begin{pmatrix} \tfrac{3}{5} & \tfrac{3}{5} & \tfrac{2}{5} \\ \tfrac{3}{5} & 1 & \tfrac{2}{5} \\ \tfrac{1}{5} & 1 & \tfrac{2}{5} \\ \tfrac{1}{5} & 1 & 0 \end{pmatrix} \qquad (4.3.1.4)$$

Computing the model output Y for each row of $\mathbf{B^*}$ and applying expression 4.3.1 an elementary effect may be estimated for each input factor. For example, an elementary effect for the third input factor is estimated by applying 4.3.1 to the output obtained for the third and fourth rows of $\mathbf{B^*}$. In order to get an estimation of the whole distribution of elementary effects for each input factor, this process must be repeated as many times as considered necessary, for example *r* times. So, the design matrix will be

$$\mathbf{X} = \begin{pmatrix} \mathbf{B^*_1} \\ \mathbf{B^*_2} \\ ... \\ \mathbf{B^*_r} \end{pmatrix} . \qquad (4.3.1.4)$$

This way, the total number of code runs or design points is (k+1)×r.

Morris' design is considered a OAT design because only one factor is changed in two successive experiments. Examples of such designs are presented in figure 4.3.1.1:

- to the left, $d=2$, $r=5$ and $p=5$; an individual OAT is in this case formed for instance by the points A, B, C.
- to the right, $d=3$, $r=1$ and $p=1$, the only individual OAT design is (A, B, C, D).
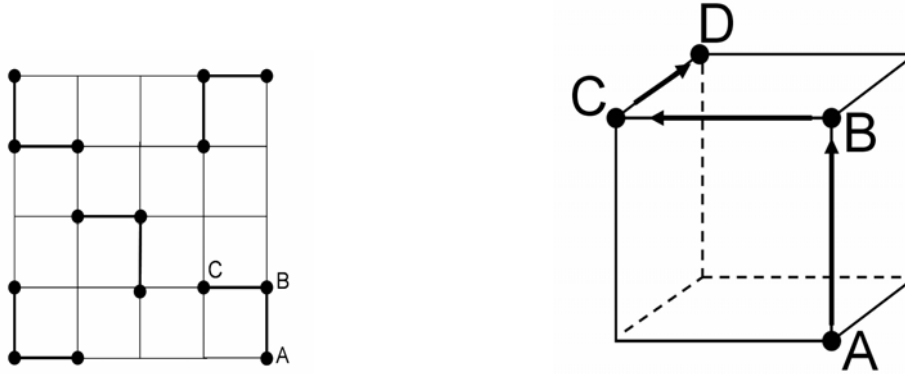
Figure 4.3.1.1.- Example of Morris' OAT designs in 2 (left) and 3 (right) dimensions

If we call $\{D_i^1, \ldots, D_i^r\}$ to the set of estimates obtained for the elementary effects of factor X_i when applying 4.3.1 to the adequate sample points, and use the usual estimators of the mean and the standard deviation (the sample mean $\overline{D}_i$ and the sample standard deviations s_i), these estimates may be used as sensitivity estimates. The interpretation of these sensitivity indices is as follows:
- a large measure of the central tendency (i.e. $\overline{D}_i$) indicates an input with an important overall influence on the output;
- a large measure of dispersion (i.e. s_i) means that there are significantly different values in the corresponding elementary effect distribution and consequently the dependence of the output on the considered factor is either nonlinear or in interaction with other factors (just think that D_i is an approximation of the derivative of Y with respect to X_i).

The plot of the means versus the standard deviations of these samples will indicate how to split the factors into the three categories mentioned at the beginning of this section:
- low values of the means → factors with negligible effect on the output.
- large values of the means and low values of the standard deviations → factors with linear effects but without interactions.
- large values of the means and of the standard deviations → factors with non-linear effects and/or interactions.

The main advantage of this screening method is its relatively low computational cost, (k+1)×r (linear function of the number of inputs factors), while the main disadvantage that it is not possible to estimate individual interactions among factors. Another disadvantage the presents the method is the possible lack of importance attributed to input factors whose variation may produce large elementary effects positive but also negative. In that case, cancellations made during the averaging process of computing a mean can render misleading results.

After the publication of Morris' original work, several authors have proposed the following modifications:

1. In order to avoid one of the disadvantages just mentioned (cancellation of terms of different sign in the estimation of the mean, underestimating the importance of some relevant factors), Campolongo et al. (2007) propose to replace the mean of the elementary effects by the mean of their absolute values (see also Saltelli et al. (2004)).
2. Campolongo et al. (2007) propose to use a space filling design (SFD) for choosing the starting point for each individual OAT.
3. Pujol (2008) propose to use a simplex design instead of a OAT design, which has two main advantages:
   - better properties in terms of projection on subspaces.
   - possibility to use a pre-existing database of simulations to form the simplex design.

4.3.2. Example of application of Morris' OAT design

The classical example for this screening method is the Morris analytical function (Morris (1991)), which has $k = 20$ input factors and is defined by:

$$y = \beta_0 + \sum_{i=1}^{20} \beta_i w_i + \sum_{i<j}^{20} \beta_{i,j} w_i w_j + \sum_{i<j<l}^{20} \beta_{i,j,l} w_i w_j w_l + \sum_{i<j<l<s}^{20} \beta_{i,j,l,s} w_i w_j w_l w_s \qquad (4.3.2.1)$$

where $w_i = 2(x_i - \frac{1}{2})$ except for $i = 3,5,7$ where $w_i = 2(1.1x_i /(x_i + .1) - \frac{1}{2})$ and x_i are rv following uniform distributions on [0,1], i.e. $x_i \sim U(0,1)$. The β coefficients are:

$$\beta_i = 20, i = 1,\ldots,10, \quad \beta_{i,j} = -15, \ i,j = 1,\ldots,6, \quad \beta_{i,j,l} = -10, \ i,j,l = 1,\ldots,5,$$
$$\text{and } \beta_{i,j,l,s} = 5, \ i,j,l,s = 1,\ldots,4.$$

The rest of the first and second order coefficients were generated independently from a normal distribution $N(0,1)$ and the rest of the third and fourth order coefficients were set to 0. The number of levels for each factor is $p = 4$, and the number of individual OAT designs is $r = 4$. In this case there will be $21 \times 4 = 84$ code runs. Using these 84 values of y, a random sample of 4 elementary effects is observed for each input factor; for each of these random samples the mean of the absolute values and the standard deviations are computed.

The plot of the means of the absolute values of the elementary effects versus their standard deviations is showed in figure 4.3.2.1, and allows us to separate the factors into the 3 groups:
   - the ones with negligible effect on the output : factors 11 to 20;
   - the ones with linear effects without interactions : factors 8, 9, 10;
   - the ones with non-linear effects and/or interactions : factors 1,…, 7.
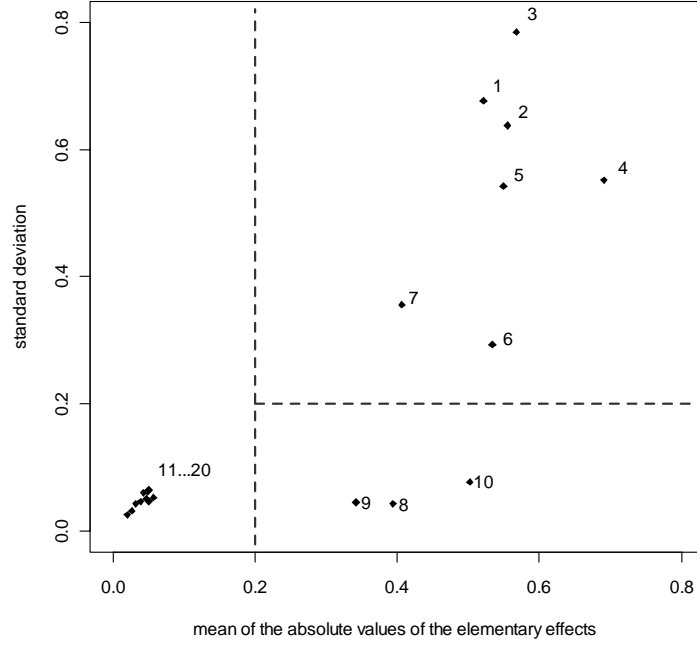
Figure 4.3.2.1.- Results of the Morris' method applied to Morris' function, the dotted lines are separators for the 3 groups

4.4. Sequential bifurcation

This method has been developed in Bettonvil and Kleijnen (1996) and is a group screening technique. It allows screening a large number of factors. One of the main advantages is that the number of simulations to be performed is smaller than the number of factors to be screened. The drawback is that the relationship between each input factor and the output has to be monotonic and that the type of monotony has to be known a priori. Whenever this condition is fulfilled, the method is very effective.

4.4.1. The method

The method is a group screening one; at each iteration the most influent group is split into two subgroups. This is the way the most influent factors are identified. In order to measure the influence of each group, the method offers two alternatives:

1. either the relationship between the inputs and the output is linear, i.e. the following model holds

$$Y = \beta_0 + \beta_1 X_1 \ldots + \beta_k X_k \qquad (4.4.1.1)$$

2. or the relationship is linear with interactions, i.e. the following model holds

$$Y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{\substack{i,j=1 \\ i<j}}^{k} \gamma_{ij} X_i X_j . \qquad (4.4.1.2)$$

Each factor X_i is uniformly varying on $[-1,1]$. The signs of the β_i coefficients have to be known (without any loss of generality, we can suppose that they are positive).

The effect of the group of factors included between the ith factor and the jth factor is denoted by e_{ij} and is defined as the difference between:

— the average of the output Y knowing that the factors $X_i \ldots X_j$ have been fixed at the value 1 (or the conditional expectation of Y knowing that $X_i=1,\ldots,X_j=1$) and
— the average of the output Y knowing that the factors $X_i \ldots X_j$ have been fixed at the value -1 (or the conditional expectation of Y knowing that $X_i=-1,\ldots,X_j=-1$).

This yields:

$$e_{ij} = E\big[Y \mid X_i = 1,\ldots,X_j = 1\big] - E\big[Y \mid X_i = -1,\ldots,X_j = -1\big] = 2\big(\beta_i + \ldots + \beta_j\big) \quad (4.4.1.3)$$

The way to estimate these effects is slightly different if we use the linear model or the linear with interactions model. For the first case (3.4.1) we use:

$$e_{ij} = f(x_{(j)}) - f(x_{(i-1)}) \qquad (4.4.1.4)$$

and for the second one, (3.4.2), we use:

$$e_{ij} = \frac{\big(f(x_{(j)}) - f(-x_{(j)})\big) - \big(f(x_{(i-1)}) - f(-x_{(i-1)})\big)}{2}, \qquad (4.4.1.5)$$

where $x_{(l)}$ denotes the vector where the first l components are set to 1 and the following ones are set to -1.

In order to estimate the effect of one group we need 2 runs for the first type of model, and 4 runs for the second type. The procedure being iterative, the total number of simulations may be diminished: at every iteration, we split a group for which we have already estimated the effect in two subgroups for which we want to estimate the effects. We need then only one supplementary run for the linear model and two for the linear with interactions model to perform the estimations of the effects of the subgroups. The maximal number of runs is then $k+1$ for the linear model and $2k$ for the linear with interactions model. In practice, this computational cost is even lower, because the iterations should stop when all the influent parameters have been found.
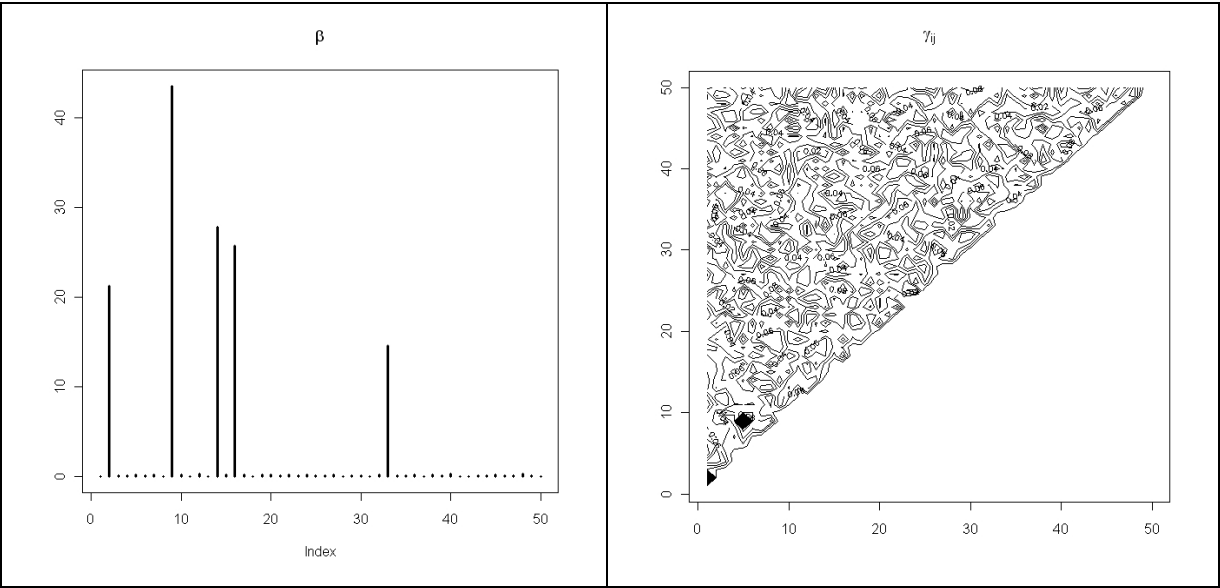
4.4.2. Example

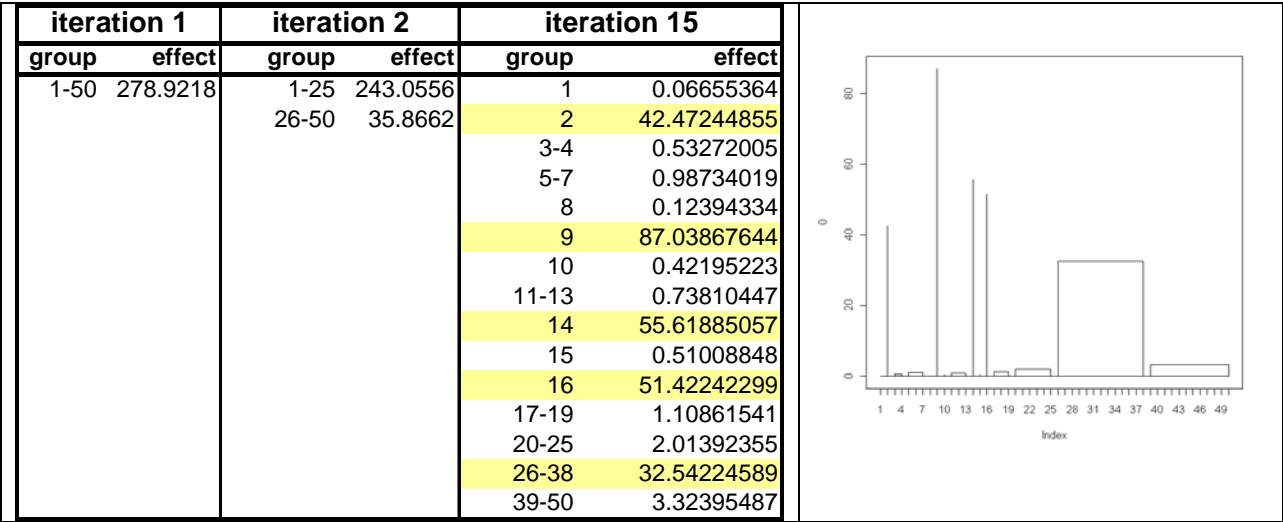This is an analytic example available in the package *sensitivity* in R. It is a linear model with interactions:

$$Y = \beta_0 + \sum_{i=1}^{d} \beta_i X_i + \sum_{\substack{i,j=1 \\ i<j}}^{d} \gamma_{ij} X_i X_j \qquad (4.4.2.1)$$

There are $d=50$ independent input factors. The coefficients of the model are represented in figure 4.4.1.1. There are 5 important β coefficients. As for the γ coefficients, they are varying uniformly between 0 and 0.1 except for two values: $\gamma_{12} = 5$ and $\gamma_{59} = 12$.

After performing 15 iterations of this method, the 4 largest main effects are identified as the variables number 9, 14, 16, 2 (in decreasing order of the corresponding main effects) and the group formed by the variables 26 – 38 have the next greatest main effect (by construction, the variable number 33 has the next most important main effect). The results for the 1st, 2nd and 15th iteration of the method are given in figure 4.4.1.2. The results have been obtained using expression 4.4.1.5.

Figure 4.4.2.1.- Coefficients of the model (4.4.2.1)

iteration 1		iteration 2		iteration 15		
group	effect	group	effect	group	effect	
1-50	278.9218	1-25	243.0556	1	0.06655364	
		26-50	35.8662	2	42.47244855	
				3-4	0.53272005	
				5-7	0.98734019	
				8	0.12394334	
				9	87.03867644	
				10	0.42195223	
				11-13	0.73810447	
				14	55.61885057	
				15	0.51008848	
				16	51.42242299	
				17-19	1.10861541	
				20-25	2.01392355	
				26-38	32.54224589	
				39-50	3.32395487	

Figure 4.4.2.2.- Results for the sequential bifurcation example - to the left the groups of variables together with their estimated effects for iteration number 1, 2 and 15; to the right the same results for the 15th iteration but in a graphical representation.

5. Global methods

Global methods focus on how the whole input space (taking into account input distributions) maps into the output space. Four sets of global methods have been considered in this study: graphical methods, Monte Carlo based methods, variance decomposition based methods and distribution sensitivity methods. In the following pages most interesting techniques are described.

5.1. Graphical methods

Graphical methods are important tools to support, guide and interpret the results provided by numerical sensitivity analysis techniques. They may also be used as standalone techniques to get further insights about the model under study. Widely used graphical tools to analyse relations between inputs and outputs are scatter-plots and cobweb plots. In this report we also include the recently revived and improved Contribution to the Sample Mean Plots (CSM plots). Extensions of some of them are also considered.

5.1.1. Scatter-plots

Let us call $X=(X_1,X_2,...,X_k)$ the vector of input parameters and Y to a given scalar output variable. For a given input X_i, the scatter-plot is the projection of the sample points (X,Y) on the (X_i,Y) plane. This representation allows the examination of the dependence between Y and X_i. Scatter-plots are very helpful to identify linear relations, monotonic relations and the existence of thresholds among other potential trends. The use of transformations may also provide a lot of information about input/output relations. They may be used as supporting material to explain the results obtained by means of numeric sensitivity techniques, but also to prevent the use of inadequate techniques. The most frequently used transformations are

1. Logarithmic (base 10)
2. Ranks

Both transformations are useful, though they also have their shortcomings. The logarithmic transformation is more intuitive, but may not be used when a fraction of the values (usually output values) take value 0, unless the software at hand has been designed to cope with such problem and it avoids null values before applying the transformation. The transformation into the ranks is not affected by such problem. In this transformation the smallest sample value is transformed into 1, the second smallest into 2 and so on until the largest value, which is transformed into n (sample size). So, the new scale is between 1 and n. Nevertheless, this transformation is not so intuitive (just think that two values separated by several orders of magnitude can get contiguous ranks, say h and h+1, the same as two other very close values). In case of ties, equal values are assigned the same rank. For example, if three values are equal, and should occupy ranks t-1, t and t+1, all of them are assigned rank [(t-1)+t+(t+1)/3]=t. The strongest reason to use the rank transformation in SA is that this transformation converts any monotonic relation between two variables into a linear one. Table 5.1.1.1 provides an example of a transformation into ranks. In many cases, the combined information provided by scatter-plots obtained using different transformations will help understanding the set of data under analysis.

Table 5.1.1.1.- Sample and corresponding ranks.

| Parameter sample	
Raw values	Ranks
18	2
96	7
45	5.5
31	3
15	1
99	8
45	5.5
39	4

Figures 5.1.1.1 to 5.1.1.6 are examples of scatter-plots obtained from the Level_E test case described in annex 1 using a simple random sample of size 459. Figures 5.1.1.1 to 5.1.1.3 are the scatter-plots for the dose at 10^4 y versus a composite input parameter (created ah-hoc as a function of other input parameters) for the raw values, the logarithms and the ranks respectively. Figure 5.1.1.1 hardly allows see anything related to the dependence input-output, except some kind of possible monotonocity. Figure 5.1.1.2 shows the same values transformed into their decimal logarithms. The software used has deleted all points whose x coordinate was null, keeping the ranges of the non-null values in both axes. In fact only the output variable contains null values, which is due to a computational threshold set to 10^{-15} (all output values below this threshold are set to zero). This figure shows the spread of the non-null part of the output over 10 orders of magnitude. Figure 5.1.1.3 shows the ranks of the output versus the rank of the input. Immediately, it can be recognised that around 350 out of 459 runs produced null output values (see the horizontal line and remind the rule given above to assign ranks in case of ties). Additionally, a threshold may be seen in the plot; roughly the 70 smallest input samples produced output values above the threshold (non-null) and no such output was obtained for input values above the 170th smallest one.

Figures 5.1.1.4 to 5.1.1.6 describe the behaviour of the peak dose versus the input parameter W. Figure 5.1.1.4 does not provide much information about the dependence between input and output due to the spread of both over several orders of magnitude. Figure 5.1.1.5s show the linear dependence between the logarithms of both variables. Figure 5.1.1.5 shows the monotonic relation between both. The three plots show that, if a regression model is used study the sensitivity of the peak dose versus W, it would be more convenient either to study the relation between the logarithms of both or to study their monotonic relation. In fact, their Pearson correlation coefficient takes value –0.25 while the Pearson correlation coefficient between both logarithms takes values –0.69 and their Spearman rank correlation is –0.71.
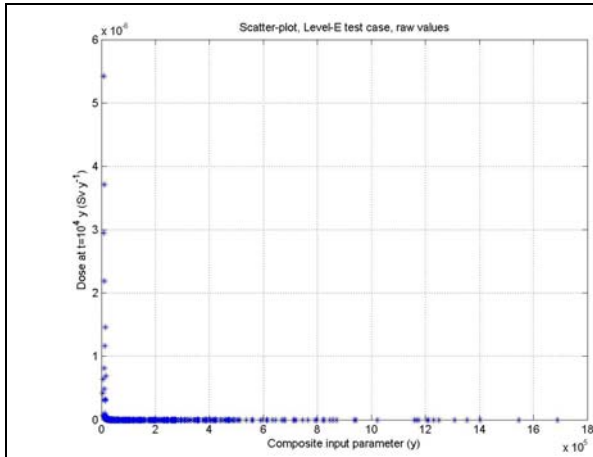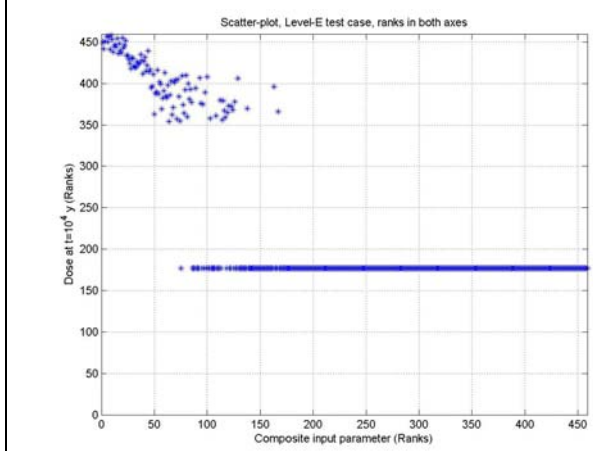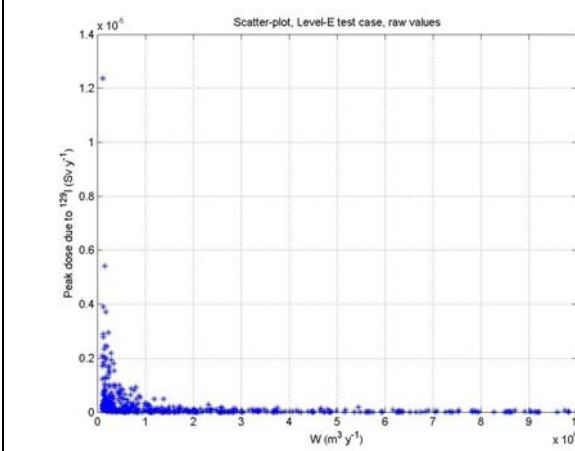
Figure 5.1.1.1.- Dose at 10^4 y versus composite input parameter (raw values in both axes). Level_E test case.
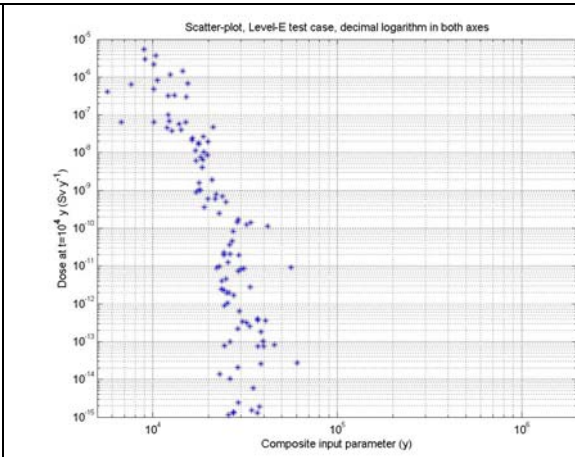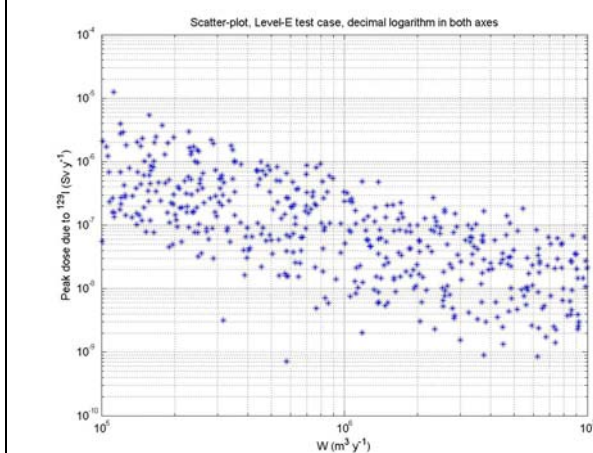

Figure 5.1.1.2.- Dose at 10^4 y versus composite input parameter (decimal logarithm in both axes). Level_E test case.
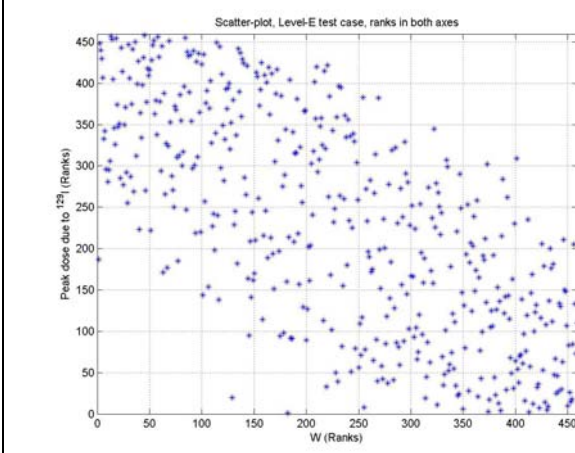

Figure 5.1.1.3.- Dose at 10^4 y versus composite input parameter (ranks in both axes). Level_E test case.

Figure 5.1.1.4.- Peak dose versus W (raw values in both axes). Level_E test case.

Figure 5.1.1.5.- Peak dose versus W (decimal logarithm in both axes). Level_E test case.

Figure 5.1.1.6.- Peak dose versus W (ranks in both axes). Level_E test case.

Scatter-plots may also be used to study the dependence between output variables. Though this cannot be considered proper SA, it may provide very useful information about the system model. Figures 5.1.1.7 and 5.1.1.8 show, respectively, the dependence between the total peak dose and the peak dose due to ^{129}I and between the total peak dose and the peak dose due to ^{36}Cl in a given repository. In the upper-right corner of figure 5.1.1.7 and in the central part of figure 5.1.1.8, two rows of points set on

straight lines may be identified. In fact both lines are close to the straight-line y=x. This means that the largest peak doses are produced mostly by ^{129}I while ^{36}Cl is responsible for the smallest peak doses.

| **Figure 5.1.1.7.-** Total peak dose versus peak dose due to ^{129}I in a system model (decimal logarithm in both axes). | **Figure 5.1.1.8.-** Total peak dose versus peak dose due to ^{36}Cl in a system model (decimal logarithm in both axes). |
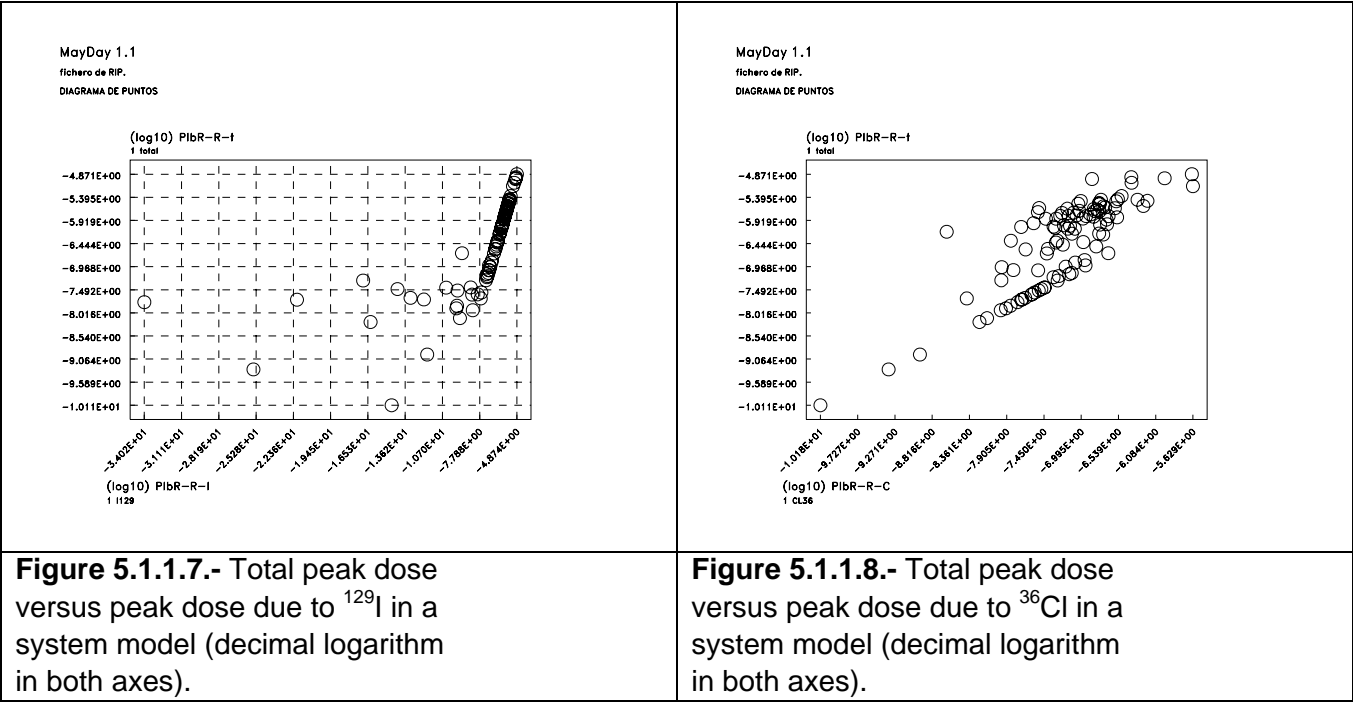
Three-dimensional (3-D) scatter-plots or XYZ plots show the projection of the sample points (**X**,Y) on the (X$_i$,X$_j$,Y) space. The information they are able to provide is also valuable. The extraction of such information is limited, though challenging, due to obvious interpretation problems when a 3-D figure is shown on a 2-D display. Software packages that allow changing the angle of the view may enhance and broaden their applicability. As in the case of normal 2-D scatter-plots, the use of convenient scale transformations may help identifying interesting model features. Figures 5.1.1.9 and 5.1.1.10 show the 3-D scatter-plots of the peak dose versus V$_1$ and W. In the first one raw values are shown in the three axes, while both input parameters have been transformed into their decimal logarithms in the second one. While figure 5.1.1.10 shows clearly the effect of the interaction between both inputs on the output, this is not seen so clearly in figure 5.1.1.9 (largest outputs values are obtained when V$_1$ takes very large values and W takes very small values).

| **Figure 5.1.1.9.-** Peak dose due to | **Figure 5.1.1.10.-** Peak dose due |

26
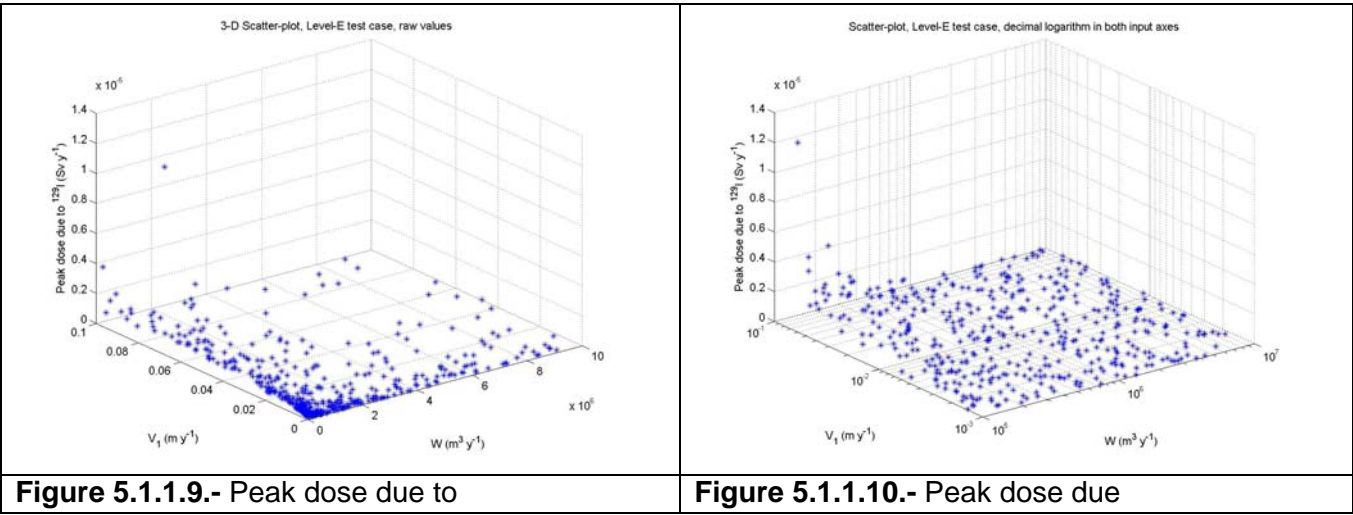
| ^{129}I versus V_1 and W (raw values in all axes). Level_E test case.	to ^{129}I versus V_1 and W (decimal logarithm in both input axes). Level_E test case.

Extensions of scatter-plots are matrices of scatter-plots and overlay scatter-plots. Matrices of scatter-plots show simultaneously, under a matrix format, the scatter-plots of different pairs of input parameters/output variables. They allow identifying quite quickly the pairs with most remarkable relations, but they are also affected by the loss of accuracy due to including several plots in a reduced space, typically a fraction of a page. Overlay scatter-plots allow showing the same plot the scatter-plot of one output and several inputs. In order to distinguish the points corresponding to different inputs, different symbols (dots, circles, crosses, diamonds, etc.) and different colours are used. Frequently only a few inputs may be represented due to either the different scales used in the plot or to the difficulties to interpret correctly so many overlapped different symbols.
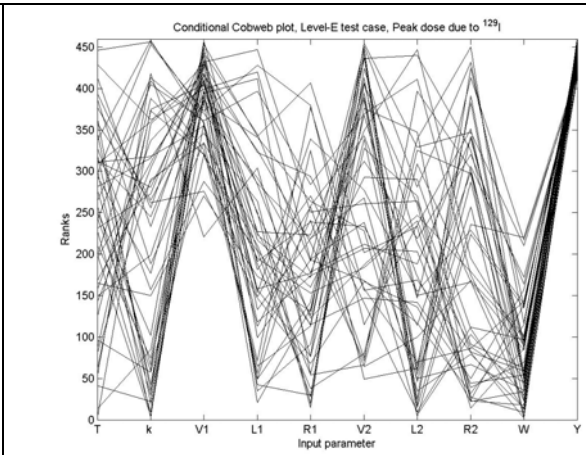
5.1.2. Cobweb plots

Cobweb plots have been designed to show multidimensional samples in a two-dimensional graph, see Cooke and Van Noortwijk (1999). Vertical parallel lines separated by equal distances are used to represent the sampled values of a given number of inputs/outputs, usually not more than ten or twelve, in order to keep the plot sufficiently clear. Each vertical line is used for a different input/output and either the raw values or the ranks may be represented (either raw values or ranks in all lines, never mixed). Sampled values are marked in each vertical line and jagged lines connect the values corresponding to the same run. Coloured lines can be used to display the different regions of any input parameter or output variable. Moreover, flexible conditioning capabilities enable an extensive insight into particular regions of the mapping. The cobweb plots are sometimes provided together with 'cross densities' showing the density of line crossings midway between the vertical axes. Therefore, an informed and careful analysis of cobweb plots enables the characterisation of dependence and conditional dependence.

Figures 5.1.2.1 to 5.1.2.4 are cobweb plots that show the relation between the 9 input parameters considered in the Level_E test case and the output variable peak dose. All these cobweb plots are based on the ranks; no one is based on the raw values. Figure 5.1.2.1 is an unconditional cobweb plot, where coloured lines have been used to distinguish between runs related to the lower (yellow), lower-medium (green), upper-medium (blue) and upper (black) quartile regions of the output variable. The output variable is represented in the last column; the rest of the columns are dedicated to each input parameter according to the legend behind them. Paying attention to what colours predominate in each region of each input parameter, we may get an idea about the complex relation between inputs and output.
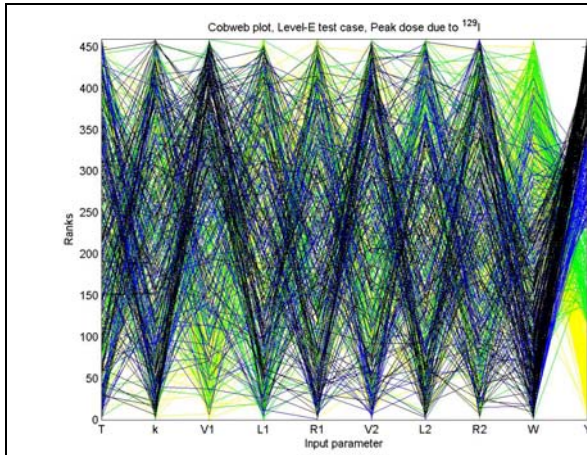
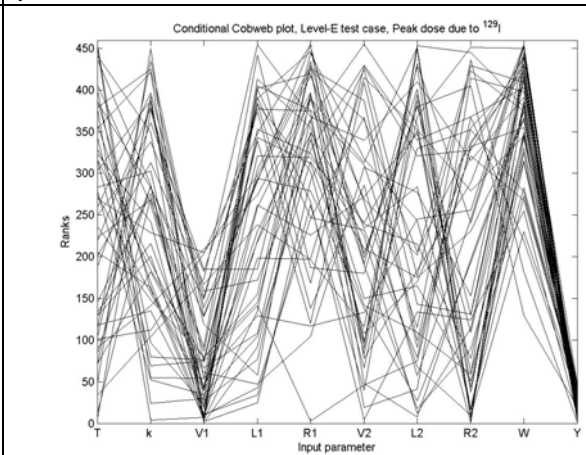|	
Figure 5.1.2.1.- Unconditional cobweb plot (ranks) for the peak dose due to ^{129}I and all input parameters. Level_E test case.	**Figure 5.1.2.2.-** Conditional cobweb plot (ranks, condition: 10% largest output values) for the peak dose due to ^{129}I and all input parameters. Level_E test case.
Figure 5.1.2.3.- Conditional cobweb plot (ranks, condition: 10% intermediate output values) for the peak dose due to ^{129}I and all input parameters. Level_E test case.	**Figure 5.1.2.4.-** Conditional cobweb plot (ranks, condition: 10% smallest output values) for the peak dose due to ^{129}I and all input parameters. Level_E test case.
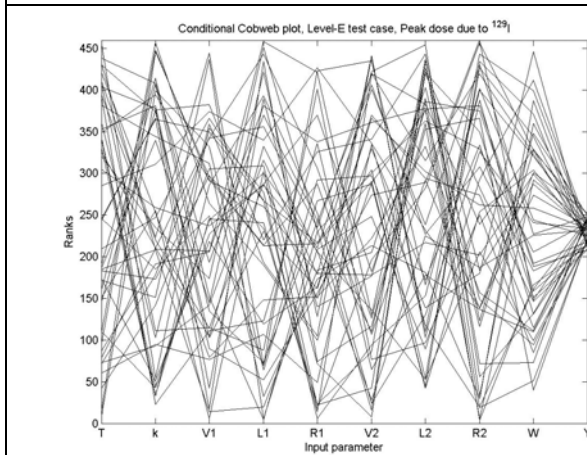
Nevertheless, the authors of this report find more convenient the use of conditional cobweb plots. In this type of plots only a fraction of the runs obtained are represented. Figure 5.1.2.2 shows the runs that produced the 10% highest peak doses. We can see in the plot that these doses are always obtained when W takes values below its own median and V1 takes values above its own median (with only one exception). For the rest of the input parameters, such a clear relation cannot be observed, in fact, what we see is that almost any region of the other input parameters may produce large values of the output. In order to produce figure 5.1.2.3, we have conditioned the plot to the 10% of intermediate values of the peak dose. In this case, no clear relation may be seen between that region of the output and any specific region of any input parameter. In figure 5.1.2.4 the 10% of smallest values of the peak dose have been selected to condition the plot. It may be seen that those outputs are related to small values of V_1 and high values of W and R_1.

5.1.3.   Contribution to the sample mean plot (CSM plot)

The Contribution to the Sample Mean plots (CSM plots) were developed in the early 1990's. Sinclair (1993) was investigating the way infinitesimal changes to the probability density function (*pdf*) of an input variable X_i can alter overall features of performance (mean and variance of *Y*). The marginal dependence of *E(Y)* on the various input factors was employed and portrayed graphically. Nevertheless, Sinclair considered his 'sensitivity plot', as he called it, as a useful graphic tool for estimating sensitivity 'by eye'.

In order to create a Contribution to the Sample Mean Plot (CSM plot), we assume that a random sample **S** of size n of the input factors and the corresponding sample of the output variable considered are available. We do also assume that the random sample has been obtained via a sampling technique that introduces no bias. Suitable sampling schemes might be, for example, simple random sampling, LHS and proportional stratified sampling, while non-proportional stratified sampling (i.e.: optimal stratified sampling) or importance sampling would not be acceptable schemes. To build the CSM plot for a given input variable, let us say X_i, and the response *Y*, the following procedure is applied:

1.   the realisations of X_i are sorted generating the series of values $\{x_i^{(1)}, x_i^{(2)}, ..., x_i^{(n)}\}$,
2.   the corresponding series of values $\{y^{[1]}, y^{[2]}, ..., y^{[n]}\}$ is created,
3.   the ancillary variable M_i is defined, whose sampled values are obtained from the sampled values of X_i and *Y* as

$$ m_i^q = \frac{1}{n} \sum_{j=1}^{q} y^{[j]}, \quad q = 1, 2, ..., n , \qquad (5.1.3.1) $$

4. M_i is normalised dividing the values m_i^q by the sample mean of *Y*,
5.   The sampled values of M_i are plotted versus the cumulative distribution of X_i.

Using the approach described previously, the estimates of the following quantity are represented on the y-axis

$$ \frac{\int_{\Omega_{\mathbf{x}(-i)}} d\mathbf{x}_{(-i)} \int_{x_i \leq x_i^q} f_{\mathbf{x}}(\mathbf{x}) y(\mathbf{x}) dx_i}{\int_{\Omega_{\mathbf{x}}} f_{\mathbf{x}}(\mathbf{x}) y(\mathbf{x}) d\mathbf{x}} , \qquad (5.1.3.2) $$

which is the fraction of the output mean corresponding to values of X_i smaller or equal to its quantile of order *q*. The subindex (-i) indicates the exclusion of the input parameter X_i. In expression 5.1.3.2 $\Omega_{\mathbf{x}}$, $\Omega_{\mathbf{x}(-i)}$ and $x_i \leq x_i^q$ mean that the respective integrals are computed on the whole input space, on the whole input space excluding input parameter X_i and on X_i up to its quantile of order *q*. Given the definition of the plot in step 5, each point in a CSM plot represents the fraction of the output mean due to any given fraction of smallest values of an input parameter.

A CSM plot represents indirectly a contribution to the variance. Indeed, if for a given quantile range, all realisations of *Y* are very close to the mean, this also implies that there is a very low contribution to the variance. Any significantly low and significantly high contribution to the mean represents locally an important contribution to the variance.

Contribution to the sample mean plot
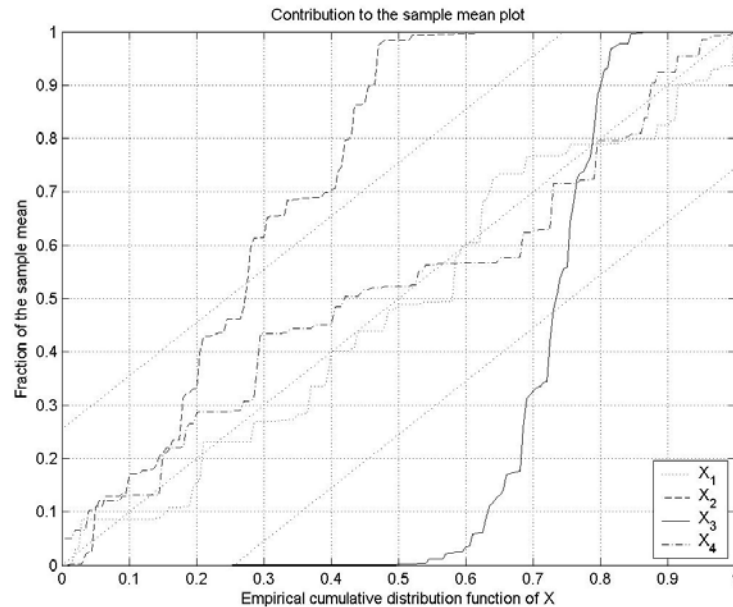
Figure 5.1.3.1.- CSM plot for four input parameters and an output variable. The 95% confidence band around the diagonal is included .

Figure 5.1.3.1 shows the CSM plot for one output variable and four input parameters of a simulation model. The sample used, a simple random sample, contains 100 Monte Carlo realisations. Each curve is characterised by a fairly different behaviour. Roughly speaking, each region of equal probability of X_1 and X_4 are responsible for the same percentage of the output sample mean (the line is always close to the diagonal). Regarding X_2, its 60% smallest values are responsible for more than 99% of the output sample mean. Only values of X_3 between its median and its quantile of order 0.85 produce output values significantly different from 0. This region is responsible for more than 99% of the output sample mean. Other similar statements could be made, as for example: values between the quantiles of order 0.70 and 0.80 of X_3 produce more than 55% out the output sample mean. The meaning of the two dotted lines parallel to the diagonal will be explained later in this section.

The main use of CMS plots is to identify important input parameters. In principle, an input parameter could be considered as non-important if knowing its value doesn't provide much information about the value of the output, which means that the value of the output depends more on the values of other input parameters than on its own values. In this case, a completely non-important variable, in relation with a given output variable would be characterised by the fact that the values of both would be randomly associated. High, low and intermediate output values would be equally obtained in any region of a non-important variable, which means that a behaviour similar to the ones of X_1 and X_4 in figure 5.1.3.1 could be expected (lines close to the diagonal).

Input parameters could be considered as important if knowing its value provides relevant information about the value of the output. This means that concentrations of low, intermediate and high values of the output could be expected to be associated to different regions of the input parameter. This is the type of behaviour observed in input parameters X_2 and X_3 in figure 5.1.3.1, where clear departures from the diagonal can be observed.

The most similar plot available in scientific literature is the Lorenz curve for measuring the concentration of wealth; see Lorenz (1905). The Lorenz curve shows the distribution of income among

families in a given region or country. In the y-axis the percentage of income is represented, while in the x-axis the percentage of poorest families is represented. Each point of the curve represents the percentage of the total income obtained by a given percentage of the poorest families. A potential Lorenz curve could show that the 50% of the poorest families obtain 10% of the total income while the 5% wealthiest families get 40% of the income, which would be the case of a country with very unequal distribution of wealth. The diagonal represents an ideal situation where all families get the same income. These curves are frequently used to compare the situation in different countries or the evolution of the concentration of wealth over time in a country. The main differences between these plots and CMS plots are that these plots are usually created from aggregated data obtained via official statistics instead of using the raw sampled data and that, by construction, the Lorenz curve takes all their values on or below the diagonal.

CMS plots should be used only when non-biasing sampling schemes have been applied to obtain the data. If a sampling technique that introduces biases is used (i.e.: importance sampling) regions of equal length in the x-axis do not represent any more equally likely regions. Under this circumstance the diagonal doesn't hold as the reference to measure lack of importance, and the interpretation of the plot becomes really difficult and different for different input parameters since the bias introduced could vary among the different parameters.

CSM plots as designed by Sinclair (1993) are suitable only for output variables that take positive or null values. Scale transformations, as for example taking the absolute value or shifting the output variable values by adding the opposite of its minimum value, are pertinent in case of either having output variables that either take only negative values or take negative and positive values.

A particularly relevant feature of these plots is the possibility of representing in the same figure the relation of many input parameters with one output variable. This is a clear advantage with respect to scatter-plots. Though overlay scatter-plots provide some flexibility regarding this point, the extraction of relevant information from this representation is limited. CMS plots could also be used to study the relation between one input parameter and many output variables, even to represent the relation between different inputs and outputs. Nevertheless, the authors of this report consider the first use (several input parameters and one output variable) as the standard and most useful one.

CMS plots provide interesting information about the relation between inputs and outputs but it is only qualitative. After the analysis of figure 1, it could be concluded that X_2 and X_3 are important parameters producing a visible impact on the output variable, while X_1 and X_4 are not. This is a statement based on our visual perception of the information contained in the plot, which is not supported by any numeric measure so far. In fact, no measure is available yet even to rank the input parameters in order of importance; who has a stronger impact on the output, X_2 or X_3? Could the behaviour shown by X_3 have been obtained just by chance?

Bolado et al. (2008) have proposed a test to study when the deviations from the diagonal observed in a CSM plot are statistically significant and when they may be obtained due to randomness. This is a permutations based test, which is explained in the next paragraphs

The inputs plus the output of interest are grouped in a (X,Y) random vector containing k+1 components characterised by its joint multivariate probability density function $f_{X,Y}(\mathbf{X},Y)$. An input parameter X_i is completely non-important if the value taken by the output depends only on the values of the other k-1 input parameters. Under this hypothesis, the conditional distribution of Y given the value of X_i is

independent of that value. In other words, this means that the conditional distribution of Y given a value of X_i equals the marginal distribution of Y ($f_{Y|X_i}(y|X_i = x_i) = f_Y(y)$), whatever the values of X_i.

When the factor Xi is not influential on the output Y, if a permutation is carried out on the realisations of Xi, since Y only depends on the other (unchanged) k-1 inputs, the realisations of Y are not altered and the same curve in CSM plot will be obtained. However, when Xi is somehow influent on Y, the permutation will lead to 2 distinct curves.

Let us consider a sample **S** of size n of the vector (**X**,**Y**). Computing all possible permutations (n!), all possible CSM curves can be drawn for the pair (X_i,Y). In order to restrict the analysis to the information already available in the sample (no additional model run), only one model input is permuted at the time.

The rationale carried out in the last two paragraphs characterise the structure of the test to be developed. In order to set up this test, the hypothesis under which the test may be applied is specified, the null and the alternative hypotheses are provided and the test statistic is defined:

- *Assumption*: a sample **S** of size N for the vector (**X**,**Y**) is available. The sample of **X** has been obtained via a random sampling technique which does not introduce any bias (see section 2). The sample of Y has been obtained via simulation using the sample of **X**.
- *Hypotheses* (null hypothesis H_0 and alternative hypothesis H_1):
  - H_0: $f_{Y|X_i}(y|X_i = x_i) = f_Y(y)$ $\forall x_i \in R_i$,
  - H_1: $\exists x_i, x_i' \in R_i / f_{Y|X_i}(y|x_i) \neq f_{Y|X_i}(y|x_i')$, where R_i is the support of X_i.
- *Test statistic*: D_m, the maximum vertical distance (absolute value) between the line built according to the procedure described in section 2 and the plot diagonal. This is the measure of discrepancy with the null hypothesis.

The distribution of the test statistic can be computed using the permutations described previously. However, since the total number of permutations (n!) increases rapidly with the sample size n (ex: 10!= 3628800), only part of them are carried out in practice. The larger n and the number of permutations considered, the better the approximation of the "maximum distance to the diagonal" distribution. Note that the permutations do not imply any additional model run. It is important to emphasize that since the distribution is calculated from the original sample, a different sample will provide another estimate for the "maximum distance to the diagonal" distribution.

Given a sample of (**X**,**Y**), the "sensitivity test" for a factor X_j can be summarised by the steps described below:

1. Estimate the distribution of the test statistic via Monte Carlo:
    a. An important number (ex. 10^3) of permutations are carried out for the values of X_j.
    b. A CMS plot is generated for each permutation.
    c. The test statistic D_m (maximum distances to the diagonal) is computed for each CSM.
    d. The cumulative distribution function of D_m is estimated using standard statistical methods (empirical distribution function and all quantiles via order statistics).
2. Set a critical level α to perform the test (typically 0.10, 0.05, 0.01)
3. $D_{m\alpha}$, the value of the test statistic corresponding to α (quantile 1- α of the test statistic under the null hypothesis) is computed.
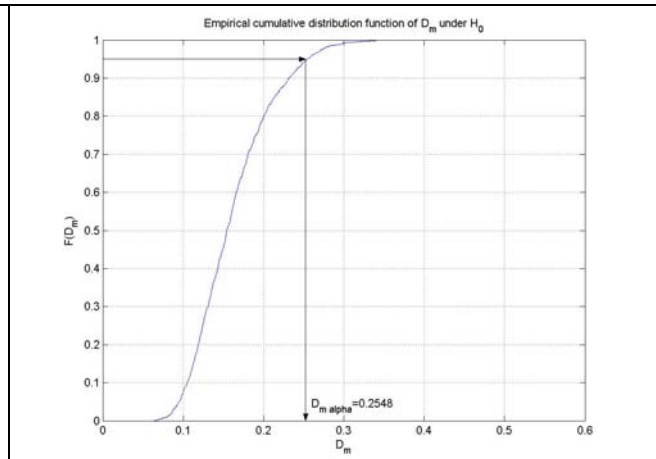
4. The CMS plot is generated with the original sample and the corresponding test statistic D_{mj} is computed.
5. The null hypothesis H_0 is rejected if $D_{mj} > D_{m\alpha}$, otherwise it is accepted.

In order to illustrate the approach described previously, the procedure is applied in a stepwise manner and the parameters importance is inferred. Figure 5.1.3.2 shows the results of computing 10^3 permutations and creating the corresponding lines in a CMS plot with the same data used to get figure 5.1.3.1. The maximum distance to the diagonal has been computed for each line. Figure 5.1.3.3 shows the empirical cumulative distribution obtained from that set of distances. When $\alpha=0.05$, $D_{m\alpha}=0.2548$ and the maximum distances to the diagonal obtained for X_1, X_2, X_3 and X_4 are, respectively, 0.0850, 0.5058, 0.5692 and 0.1394. When comparing these four values with $D_{m\alpha}$, the null hypothesis should be rejected for X_2 and X_3, and it should be accepted for X_1 and X_4. This means that a maximum distance to the diagonal like the one obtained for X_1 or larger could have been quite likely achieved under the null hypothesis (approximate p_value=0.982). That is also the case of X_4 (p_value=0.628) while that is not true for X_2 and X_3, in fact such large distances are very unlikely under the null hypothesis. The p-values are smaller than 0.001 in both cases and the estimate of the quantile of order 0.999 of D_m under the null hypothesis is 0.3527. P-values for each input may be estimated by interpolation in the empirical distribution function of D_m.
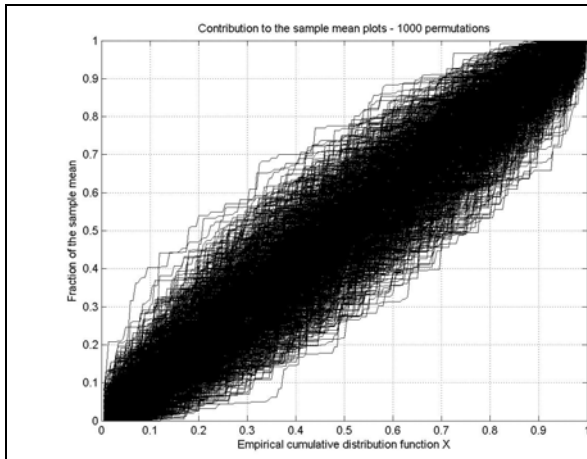
Figure 5.1.3.2.- 1000 CSM lines obtained by permuting the values of the output. The data used are the same used to create figure 5.1.3.1.	Figure 5.1.3.3.- Empirical cumulative distribution function of D_m under the null hypothesis (non important input parameter).

The result of the test may also be seen graphically in figure 5.1.3.1. The dotted lines parallel to the diagonal are obtained by shifting it a length $D_{m\alpha}$ upwards and downwards. They define a band in the plot. If a line trespasses (outwards) the limits of that band, it means that its maximum distance to the diagonal exceeds $D_{m\alpha}$; in this case the null hypothesis is rejected. Figure 5.1.3.1 also emphasises that the null hypothesis is rejected in the case of X_2 and X_3 but not in the case of X_1 and X_4.

Moreover, the four input parameters could be ranked in order of importance according to the measure of importance developed (maximum distance to the diagonal – test statistic). X_3 would be the most important one ($D_m=0.5692$), followed by X_2 ($D_m=0.5058$), X_4 ($D_m=0.1394$) and by X_1 ($D_m=0.0580$). The authors of this report consider that only input parameters that result in a rejection of the null hypothesis ($D_m>D_{m\alpha}$), and perhaps those close to the rejection area, should actually be ranked. Usually,

ranking input parameters that fall clearly in the null hypothesis acceptance region is completely meaningless, and their ranking could dramatically change from one sample to another one. This is the case of X_1 and X_4.

5.2. *Monte Carlo based methods*

The Monte Carlo method consists in sampling at random the vector of input parameters, running the system model computer code for each sample of that vector and getting a sample of the vector of output variables. Later on, the characteristics of the output variables may be estimated using the output samples obtained. One of the advantages of using the Monte Carlo method is that all statistical standard methods we need to estimate the output variables distributions and to test any hypothesis may be used. This makes it the most straightforward and powerful method available in the scientific literature to deal with uncertainty propagation in complex models, as it is the case of PA models. This method is valid for models that have static and also dynamic outputs. It is adequate for working with discrete and continuous inputs and outputs, and the implementation of computational algorithms required has no fundamental complexity. SA methods adapted to Monte Carlo samples are extremely convenient since they allow performing SA and UA using the same sample.

### 5.2.1. Correlation and regression – based methods

Several sampling strategies are available when using Monte Carlo to propagate uncertainties and perform SA, but the most used are Simple Random Sampling (SRS) and Latin hypercube Sampling (LHS). The most commonly used analysis is the one based on the computation of the correlation coefficient. The correlation coefficient provides a measure of the strength of the ***linear*** relationship between any input factor X_j and the output Y. In this section the input factors are supposed independent.

Correlations: Pearson correlation coefficient

This coefficient is the linear correlation coefficient of the sample and it is defined as:

$$CC(x_j, y) = \frac{\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)(y_i - \bar{y})}{\left[\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2\right]^{1/2}\left[\sum_{i=1}^{n}(y_i - \bar{y})^2\right]^{1/2}} \tag{5.2.1.1.1}$$

where $\bar{x}_j = \sum_{i=1}^{n} x_{ij}/n$ and $\bar{y} = \sum_{i=1}^{n} y_i/n$ are the sample means. The values of this coefficient are between -1 and 1. A positive value means that both X_j and Y are increasing or decreasing together while a negative value means that X_j and Y tend to move in opposite directions. An absolute value of $CC(x_j, y)$ close to one corresponds to a linear relationship, while an absolute value close to zero corresponds to the fact that there is no linear relationship between X_j and Y.
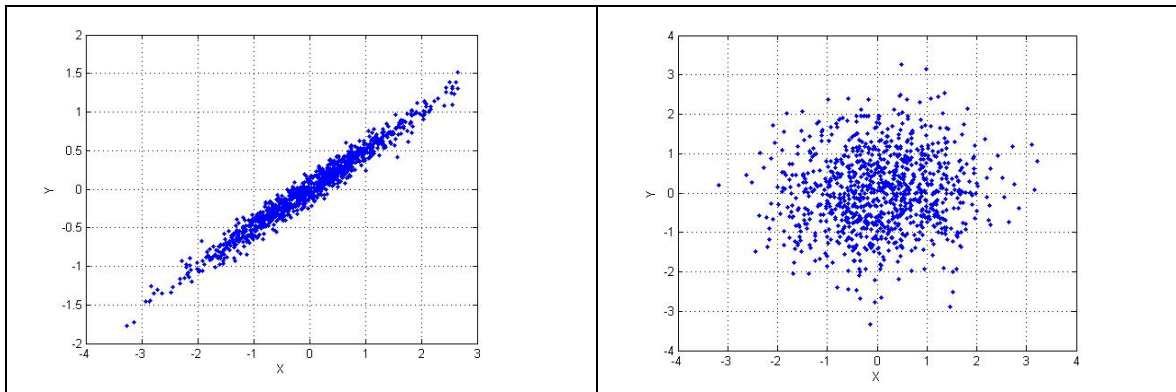
Figure 5.2.1.1.1.: Samples with strong linear relationship (left) and no linear relationship (right) between X and *Y*

We present in figure 5.2.1.1.1 two examples, one with a strong linear relationship between *X* and *Y*, for which the Pearson correlation coefficient is equal to 0.9825 and another one with no linear relationship between the two variables and for which the correlation coefficient is equal to 0.0699. The Pearson correlation coefficient is related to the results of a linear regression for *Y* and *X*, i.e. it is equal to the standardized regression coefficient of the regression, and its square is equal to the coefficient of determination (R^2) of the regression.

Correlations: Spearman correlation coefficient

Whenever a nonlinear but monotonic relationship between X_j and *Y* exists, a rank transformation can be used to get a linear relationship. This transformation replaces the values of X_j and *Y* by their corresponding ranks, see section 5.1.1. Spearman correlation coefficient (denoted by *RCC* for rank correlation coefficient) is computed using the same expression 5.2.1.1.1 as the Pearson correlation coefficient except that the ranks of each variable are used instead of the raw values.
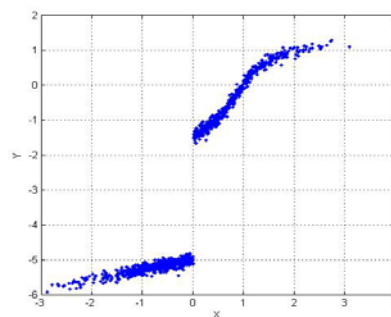
Figure 5.2.1.2.1.- Example of data for which the Spearman and the Pearson correlation coefficients are compared.

If we compute the Spearman and the Pearson correlation coefficients for the data in figure 5.2.1.2.1, we obtain: *RCC*=0.9792 and *CC*=0.8931. The Spearman coefficient is larger than the Pearson coefficient because it reflects the fact that the relationship between the two variables is monotonic instead of linear.

Regression: general framework

Regression is a technique that allows building an approximate empirical model starting from a sample of the input and output variables. The simplest models are those that can be written as

$$y(x) = \beta_0 + \beta_1 f_1(x) + \ldots + \beta_M f_M(x) + \varepsilon \qquad (5.2.1.3.1)$$

where $\varepsilon \sim N(0, \sigma^2)$ (normal distribution with null mean and variance σ^2) is a white noise independent of x_i. The model is linear in its parameters $\beta = (\beta_0, \beta_1, \ldots, \beta_M)$. The functions $f_1, \ldots, f_M$ are predefined. They can be the input variables, some transforms of those variables (such as logarithms, powers, square roots...), functions of several variables, etc.

Regression: first order polynomial

In the class of linear models, the simplest ones are the first order polynomials:

$$y(x) = \beta_0 + \beta_1 x_1 \ldots + \beta_k x_k + \varepsilon . \qquad (5.2.1.3.2)$$

The coefficients $\beta = (\beta_0, \beta_1, \ldots, \beta_k)^T$ are computed using the sample, such that the error ε is minimized in the least squares sense.

Let us recall the classical notations in regression:

- $x = (x_1, \ldots, x_k)$ a realization of the vector of input factors.
- $(x_1, \ldots, x_n)$: a sample of n realizations; each x_j has k coordinates. For simplicity sake, this sample is written in matrix notation as

$$X = \begin{bmatrix} 1 & x_{11} & \ldots & x_{1k} \\ 1 & x_{21} & \ldots & x_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \ldots & x_{nk} \end{bmatrix} \text{ where a column of ones have been added.}$$

- $y = (y_1, \ldots, y_n)^T$: the sampled output.
- $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)^T$: a vector of random errors.

With the matrix notations the model 5.2.1.3.2 becomes:

$$y = X\beta + \varepsilon \qquad (5.2.1.3.3)$$

The least squares estimator of β is

$$\hat{\beta} = \left(X^T X \right)^{-1} X^T y \qquad (5.2.1.3.4)$$

and the fitted regression model is

$$\hat{y} = X\hat{\beta} . \qquad (5.2.1.3.5)$$

An important feature of the linear regression is the decomposition of the total sum of squares $SS_T = \sum_{i=1}^{n}(y_i - \bar{y})^2$ into a sum of squares due to the regression $SS_R = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$ and a sum of squares due to the error $SS_E = \sum_{i=1}^{n}(\hat{y}_i - y_i)^2$:

$$SS_T = SS_R + SS_E . \qquad (5.2.1.3.6)$$

The ratio

$$R^2 = \frac{SS_R}{SS_T} = \frac{\sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \qquad (5.2.1.3.7)$$

measures the extent to which the regression model matches the data and is called the coefficient of multiple determination. A value of R^2 close to 1 indicates that the regression model is accounting for most of the uncertainty in y, while a value of R^2 close to 0 indicates that the regression model do not explain the uncertainty in y.

When the input factors are independent, the value of R^2 can be decomposed as $R^2 = R_1^2 + R_2^2 + \ldots + R_k^2$, where each individual R_j^2 represents the contribution of x_j to the R^2 value. R_j^2 is computed as the R^2 value for the model where the only input factor is x_j.

The equation 5.2.1.3.5 describes a hyper plane in the k-dimensional space of the input variables. The parameter $\hat{\beta}_0$ represents the intercept of the hyper plane, while each of the parameters $\hat{\beta}_j$ represents the expected change in the output y per unit change in x_j when all the remaining independent variables are constant. With this interpretation, the parameters $\hat{\beta}_j$ are candidates for sensitivity indicators except that each one is influenced by the units in which the corresponding x_j is expressed, and that it doesn't give any information on the distribution of X_j. To fix this problem, the regression model 5.2.1.3.2 is replaced by a model where all the variables have been standardized:

$$y \leftarrow \frac{y - \bar{y}}{s}, \quad x_j \leftarrow \frac{x_j - \bar{x}_j}{s_j}, \ j = 1, \ldots, k , \qquad (5.2.1.3.8)$$

s, s_j being the sample standard deviations for y and x_j:

$$s = \left[\frac{1}{n-1} \sum_{i=1}^{n}(y_i - \bar{y})^2 \right]^{1/2}, \quad s_j = \left[\frac{1}{n-1} \sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2 \right]^{1/2} . \qquad (5.2.1.3.9)$$

The regression coefficients of this new model are called ***standardized regression coefficients*** (*SRC*). They provide a sensitivity measure, or more precisely a measure of variables importance:
— a variable X_j is more important than a variable X_l if the absolute values of their standardized regression coefficients are satisfying $|SRC_j| > |SRC_l|$
— the sign of SRC_j indicates whether X_j and Y tend to move in the same direction or in opposite ones.

Moreover if the input factors X_j are independent, the inclusion or exclusion of one factor has no effect on the SRCs of the other factors in the model. If the input factors are not independent, the information provided by the SRCs is not reliable (for the variable importance).

The relationship between the standardized regression coefficients SRC_j and the regression coefficients $\hat{\beta}_j$ is

$$SRC_j = \frac{s_j}{s}\hat{\beta}_j \qquad (5.2.1.3.10)$$

Taking into account all the previous considerations, a **stepwise procedure** to build a regression model can be conceived. First model is build with the most influential variable (based on R^2 values for regression models with only one variable). Then a regression model in build with this first selected variable and the next most influential one (based on R^2 values for regression models with the first selected variable and each of the remaining ones). The procedure is repeated until no more variable with significant change in the cumulative R^2 can be found.

Regression: example of transport of a radionuclide in a nuclear waste repository

This example deals with the transport of one radionuclide (^{129}I) in a nuclear waste repository. The computation is restricted to a 2-D section of the disposal site, which has three different geological layers; the nuclear waste being disposed in the first one (the deepest one).
The numerical code used for this model is CAST3M (http://www-cast3m.cea.fr/). The computations linked to the sensitivity computations have been performed using R. The example have been studied in a Momas project**: (**http://www.gdrmomas.org/Activites/2007/MoMaS_Frejus/Vendredi/Badea.pdf**).**

The input of the numerical code consists of six environmental parameters:
— $Kh1$: horizontal permeability of the first layer
— $Kv1$: vertical permeability of the first layer
— $K2$: permeability of the second layer
— $K3$: permeability of the third layer
— $poro$: effective porosity
— de : effective diffusion coefficient

The output y is the maximal release (concentration) of ^{129}I up to 10^6 years at a predefined point located on the top of the third layer (and called exutory). The sampling has been done by latin hypercube sampling with $n=60$. The distributions for the input parameters are: log-normal for the permeabilities and the effective diffusion coefficient and uniform for the effective porosity.

We consider the model

$$y = \beta_0 + \beta_1 Kh_1 + \beta_2 Kv_1 + \beta_3 K_2 + \beta_4 K_3 + \beta_5 poro + \beta_6 de + \varepsilon .$$

The results for this regression analysis are given in table 5.2.1.5.1. The overall R^2 value is $R^2 = 0.4657$, which is not very close to 1, meaning that the regression model is not accounting for most of the uncertainty in y. However, the standardized regression coefficients are indicating that the first most important variables are, in this order, $poro$, $Kv1$, $K3$. These three variables are accounting

for 96% of the overall R^2 value. We can also see that the signs of the SRC for *poro,* and *K*3 indicate that they tend to move in opposite direction as the output while *Kv*1 tend to move in the same direction as the output.

Table 5.2.1.5.1.- Results for the regression analysis in the example of the transport of a radio nuclide.

Variable name	Regression coefficients	Standardized regression coefficients	Order of selection in stepwise regression	Cumulated R^2 in stepwise regression	Partial correlation coefficients
	$\hat{\beta}_0 = 1.528e{-}04$				
Kh1	$\hat{\beta}_1 = 9.252e{+}05$	$SRC_1 = 5.099e{-}03$	6	0.4657	$PCC_1 = 6.788e{-}03$
Kv1	$\hat{\beta}_2 = 5.548e{+}08$	$SRC_2 = 3.519e{-}01$	2	0.3748	$PCC_2 = 4.247e{-}01$
K2	$\hat{\beta}_3 = 4.437e{+}03$	$SRC_3 = 7.112e{-}02$	5	0.4656	$PCC_3 = 9.555e{-}02$
K3	$\hat{\beta}_4 = -3.86e{+}01$	$SRC_4 = -2.915e{-}01$	3	0.4454	$PCC_4 = -3.636e{-}01$
poro	$\hat{\beta}_5 = -1.03e{-}03$	$SRC_5 = -3.960e{-}01$	1	0.2496	$PCC_5 = -4.655e{-}01$
de	$\hat{\beta}_6 = 1.028e{+}07$	$SRC_6 = 1.320e{-}01$	4	0.4607	$PCC_6 = 1.711\ e{-}01$

Regression: partial correlation

Sometimes the correlation between X_j and Y may be due to a third variable. In order to avoid that, the partial correlation coefficient is defined as follows.
Two regression models have to be constructed

$$x_j = \alpha_0 + \sum_{\substack{i=1 \\ i \neq j}}^{d} \alpha_i x_i + \delta \quad \text{and} \quad y = \beta_0 + \sum_{\substack{i=1 \\ i \neq j}}^{d} \beta_i x_i + \varepsilon , \tag{5.2.1.6.1}$$

with the corresponding fitted regression models

$$\hat{x}_j = \hat{\alpha}_0 + \sum_{\substack{i=1 \\ i \neq j}}^{d} \hat{\alpha}_i x_i \quad \text{and} \quad \hat{y} = \hat{\beta}_0 + \sum_{\substack{i=1 \\ i \neq j}}^{d} \hat{\beta}_i x_i . \tag{5.2.1.6.2}$$

The partial correlation coefficient (denoted *PCC*) is then the Pearson correlation coefficient defined by expression 5.2.1.1.1, for the variables $x_j - \hat{x}_j$ and $y - \hat{y}$.

Both *PCC*s and *SRC*s provide measures of variable importance. PCC_j characterizes the linear relationship between X_j and Y after excluding the linear effects on Y of the other input factors. When the input factors are independent, *PCC*s and *SRC*s give the same ranking of variable importance, i.e. an ordering based on the absolute value of *PCC*s is the same as an ordering based on the absolute value of *SRC*s.

One has also to keep in mind that if the input factors are correlated, the results based on *SRC*s or on *PCC*s may be misleading, as some authors remark, see Helton et al. (2006).

The *PCC*s for the example in the previous paragraph are also given in table 5.2.1.5.1. The ranking of variable importance is the same whether if we use *SRC*s or *PCC*s, though this is not always true. In many cases the ranking produced by both sensitivity indices is not the same, though it does not differ much.

Regression: rank transformations

In the same way as for the Spearman correlation coefficient, whenever a nonlinear but monotonic relationship between X_j and Y exists, a rank transformation can be used to get a linear relationship. Using the rank transformation leads to rank regressions and consequently to standardized rank regression coefficients (*SRRC*s) and partial rank correlation coefficients (*PRCC*s). The results of sensitivity analysis can be improved by using these coefficients when monotonic relationships between inputs and output exist. The results for the rank regression analysis for the previous example are given in table 5.2.1.7.1.

Table 5.2.1.7.1.- Results for the rank regression analysis in the example of the transport of a radionuclide.

Variable name	Standardized rank regression coefficients	Partial rank correlation coefficients	Order of variable importance
Kh1	$SRRC_1 = 8.29\mathrm{e}{-03}$	$PRCC_1 = 2.578\mathrm{e}{-02}$	6
Kv1	$SRRC_2 = 3.362\mathrm{e}{-01}$	$PRCC_2 = 7.238\mathrm{e}{-01}$	3
K2	$SRRC_3 = 8.726\mathrm{e}{-02}$	$PRCC_3 = 2.626\mathrm{e}{-01}$	4
K3	$SRRC_4 = -5.325\mathrm{e}{-01}$	$PRCC_4 = -8.564\mathrm{e}{-01}$	2
poro	$SRRC_5 = -6.338\mathrm{e}{-01}$	$PRCC_5 = -8.922\mathrm{e}{-01}$	1
de	$SRRC_6 = 3.048\mathrm{e}{-02}$	$PRCC_6 = 9.442\ \mathrm{e}{-02}$	5

The three most important variables are the same as in the linear regression case, even if their order of importance is changed; for the rank analysis the ranking is *poro, K3, Kv1*, while for the standardized regression the order was poro, *Kv1, K3*. Moreover the overall R^2 value for this model is $R^2 = 0.8987$ (it was 0.4657 for the model using the standardized variables).

Regression: extensions

Linear regression with first order polynomials is not enough in most cases under study, because the relationship between output and input factors is not a linear one. It is more interesting to study the standardized regression coefficients for different types of regression, as presented in the following.

Output and input transformation

In many PA applications, the variable of interest is not the output of the computer code, but a function of it, in other cases the relation between inputs and outputs is more easily analysed if some of them or both of them are transformed. In the PA area, many input parameters and output variables are spread over several orders of magnitude. In these cases, a logarithmic transformation of all parameters and variables with such spread of values could be of interest. For instance, for the previous example, we consider the following model:

$$\log_{10} y = \beta_0 + \beta_1 \log_{10} Kh_1 + \beta_2 \log_{10} Kv_1 + \beta_3 \log_{10} K_2 + \beta_4 \log_{10} K_3 + \beta_5 poro + \beta_6 \log_{10} de + \varepsilon$$

(for every variable, except *poro*, a logarithm have been applied). The overall R^2 value is $R^2 = 0.9141$, which means that the quality of the model is quite good. The standardized regression coefficients are given in table 5.2.1.8.1. The results are more or less the same as those obtained for the rank regression. The order of importance changes only between variables *K2* and *de*, which where not the most significant ones.

Table 5.2.1.8.1.- Regression results for the transformed data in the example of the transport of a radionuclide.

Variable name	Standardized regression coefficients	Order of variable importance
$\log_{10}(Kh1)$	$SRC_1 = 6.454\text{e}{-03}$	6
$\log_{10}(Kv1)$	$SRC_2 = 3.516\text{e}{-01}$	3
$\log_{10}(K2)$	$SRC_3 = 8.783\text{e}{-02}$	5
$\log_{10}(K3)$	$SRC_4 = -5.121\text{e}{-01}$	2
poro	$SRC_5 = -6.278\text{e}{-01}$	1
$\log_{10}(de)$	$SRC_6 = 9.475\text{e}{-02}$	4

We can conclude that in some cases, by applying some usual transforms to the original variables, we can both conserve the simplest regression model and improve a lot the quality of the model (expressed in terms of R^2).

Second order polynomials

In other cases some more complicated linear regression models may be considered, such as second order polynomials (or only first order and interaction terms), which are written as:

$$y = \beta_0 + \sum_{i=1}^{d} \beta_i x_i + \sum_{\substack{i,j=1 \\ i \le j}}^{d} \beta_{ij} x_i x_j + \varepsilon .$$
(5.2.1.8.1)

Similar interpretation as in the case of the first order polynomials might be given to the regression coefficients. However, one has to be aware of the fact that for instance the importance of variable x_1 will be the result of an accumulation of different coefficients of the terms in which this variable appears.

Functional outputs

Many of the output variables considered in PA models are time dependent functions. In these cases, all the previously described coefficients may be computed at every time step, yielding time dependent curves.

Example (NRG)

This example comes from a joint work JRC/NRG concerning the probabilistic uncertainty analysis for the abandonment scenario for disposal facilities in rock salt (see figure 5.2.1.8.1 (rleft)). The conceptual model of the generic repository design with the option to retrieve waste, as has been implemented in the EMOS. There are 6 input factors denoted by A_{ps}, B_{recr}, *F09*, *n*, *F47*, *F46* (with the following probability distributions: log uniform for A_{ps}, B_{recr}, *F47*, *F46*, log normal for *F09* and normal for *n*). A simple random sample of size 1000 has been used in this test case.

There are 4 scalar outputs, and 7 time dependent ones. We present here some time dependent results for only one output, "B.2, Permeability of the plug" (the 1000 realizations for this output are presented in figure 5.2.1.8.1 (right)):

- correlation coefficients: Pearson (figure 5.2.1.8.2), Spearman (figure 5.2.1.8.3) and
- regression based coefficients: SRC (figure 5.2.1.8.4), PCC (figure 5.2.1.8.5), SRRC (figure 5.2.1.8.6), PRCC (figure 5.2.1.8.7)
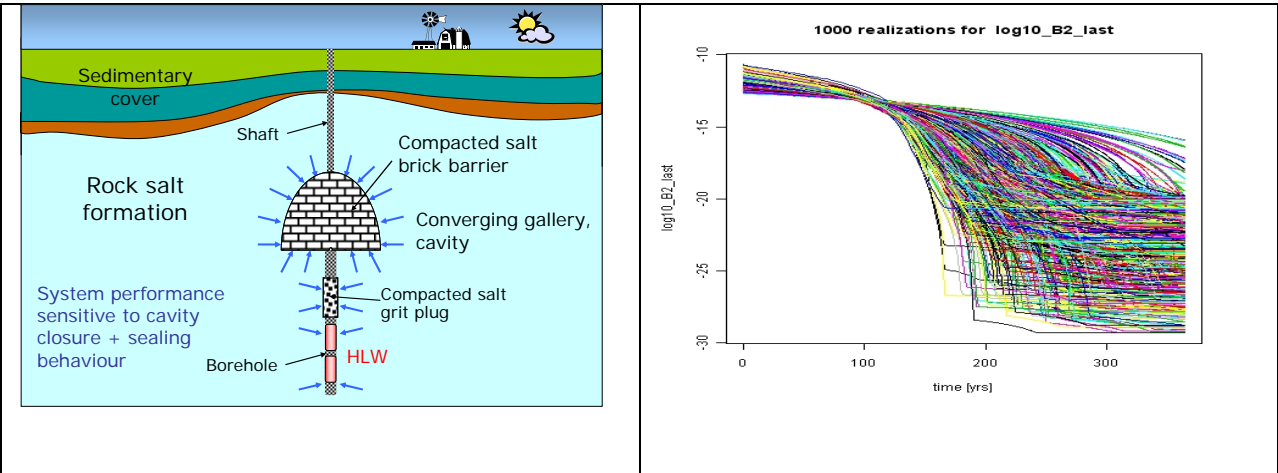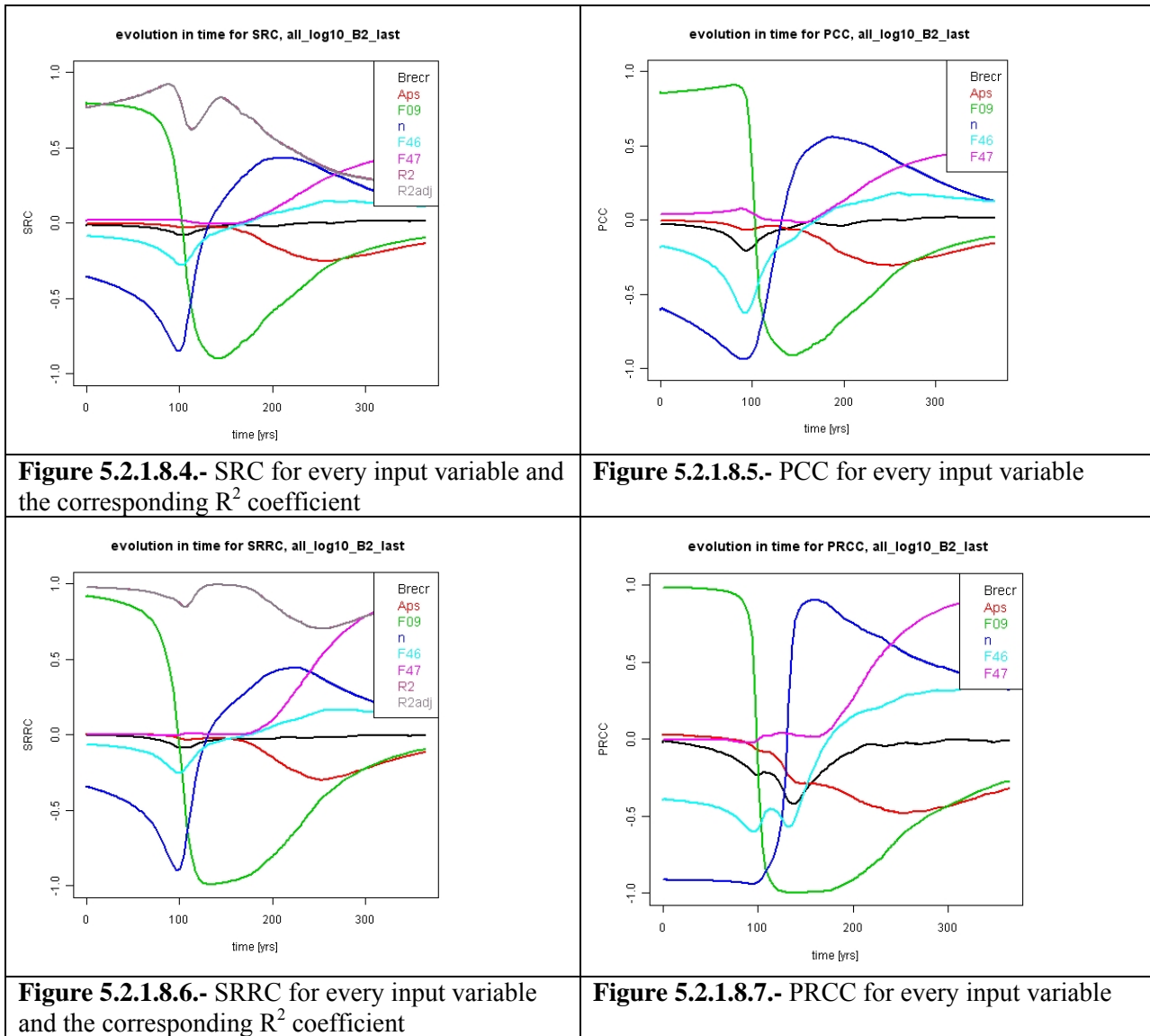

Figure 5.2.1.8.1: The abandonment scenario for disposal facilities in rock salt (left); 1000 realizations for the output "Permeability of the plug" (right)
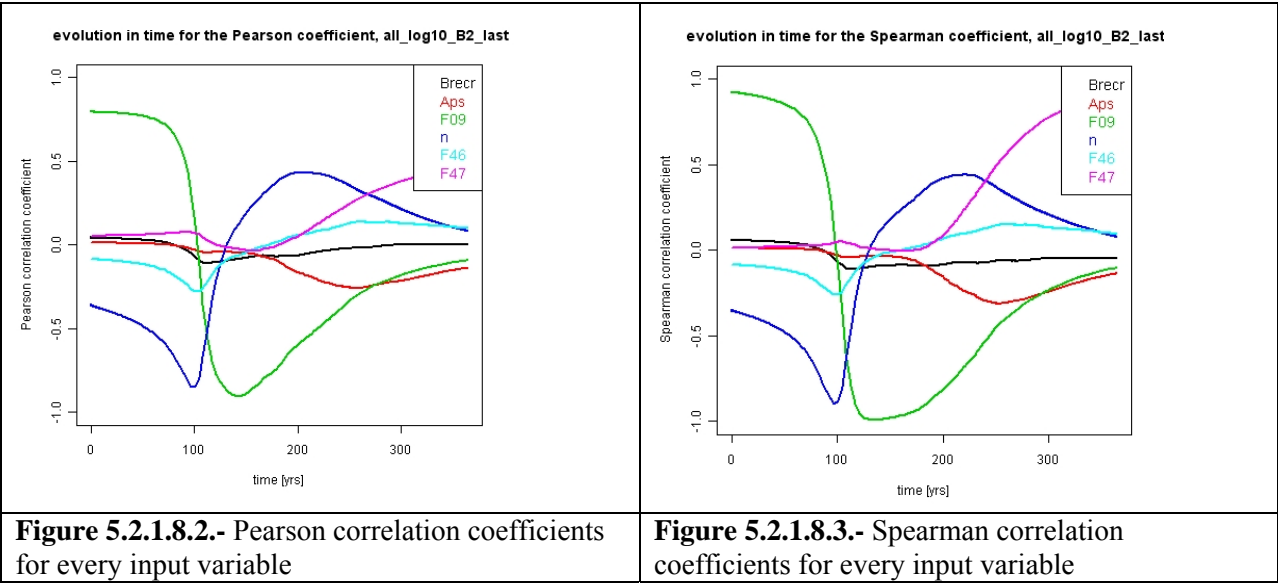
Figure 5.2.1.8.2.- Pearson correlation coefficients for every input variable	**Figure 5.2.1.8.3.-** Spearman correlation coefficients for every input variable

Figure 5.2.1.8.4.- SRC for every input variable and the corresponding R^2 coefficient

Figure 5.2.1.8.5.- PCC for every input variable

Figure 5.2.1.8.6.- SRRC for every input variable and the corresponding R^2 coefficient

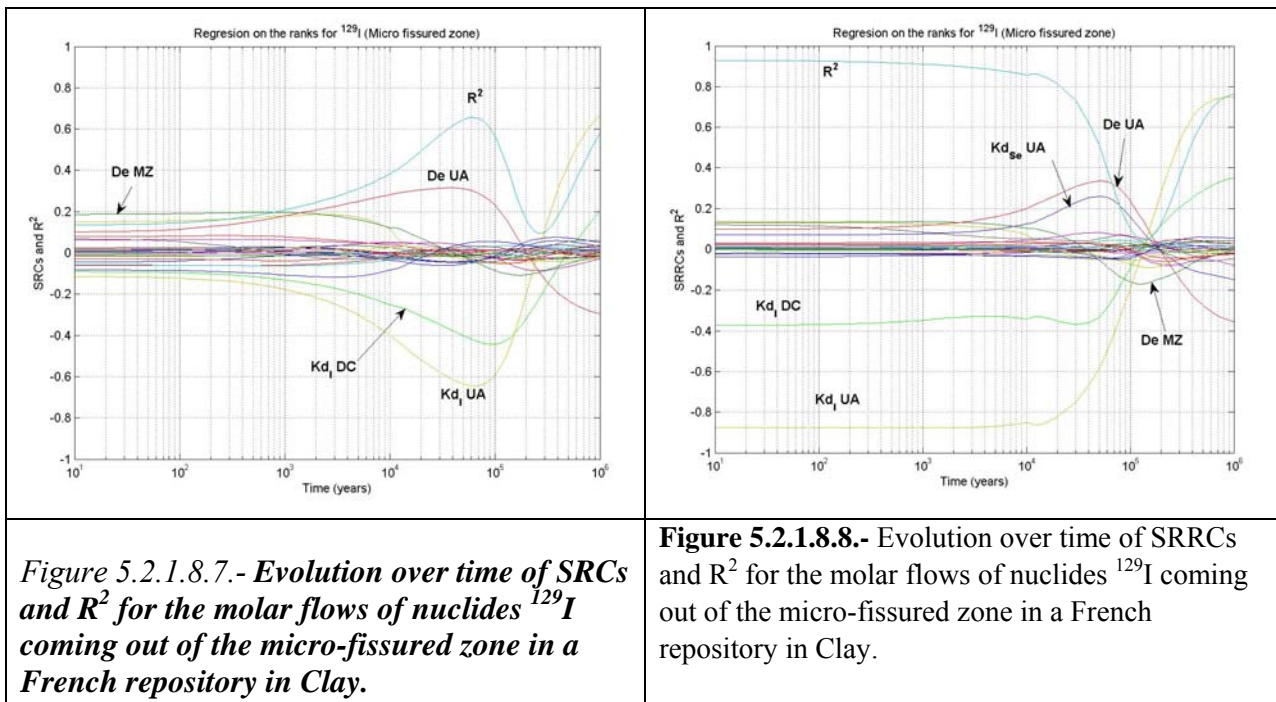**Figure 5.2.1.8.7.-** PRCC for every input variable

Several remarks may be made about this set of plots;

- the influence of the model input factors on the permeability of the borehole plug changes significantly over time.
- the rank based regressions provide more significant results. R^2 is larger in the rank based regressions than in the regressions based on raw values at all time steps. In fact R^2 is always larger than 0.7 in the first case while it is below that value a large fraction of the time in the second case. Remind that for values of R^2 smaller than 0.6, the results of the regression should not be taken as very reliable. Moreover, statistics based on ranks (RCC, SRRC and PRCC) tend to take more extreme values (closer to ±1) than statistics based on raw values (CC, SRC and PCC).
- All techniques provide similar results, identifying as relevant input parameters the same set.
- Two parameters change clearly the sign of their sensitivity indices over time (F09 and n). This behaviour is detected quite frequently in PA studies.

These remarks remain true in many other applications, as for example the one shown in figures 5.2.1.8.8 and 5.2.1.8.9, obtained for a French repository in clay. Pay special attention to the huge improvement in the value of R^2 and the SRRC associated to the most relevant input parameters at early

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and intermediate times, with respect to the corresponding SRCs . Many other similar examples may be seen in Prváková et al. (2008).

*Figure 5.2.1.8.7.- **Evolution over time of SRCs and R^2 for the molar flows of nuclides ^{129}I coming out of the micro-fissured zone in a French repository in Clay.***	**Figure 5.2.1.8.8.-** Evolution over time of SRRCs and R^2 for the molar flows of nuclides ^{129}I coming out of the micro-fissured zone in a French repository in Clay.

5.2.2.   Monte Carlo filtering

In the previous sections we could see a set of techniques that took as a base to interpret sensitivity the ideas of linearity and monotony. Nevertheless, sensitivity may be interpreted in different ways that have nothing to do with these two ideas. In some cases, we could consider an input parameter as important with respect to a given output variable if we are able to uncover a clear link between specific regions of both. Monte Carlo Filtering (MCF) is based on dividing the output sample in two or more subsets according to some criterion (achievement of a given condition, exceeding a threshold, etc.) and testing if the inputs associated to those subsets are different or not. As an example, we could divide the output sample in two parts, the one that exceeds a safety limit and the rest. We could wonder if points in both subsamples are related to different regions of a given input or if they may be related to any region of that input. In the first case knowing the value of that input parameter would be important in order to be able to predict if the safety limit will be exceeded or not, while in the second case it would not be. The tools used to provide adequate answers to this type of questions are a set of parametric and non-parametric statistics and their associated tests, among them the most popular are

- The two-sample Smirnov test
- The Mann-Whitney (or Wilcoxon) two-sample test
- The two-sample t-test

The two-sample Smirnov test is based on comparing empirical cumulative distribution functions, the Mann-Whitney test is based on ranks, the two-sample t-test is based on the sampling distribution of the mean of normal variables. Other tests, as for example the Kruskal-Wallis test and the k-sample Smirnov test are also available in the Statistics literature, see Conover (1980), which are respectively

extensions of the Mann-Whitney and the Smirnov tests to several samples. These tests will not be included in this study because they have hardly ever been used with SA purposes, though formally they could be.

Normally, when any of these tests is applied in other areas, two samples (Smirnov, Mann-Whitney and t-test) are taken via random sampling from two or more populations, as for example the height of a set of boys and girls 10 years old in a given country. In our case, when the test is used with SA purposes, the samples used to perform the test are in fact subsamples of an input parameter sample. Let us see how those two samples are obtained

Consider the samples obtained via simulation for a given input parameter X and an output variable Y: $(x_1, x_2, ..., x_n)$ and $(y_1, y_2, ..., y_n)$

1. Then, sort $(y_1, y_2, ..., y_n)$, obtaining $(y^{(1)}, y^{(2)}, ..., y^{(n)})$, and re-order $(x_1, x_2, ..., x_n)$ according to the order of the sample of Y, obtaining $(x^{[1]}, x^{[2]}, ..., x^{[n]})$.

2. Set a threshold on $(y^{(1)}, y^{(2)}, ..., y^{(n)})$ based on a given criterion and divide it in the corresponding two subsamples $(y^{(1)}, y^{(2)}, ..., y^{(h)})$ and $(y^{(h+1)}, y^{(h+2)}, ..., y^{(n)})$. Let us call 'C' the criterion.

3. Divide accordingly the sample $(x^{[1]}, x^{[2]}, ..., x^{[n]})$ in the two subsamples $(x^{[1]}, x^{[2]}, ..., x^{[h]})$ and $(x^{[h+1]}, x^{[h+2]}, ..., x^{[n]})$. These two subsamples will be the samples used to perform the test.

The procedure to follow is the same if three or more samples are required, just set two or more thresholds in step 3 and act consequently in step 4. In the next sections a detailed description of these tests is given.

The two-sample Smirnov test

The procedure to perform a test is roughly the same for every test: 1) set assumption to perform the test, 2) set the null (H_0) and the alternative (H_1) hypotheses, 3) establish a measure of discrepancy (test statistic) between what is expected under the null hypothesis and under different conditions and, 4) set a decision rule. In the case of the two-sample Smirnov test, this procedure is as follows

1. Assumptions:
   - Both samples are random and mutually independent
   - The variable considered should be continuous in order to get an exact test (having a discrete variable does not preclude the use of the test unless it takes only a few different values).

2. Hypotheses:
   - H_0: $F_{X|C1}(x|C1) = F_{X|C2}(x|C2) \quad \forall x \in IR$
   - H_1: $\exists x' \in IR / F_{X|C1}(x'|C1) \neq F_{X|C2}(x'|C2)$, where $C1$ indicates fulfilling the criterion and $C2$ means not fulfilling the criterion

3. Discrepancy measure (test statistic): $T_{Smirnov} = Sup_x |S_{C1}(x) - S_{C2}(x)|$, which is the maximum vertical distance between the empirical distribution functions ($S_{C1}(x)$) of $(x^{[h+1]}, x^{[h+2]}, ..., x^{[n]})$, the subsample of the input parameter linked to the subsample of the output variable that fulfils the criterion, and the empirical distribution functions ($S_{C2}(x)$) of $(x^{[1]}, x^{[2]}, ..., x^{[h]})$, the subsample which does not.

4. Decision rule: set some limits for the p-values that allow the user decide if, from the result of the test it should be concluded that that input parameter is either important or not (reject or not reject the null hypothesis). Setting these limits is up to the user opinion, though, as a generally accepted rule, the null hypothesis is accepted if the p-value of the test is above 0.05, otherwise it is rejected. The distribution of the test statistic under the null hypothesis may be found in Conover (1980). As an alternative to this general rule, Saltelli et al. (2004) propose the following decision rule

- P-value < 0.01 ==> the input parameter is critical.
- $0.01 \leq$ p-value ≤ 0.1 ==> the input parameter is important
- p-value ≥ 0.1 ==> the input parameter is not important
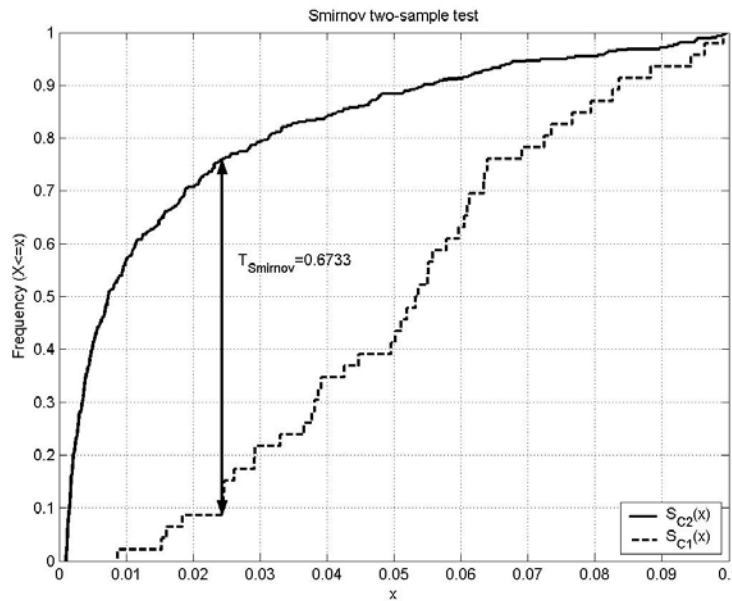
Figure 5.2.2.1.1.- Graphic representation of the computation of the two-sample Smirnov test for the peak dose due to ^{129}I (output) and V1 (input). Level_E test case. The output sample has been divided in the largest 10% observations and the 90% smallest observations.

Figure 5.2.2.1.1 represents the implementation of a Smirnov two-sample test. The sample considered to perform the test is a sample of size 459 obtained for the Level_E test case. The output variable is the peak dose due to ^{129}I and the input parameter is V1, the velocity of ground water in the first geosphere layer. We have taken as a reference the 10% largest observations obtained for the output variable and we wish to know if these observations are related to a specific region of V1 or not. This plot shows the empirical cumulative distribution functions corresponding to the two subsamples of V1, the one related to the 10% largest observations of the output variable (dashed line) and the one relasted to the other 90% observations (solid line). As indicated in the plot, the Smirnov statistic (maximum vertical distance between both curves) takes value $T_{Smirnov}=0.6733$, which corresponds to a p-value=0.0. The result of the test is conclusive, certainly the values of V1 that produce the 10% largest values of the output variable and the values of V1 that produce the rest of the values of the same output variable, belong to two subpopulations of V1 that have very different properties (distributions). The p-value shows no ambiguity in the result. This can be observed in the same figure, all the values of the the subsample of V1 related to C1 are above the median of the values of V1 related to C2. Observe the

similarity between the results of this test, included figure 5.2.2.1.1, and the information contained in figure 5.1.2.2.

Mann-Whitney two-sample test

As in the case of the Smirnov two-sample test, the assumptions, hypotheses, test statistic and decision rule are as follows

1. Assumption: Both samples are random and mutually independent.
2. Hypotheses: As for the Smirnov two-sample test.
3. Discrepancy measure (test statistic):

$$T_{Mann-Whitney} = \sum_{i=h+1}^{n} R(x^{[i]}),$$
(5.2.2.2.1)

where $R(x^{[i]})$ is the rank associated to observations $x^{[i]}$ of the input parameter corresponding to the output values that satisfy condition C1. If there are many ties, which may happen only if the input parameter is discrete, the Mann-Whitney test statistic is

$$T'_{Mann-Whitney} = \frac{T_{Mann-Whitney} - (n-h)(n+1/2)}{\sqrt{[h(n-h)/n(n-1)]\sum_{i=1}^{n} R^2(x_i) - h(n-h)(n+1)^2/4(n-1)}}$$
(5.2.2.2.2)

4. Decision rule: As for the Smirnov two-sample test.

Figure 5.2.2.2.1 represents the implementation of a Mann-Whitney two-sample test. The sample considered to perform the test and the question at stake is the same as in the previous section. This plot shows ranks corresponding to the two subsamples of V1, the one related to the 10% largest observations of the output variable (represented by symbol '*'in figure 5.2.2.2.1) and the ones related to the other 90% observations (represented by symbol 'o'in figure 5.2.2.2.1). The value of the test statistic is $T_{Mann-Whitney} = 17534$, which corresponds to a p-value=0.0. The result of the test is again conclusive, certainly the values of V1 that produce the 10% largest values of the output variable and the values of V1 that produce the rest of the values of the same output variable, belong to two subpopulations of V1 that have very different properties (ranks). The p-value shows no ambiguity in the result. This can be observed in the same figure, all the ranks of the subsample of V1 related to C1 overlap only with the largest ranks of the subsample of V1 related to C2. Observe the similarity between the results of this test, included figure 5.2.2.2.1, the results obtained in previous section with the Smirnov two-sample test and the information contained in figure 5.1.2.2.
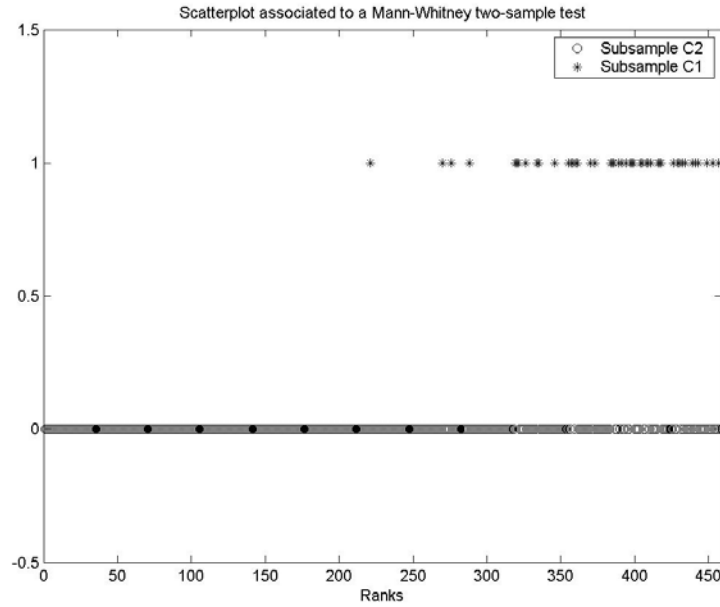
Figure 5.2.2.2.1.- Graphic representation of the computation of the two-sample Mann-Whitney test for the peak dose due to ^{129}I (output) and V1 (input). Level_E test case. The output sample has been divided in the largest 10% observations and the 90% smallest observations.

Two-sample t test

As in the case of the Smirnov two-sample test and the Mann-Whitney test, the assumptions, hypotheses, test statistic and decision rule are as follows

1. Assumption:
   - Both samples are random and mutually independent.
   - Both samples come from normal (Gaussian) populations with equal variances.
2. Hypotheses: As for the Smirnov and Mann-Whitney two-sample tests.
3. Discrepancy measure (test statistic):

$$t = \frac{\bar{x}_1 - \bar{x}_2}{\hat{S}_T \sqrt{\frac{1}{h} + \frac{1}{n-h}}}, \qquad (5.2.2.3.1)$$
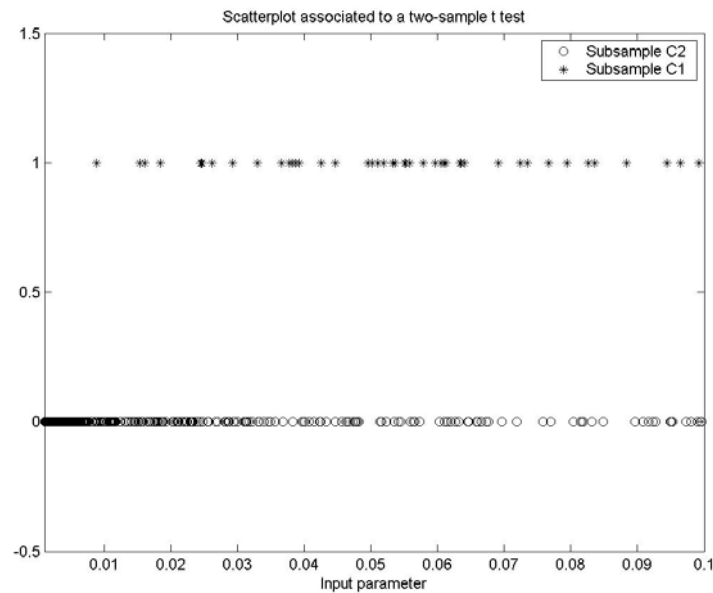
where $\bar{x}_1$ is the sample mean of $(x^{[h+1]}, x^{[h+2]}, ..., x^{[n]})$, $\bar{x}_2$ is the sample mean of $(x^{[1]}, x^{[2]}, ..., x^{[h]})$, and $\hat{S}_T$ is the weighted common estimator of the variance of both subsamples

$$\hat{S}_T = \sqrt{\frac{n-h-1}{n-2}\hat{S}_1^2 + \frac{h-1}{n-2}\hat{S}_2^2} \qquad (5.2.2.3.1)$$

where $\hat{S}_1^2$ and $\hat{S}_2^2$ are, respectively, the estimators of the variance of $(x^{[h+1]}, x^{[h+2]}, ..., x^{[n]})$ and of $(x^{[1]}, x^{[2]}, ..., x^{[h]})$.
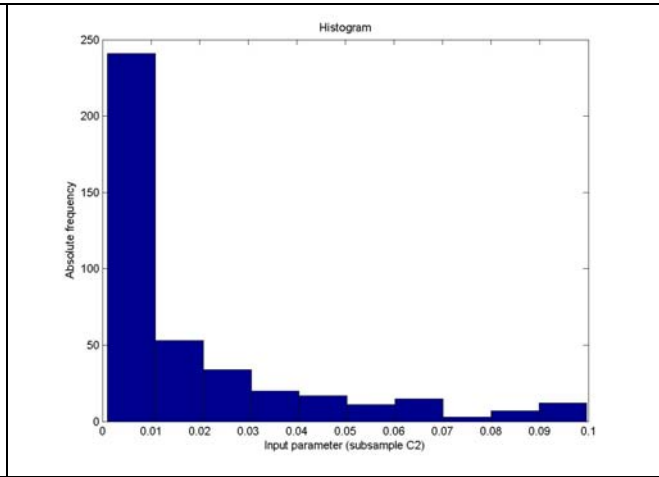
4. Decision rule: As for the Smirnov two-sample test.

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Figure 5.2.2.3.1.- Graphic representation of the computation of the two-sample t test for the peak dose due to ^{129}I (output) and V1 (input). Level_E test case. The output sample has been divided in the largest 10% observations and the 90% smallest observations.

Figure 5.2.2.3.1 represents the implementation of a two-sample t test. The sample considered to perform the test and the question at stake is the same as in the previous two sections. This plot shows the raw values corresponding to the two subsamples of V1, the one related to the 10% largest observations of the output variable (represented by symbol '*'in figure 5.2.2.3.1) and the ones related to the other 90% observations (represented by symbol 'o'in figure 5.2.2.3.1). The value of the test statistic is t=9.33, which corresponds to a p-value=0.0. The result of the test is again conclusive, certainly the values of V1 that produce the 10% largest values of the output variable and the values of V1 that produce the rest of the values of the same output variable, belong to two subpopulations of V1 that have very different properties (means). The p-value shows no ambiguity in the result. This can be observed in the same figure, all the raw values of the subsample of V1 related to C1 overlap only with the largest ranks of the subsample of V1 related to C2. Observe the similarity between the results of this test, included figure 5.2.2.3.1, the results obtained in previous sections with the Smirnov two-sample test and the Mann-Whitney two-sample test, and the information contained in figure 5.1.2.2.

Nevertheless, in this case, results should be taken cautiously. Figures 5.2.2.3.2 and 5.2.2.3.3 show respectively the histograms of samples $(x^{[h+1]}, x^{[h+2]},..., x^{[n]})$ and $(x^{[1]}, x^{[2]},..., x^{[h]})$. Though the first histogram resembles reasonably well the shape of a normal distribution, the second one is certainly far from being close to such a shape. This means that, under such violation of one of the assumptions of the test, the validity of the result is under question. Under these circumstances, the best option is to discard this test. It is also worthwhile to realise that the assumptions for the Smirnov test and the Mann-Whitney test are so broad and generic that it is difficult to find a situation in a PA when they cannot be applied. As a general conclusion, Smirnov and Mann-Whithney test have a much broad applicability in the framework of PA studies than the t test.
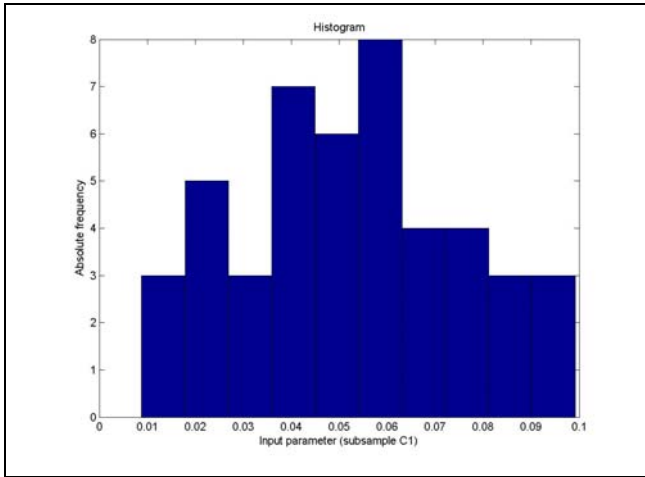
Figure 5.2.2.3.2.- Histogram of the subsample of V1 corresponding to the 10% largest values of the peak dose due to [129]I. Level_E test case.	**Figure 4.2.2.3.3.-** Histogram of the subsample of V1 corresponding to the 90% smallest values of the peak dose due to [129]I. Level_E test case.

5.3. Variance decomposition based methods

The main measure to quantify the uncertainty affecting any output variable is its variance $V(Y)$, as for any other random variable. In a PA model, as in many other simulation models, the uncertainty of any output variable is the result of propagating uncertainties from the input space into the output space. So, each input parameter is responsible for a fraction of the output variance. Variance based methods take this fraction as the reference sensitivity measure and provide the means to estimate it. In the next pages we describe the main variance based methods.

5.3.1. HDMR decomposition

Variance based methods are linked to the HDMR (High Dimensional Model Representation) which consists in decomposing $Y = f(X_1, \ldots, X_d)$ in the form:

$$Y = f(X_1, \ldots, X_k) = f_0 + \sum_i f_i(X_i) + \sum_{i<j} f_{ij}(X_i, X_j) + \ldots + f_{1\ldots k}(X_1, \ldots, X_k). \qquad (5.3.1.1)$$

This decomposition exists and is unique.

The term f_0 is the mean of Y (a constant). The first order function $f_i(X_i)$ of the decomposition represents the effect of the input factor X_i acting independently (and generally in a nonlinear way) upon the output Y. The second order function $f_{ij}(X_i, X_j)$ represents the joint effect of the input factors X_i and X_j upon the output Y. Higher order functions represent the joint effect of the input factors upon the output. The last term of the decomposition gives the residual influence of all the input factors together.

The HDMR formulation is very efficient whenever the high-order variable correlations are weak, allowing the physical model to be captured by the first few low-order terms. Very often the HDMR expression to 2nd order provides a satisfactory description of $Y = f(X_1, \ldots, X_d)$, which does not imply

that a small number of input factors are significant nor does it limit the nonlinear structure of the relationship input-output.

The component functions of the HDMR (5.3.1.1) are a set of projectors that are mutually orthogonal to one another (the integral of the product of any pair of them over the whole input space is null); their expressions are:

$$
\begin{aligned}
f_0 &= E[Y] \\
f_i(X_i) &= E[Y \mid X_i] - f_0 \\
f_{ij}(X_i, X_j) &= E[Y \mid X_i, X_j] - f_i(X_i) - f_j(X_j) - f_0 \\
f_{ijk}(X_i, X_j, X_k) &= E[Y \mid X_i, X_j, X_k] - f_{ij}(X_i, X_j) - f_{ik}(X_i, X_k) - f_{kj}(X_k, X_j) \\
&\quad - f_i(X_i) - f_j(X_j) - f_k(X_k) - f_0 \\
&\dots
\end{aligned}
\tag{5.3.1.2}
$$

Where $E[Y \mid X_i]$ is the expectation of Y conditional on X_i, $E[Y \mid X_i, X_j]$ is the expectation of Y conditional on X_i and X_j and so on. The details for obtaining these formulas may be found in Sobol (1993).

5.3.2. Variance decomposition

For *independent* input factors and using the fact that any two different components of the HDMR decomposition are orthogonal, the variance of the model $Y = f(X_1, \dots, X_d)$ can be written as:

$$
V = Var(Y) = \sum_i V_i + \sum_{i<j} V_{ij} + \dots + V_{1\dots d} \quad,
\tag{5.3.2.1}
$$

where

$$
\begin{aligned}
V_i &= Var(E[Y \mid X_i]) \\
V_{ij} &= Var(E[Y \mid X_i, X_j]) - V_i - V_j \\
V_{ijk} &= Var(E[Y \mid X_i, X_j, X_k]) - V_{ij} - V_{jk} - V_{ki} - V_i - V_j - V_k \\
&\dots
\end{aligned}
\tag{5.3.2.2}
$$

It can be shown (see for instance Sobol (1993), Jacques (2005)) that the individual terms in expression 5.3.1.2 are the variances of the functions of the corresponding indices in the HDMR decomposition 5.3.1.1, which means that:

$$
\begin{aligned}
V_i &= Var(f_i(X_i)) \\
V_{ij} &= Var(f_{ij}(X_i, X_j)) \\
V_{ijk} &= Var(f_{ijk}(X_i, X_j, X_k)) \\
&\dots
\end{aligned}
\tag{5.3.2.3}
$$

5.3.3. Sobol sensitivity indices

Using the variance decomposition 5.3.2.1, Sobol sensitivity indices are defined as:
- first order sensitivity indices

$$S_i = \frac{V_i}{V}$$
(5.3.3.1)

- second order sensitivity indices, which gives the sensitivity of the variance of the output to the interaction between the input factors X_i, X_j

$$S_{ij} = \frac{V_{ij}}{V}$$
(5.3.3.2)

- and so on until the order k.

We can divide both sides of 5.3.2.1 and obtain a very useful relation:

$$1 = \sum_i S_i + \sum_{i<j} S_{ij} + \ldots + S_{1\ldots k}.$$
(5.3.3.3)

The interpretation of the sensitivity indices is straightforward, as the sum of all indices is 1 and as they are all positive: the larger the sensitivity index (close to 1), the more influent the corresponding input (or group of inputs). However, the number of all these indices is $2^d - 1$ and when the number of input factors is too large their computation and interpretation becomes impossible. This is why Homma and Saltelli (1996) introduced the total sensitivity indices which assess the sensitivity of the variance of the output with respect to the standalone and every interaction of the considered input factor, by:

$$S_{T_i} = \sum_{\substack{k \in \text{all the sets of} \\ \text{indices containing} \\ \text{the index } i}} S_k \quad .$$
(5.3.3.4)

For a model with three input factors, we have $S_{T_1} = S_1 + S_{12} + S_{13} + S_{123}$, and similar expressions for the two other total indices. There is a simpler definition of the total indices:

$$S_{T_i} = 1 - \frac{V_{-i}}{V},$$
(5.3.3.5)

where $V_{-i} = Var(E[Y \mid X_{-i}])$ represents the variance explained by all the factors except X_i. This definition makes the total indices as easy to estimate as the first order indices.

5.3.4. Example : the Ishigami function

The Ishigami function is defined in Ishigami and Homma (1990) as:

$$Y = \sin X_1 + A \sin^2 X_2 + B X_3^4 \sin X_1,$$

with all input factors independent and following uniform distributions in the interval (-π, π), i.e. $X_i \sim U(-\pi, \pi)$.

Taking into account expressions 5.3.1.1 and 5.3.1.2, the HDMR decomposition the Ishigami function is as follows:

$$f_0 = E[Y] = A/2$$
$$f_1(X_1) = E[Y \mid X_1] - f_0 = (1 + B\pi^4/5)\sin X_1$$
$$f_2(X_2) = E[Y \mid X_2] - f_0 = A\sin^2 X_2 - A/2$$
$$f_3(X_3) = E[Y \mid X_3] - f_0 = 0$$
$$f_{12}(X_1, X_2) = E[Y \mid X_1, X_2] - f_1(X_1) - f_2(X_2) - f_0 = 0$$
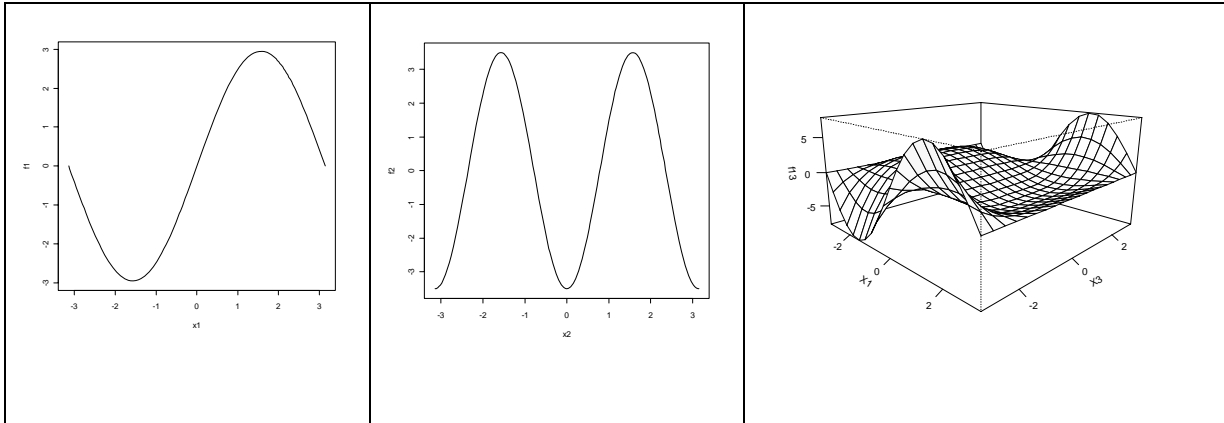$$f_{13}(X_1, X_3) = E[Y \mid X_1, X_3] - f_1(X_1) - f_3(X_3) - f_0 = B\sin X_1(X_3^4 - \pi^4/5)$$
$$f_{23}(X_2, X_3) = E[Y \mid X_2, X_3] - f_2(X_2) - f_3(X_3) - f_0 = 0$$
$$f_{123}(X_1, X_2, X_3) = \ldots = 0$$
and
$$Y = f_0 + f_1(X_1) + f_2(X_2) + f_{13}(X_1, X_3).$$

The three non zero functions, $f_1(X_1), f_2(X_2), f_{13}(X_1, X_3)$, if the Ishigami function are represented in figure 5.3.4.1.

Figure 5.3.4.1.- Representation of the functions forming the HDMR decomposition of the Ishigami function.

This leads to the following expressions for the variances

$$V_1 = Var(f_1) = \tfrac{1}{2}(1 + B\pi^4/5)^2$$
$$V_2 = Var(f_2) = A^2/8$$
$$V_{13} = Var(f_{13}(X_1, X_3)) = 8B^2\pi^8/225$$
and
$$V = Var(Y) = \frac{1}{2} + \frac{A^2}{8} + \frac{B\pi^4}{5} + \frac{B^2\pi^8}{18}$$

the other variances being equal to 0.

For the case $A = 7$ and $B = 0.1$ (which is the one presented in Ishigami and Homma (1990)) the values for the previous variances are $V_1 = 4.3459$; $V_2 = 6.125$; $V_{13} = 3.3737$; $V = 13.8446$ and the values for the sensitivity indices are:

- first order sensitivity indices:

$$S_1 = \frac{V_1}{V} = 0.3139; \ S_2 = \frac{V_2}{V} = 0.4424; \ S_3 = \frac{V_3}{V} = 0 \tag{5.3.4.1}$$

- second order sensitivity indices:

$$S_{12} = \frac{V_{12}}{V} = 0; \ S_{23} = \frac{V_{23}}{V} = 0; \ S_{13} = \frac{V_{13}}{V} = 0.2437 \tag{5.3.4.2}$$

- third order sensitivity index:

$$S_{123} = \frac{V_{123}}{V} = 0 \tag{5.3.4.3}$$

- total sensitivity indices:

$$
\begin{aligned}
S_{T_1} &= S_1 + S_{12} + S_{13} + S_{123} = 0.5596 \\
S_{T_2} &= S_2 + S_{12} + S_{23} + S_{123} = 0.4424 \\
S_{T_3} &= S_3 + S_{13} + S_{23} + S_{123} = 0.2437.
\end{aligned}
\tag{5.3.4.4}
$$

If we only compute the first order indices, the effect of X_3 is not visible and we can also conclude that 24% of the variance is due to interactions.

5.3.5. Estimation of the sensitivity indices

The computation of Sobol indices is based on the computation of the variances of conditional expectations, which are very time consuming. The following methods are generally used in this purpose:
- Sobol/Saltelli methods
- FAST (Fourier Amplitude Sensitivity Test) / E (extended) FAST method / Random balanced design method
- Correlation ratios
- McKay method
- Alternatively, a response surface may be built for the initial model and the Sobol indices may be either analytically computed or estimated for the response surface.

Sobol/Saltelli estimation method

This method, due to Sobol (1993) and addressed by Archer et al. (1997), Saltelli (2002), allows the computation of all the terms in the variance decomposition 5.3.2.1.

Let us consider a sample of size n of the input vector, $(x_{k1}, \ldots, x_{kd})_{k=1,\ldots,n}$. The expectation f_0 and the variance V of Y are estimated as usual by:

$$\hat{f}_0 = \frac{1}{n} \sum_{k=1}^{n} f(x_{k1}, \ldots, x_{kd}), \qquad (5.3.5.1.1)$$

$$\hat{V} = \frac{1}{n} \sum_{k=1}^{n} f^2(x_{k1}, \ldots, x_{kd}) - \hat{f}_0^2. \qquad (5.3.5.1.2)$$

To estimate the first order sensitivity indices we need to estimate $V_i = Var(E[Y \mid X_i])$. This variance can be written under the form :

$$V_i = Var(E[Y \mid X_i]) = \underbrace{E[E[Y \mid X_i]^2]}_{U_i} - E[E[Y \mid X_i]]^2 = U_i - E[Y]^2 \qquad (5.3.5.1.3)$$

(using the fact that $E[E[Y \mid X_i]] = E[Y]$). The quantity $E[Y]$ is estimated by 5.3.5.1.1, and for U_i, Sobol (1993) has given the following estimation:

$$\hat{U}_i = \frac{1}{n} \sum_{k=1}^{n} f(x_{k1}, \ldots, x_{k(i-1)}, x_{ki}, x_{k(i+1)}, \ldots, x_{kd}) f(x'_{k1}, \ldots, x'_{k(i-1)}, x_{ki}, x'_{k(i+1)}, \ldots, x'_{kd}) \qquad (5.3.5.1.4)$$

where $(x'_{k1}, \ldots, x'_{kd})_{k=1,\ldots,n}$ represents a second sample of size n of the input vector and the conditioning is taken into account by "resampling" all the variables except x_{ki}.

The first order sensitivity indices are then estimated by

$$\hat{S}_i = \frac{\hat{U}_i - \hat{f}_0^2}{\hat{V}} \qquad (5.3.5.1.5)$$

In the same way, for the second order sensitivity indices, the conditional variance is written as

$$Var(E[Y \mid X_i, X_j]) = \underbrace{E[E[Y \mid X_i, X_j]^2]}_{U_{ij}} - E[E[Y \mid X_i, X_j]]^2 = U_{ij} - E[Y]^2,$$

and the quantity U_{ij} is estimated by

$$\hat{U}_{ij} = \frac{1}{n} \sum_{k=1}^{n} f(x_{k1}, \ldots, x_{k(i-1)}, x_{ki}, x_{k(i+1)}, \ldots, x_{k(j-1)}, x_{kj}, x_{k(j+1)}, \ldots, x_{kd})$$
$$\times f(x'_{k1}, \ldots, x'_{k(i-1)}, x_{ki}, x'_{k(i+1)}, \ldots, x'_{k(j-1)}, x_{kj}, x'_{k(j+1)}, \ldots, x'_{kd}) \qquad (5.3.5.1.6)$$

The second order sensitivity indices are then estimated by

$$\hat{S}_{ij} = \frac{\hat{U}_{ij} - \hat{f}_0^2 - \hat{V}_i - \hat{V}_j}{\hat{V}} \tag{5.3.5.1.7}$$

with $\hat{V}_i = \hat{U}_i - \hat{f}_0^2$. The procedure continues for the estimation of all the indices. The total sensitivity indices are estimated by

$$\hat{S}_{T_i} = 1 - \frac{\hat{U}_{\sim i} - \hat{f}_0^2}{\hat{V}}, \tag{5.3.5.1.8}$$

with

$$\hat{U}_{\sim i} = \frac{1}{n} \sum_{k=1}^{n} f(x_{k1}, \dots, x_{k(i-1)}, x_{ki}, x_{k(i+1)}, \dots, x_{kd}) f(x_{k1}, \dots, x_{k(i-1)}, x'_{ki}, x_{k(i+1)}, \dots, x_{kd}). \tag{5.3.5.1.9}$$

Saltelli (2002) extends the method such that the number of $n(2d+1)$ model evaluations needed to estimate all the first order and total indices is reduced to $n(d+2)$.

Example (The Ishigami function continued)

For the Ishigami function we get, using the package *sensitivity* in R:

- with Sobol method for $n = 1000$: 7000 model evaluations for estimation of 6 indices

$$\hat{S}_1 = 0.3754, \hat{S}_2 = 0.439, \hat{S}_3 = 0.025, \hat{S}_{12} = 0.0076, \hat{S}_{13} = 0.1533, \hat{S}_{23} = 0.076 \tag{5.3.5.1.10}$$
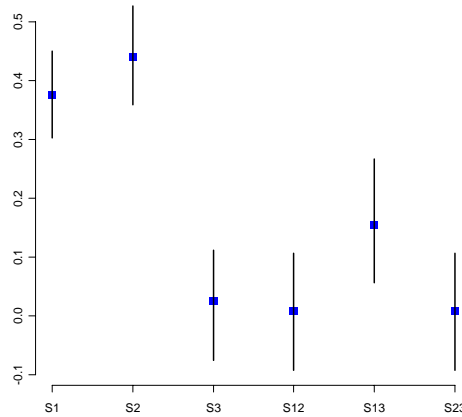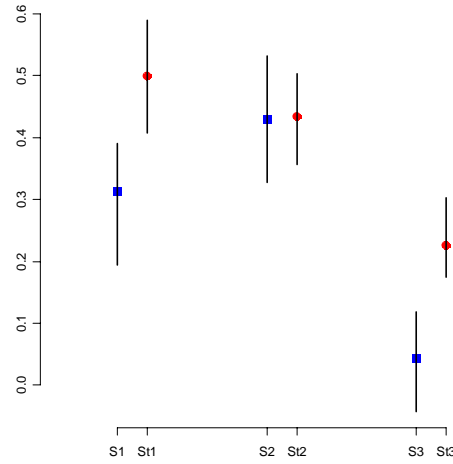

Figure 5.3.5.1.1.- First and second order sensitivity indices and their 95% confidence interval for Ishigami function (Sobol method)

- with Saltelli method for $n = 1000$: 5000 model evaluations for 6 indices

$$\hat{S}_1 = 0.3128, \hat{S}_2 = 0.4289, \hat{S}_3 = 0.043, \hat{S}_{T_1} = 0.5, \hat{S}_{T_2} = 0.434, \hat{S}_{T_3} = 0.226 \tag{5.3.5.1.11}$$

Figure 5.3.5.1.2.- First order and total sensitivity indices and their 95% confidence interval for Ishigami function (Saltelli method)

Estimation by FAST method

This method is due to Cukier et al. (1973, 1975, 1978) and Schaiby and Shuler (1975) and different algorithms have been developed in Koda et al. (1979), and Saltelli and Bolado (1998).
This method is based on the fact that it is possible to convert the *k*-dimensional integrals defining the variances in the variance decomposition 5.3.2.1 into one-dimensional integrals, by using the transformation functions $G_i, i = 1,...,k$ defined as:

$$x_i = G_i(\sin(\omega_i s)) \tag{5.3.5.2.1}$$

where *s* is a scalar variable $s \in \left]-\pi, \pi\right[$ and $\{\omega_i\}$ is a set of integer angular frequencies.
Cukier et al showed (using the properties of Fourier series) that for properly chosen ω_i and G_i, the expectation and the variance of *Y* can be approximated respectively by:

$$f_0 = E[Y] = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s)ds \tag{5.3.5.2.2}$$

$$Var(Y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f^2(s)ds - f_0^2 \approx \sum_{j=-\infty}^{\infty} (A_j^2 + B_j^2) - (A_0^2 + B_0^2)$$
$$= 2\sum_{j=1}^{\infty} (A_j^2 + B_j^2) \tag{5.3.5.2.3}$$

with $f(s) = f(G_1(\sin(\omega_1 s)),...,G_k(\sin(\omega_k s)))$ and A_j, B_j the Fourier coefficients of the cosine and sine series:

$$A_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s)\cos(js)ds, \quad B_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(s)\sin(js)ds. \tag{5.3.5.2.4}$$

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Cukier et al. (1973) showed that the part of the variance due to one input factor X_i is the sum of the squares of the Fourier coefficients due to the angular frequency ω_i and its harmonics:

$$V_i = 2\sum_{k=1}^{\infty}(A_{k\omega_i}^2 + B_{k\omega_i}^2).$$
(5.3.5.2.5)

The sensitivity S_i index is then defined as:

$$S_i = \frac{\sum_{k=1}^{\infty}(A_{k\omega_i}^2 + B_{k\omega_i}^2)}{\sum_{j=1}^{\infty}(A_j^2 + B_j^2)}.$$
(5.3.5.2.6)

Finally, Saltelli and Bolado (1998) have proved that the sensitivity indices defined by the FAST method are equivalent to the ones defined by Sobol.

However, in order to use the formula 5.3.5.2.6, several conditions have to be fulfilled:

— a bound for the infinite sum in 5.3.5.2.5 has to be fixed; it is denoted by M (Cukier et al. (1975) have empirically shown that a good compromise between a good quality of the indices and their estimation cost is $M = 4$ or $M = 6$)
— the functions G_i have to be chosen; the initial choices were given in Cukier et al. (1973) and in Koda et al. (1979) respectively

$$x_i = G_i(\sin(\omega_i s)) = x_i^0 \exp(\nu_i \sin(\omega_i s))$$
(5.3.5.2.7)

$$x_i = G_i(\sin(\omega_i s)) = x_i^0 (1 + \nu_i \sin(\omega_i s))$$
(5.3.5.2.8)

— the choice of the angular frequencies ω_i such that are free of interferences up to a certain order (here up to order 4). These frequencies are changing with the number of input variables and sets of such frequencies are given in Schaibly and Shuler (1973) for example and are reproduced in table 5.3.5.2.1.
— the sampling of the variable $s \in]-\pi, \pi[$, for the computation of the Fourier coefficients A_j, B_j has to respect the Nyquist-Shannon sampling theorem (i.e. the sampling frequency should be at least twice the maximal frequency of the function to be sampled); if we denote by N_s the size of this sample, then its minimal value should be $N_s > 2M \max(\omega_i)$. However, Cukier et al. (1975) showed that there is no significant gain in accuracy in the calculation of the Fourier coefficients for sample sizes beyond $N_s \approx M \max(\omega_i)$. In table 5.3.5.2.1 we also present, for each set of angular frequencies, the minimal number of simulations to be performed N_s.
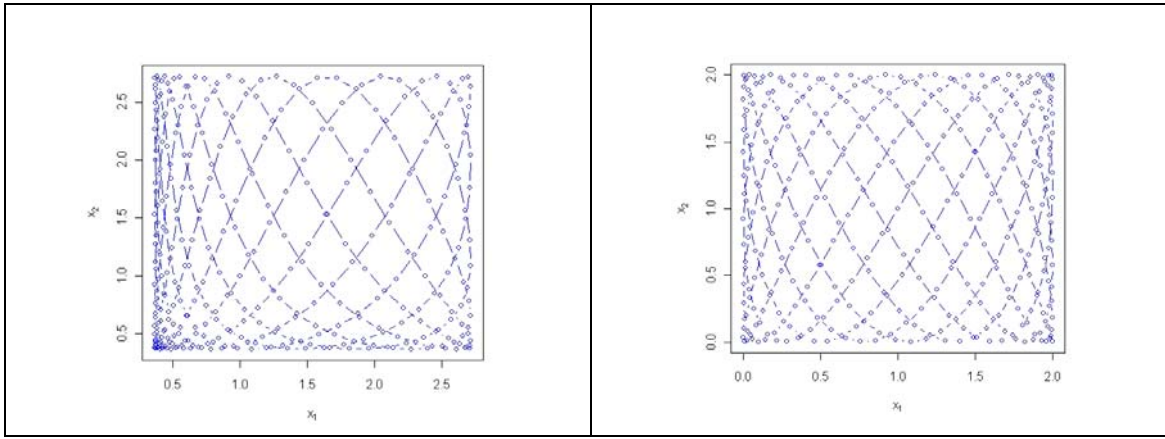
Figure 5.3.5.2.1.- Example of FAST sampling in 2 dimensions, with a set of frequencies equal to {11, 21} and N_s=691; (a) using formula 5.3.5.2.7; (b) using formula 5.3.5.2.8.

Table 5.3.5.2.1.- Set of frequencies and corresponding minimal sample size, based on the formula $N_s = M \max(\omega_i) + 1, \ M = 4$.

Number of input factors	Set of frequencies {ω_i}	Minimal sample size N_s
5	{11, 21, 27, 35, 39}	157
6	{1, 21, 31, 37, 45, 49}	197
7	{17, 39, 59, 69, 75, 83, 87}	349
8	{23, 55, 77, 97, 107, 113, 121, 125}	501
9	{19, 59, 91, 113, 133, 143, 149, 157, 161}	645
10	{25, 63, 103, 135, 157, 177, 187, 193, 201, 205}	821
11	{41, 67, 105, 145, 177, 199, 219, 229, 235, 243, 247}	989
12	{31, 87, 113, 151, 191, 223, 245, 265, 275, 281,289, 293}	1173
13	{23, 85, 141, 167, 205, 245, 277, 299, 319, 329, 335, 343, 347}	1389
14	{87, 133, 195, 251, 277, 315, 355, 387, 409, 429, 439, 445, 453, 457}	1829
15	{67, 143, 189, 251, 307, 333, 371, 411, 443, 465, 485, 495, 501, 509, 513}	2053
16	{73, 169, 245, 291, 353, 409, 435, 473, 513, 545, 567, 587, 597, 603, 611, 615}	2461
17	{85, 145, 241, 317, 363, 425, 481, 507, 545, 585, 617, 639, 659, 669, 675, 683, 687}	2749
18	{143, 229, 289, 385, 461, 507, 569, 625, 651, 689, 729, 761, 783, 803, 813, 819, 827, 831}	3325
19	{149, 275, 361, 421, 517, 593, 639, 701, 757, 783, 821, 861, 915, 935, 945, 951, 959, 963}	3853

Application example (level_E test case)

A study has been performed in order to compare results obtained via regression based techniques and via FAST. This study is based on two samples, a simple random sample of size 459 and a FAST sample of size 323 (one half of the suggestion made in table 5.3.5.2.1, though in agreement with some authors, as for example Koda et al. (1979)). The former was used to estimate sensitivity indices based on regression models (SRRCs) and CSM plots, while the latter was used to estimate variance-based sensitivity indices (first order effects contributions to the variance of the output variables). Three

output variables have been considered in this study, one of them is dynamic (the dose over time), while the others are scalar responses (the peak dose and the time to the peak dose).

Regarding the dose over time, regressions based on the raw values never reached a coefficient of determination (R^2) above 0.35, and most of the time it was between 0.10 and 0.20, see figure 5.3.5.2.2. This fact makes very limited the validity of this regression model to explain the behaviour of the dose over time. Figure 5.3.5.2.3 shows the results of the regressions based on the ranks of the values. According to this analysis it is clear that $V^{(1)}$ is the most important model input. In fact, there is a clear correlation between the R^2s and the absolute value of the SRRC associated to $V^{(1)}$. The rest of the inputs are practically non-influential (only $L^{(1)}$ reach at early time steps values around –0.30).

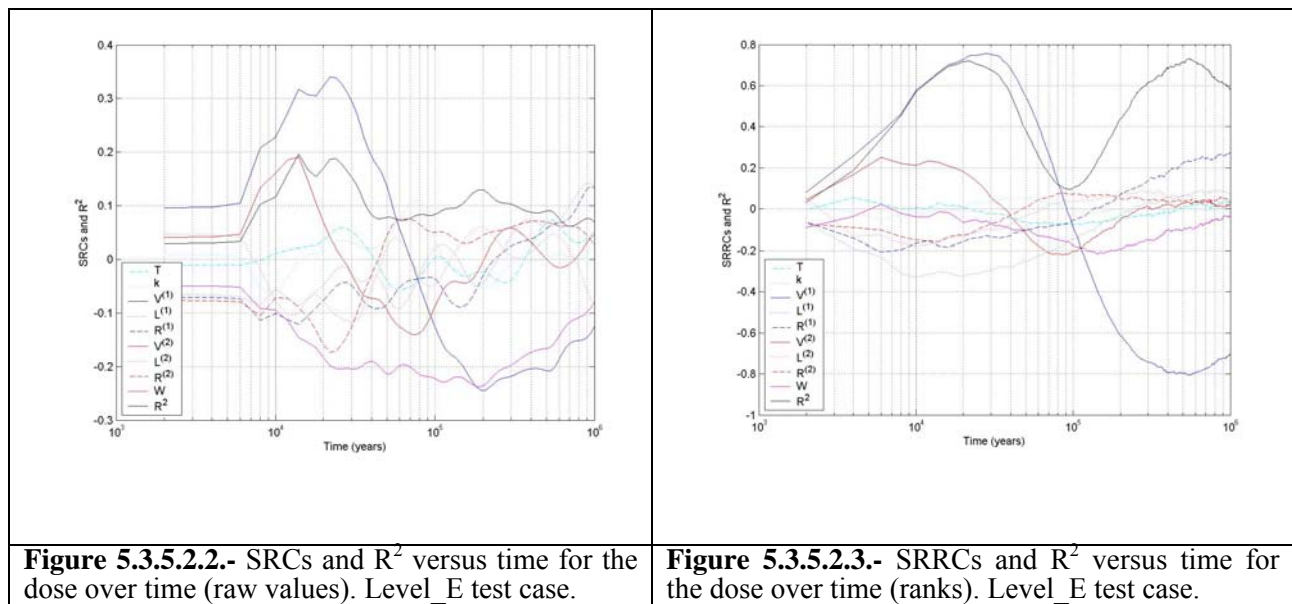|	
Figure 5.3.5.2.2.- SRCs and R^2 versus time for the dose over time (raw values). Level_E test case.	**Figure 5.3.5.2.3.-** SRRCs and R^2 versus time for the dose over time (ranks). Level_E test case.

Figure 5.3.5.2.4 shows the results of the FAST analysis. The results obtained are partially different from the ones provided by regression analysis. In this case, the two most relevant model inputs are W and $V^{(1)}$, in this order except at early and late time. The other inputs are quite less important. This figure does also show that first order effects are able to explain between 15 and 25% of the variability, depending on the time. These results do also show that the behaviour of the dose over time in this test case is complex, since a large fraction of the variability (more than 75%) is due to interactions. Figure 5.3.5.2.5 shows the maximum distance to the diagonal obtained when computing CSM plots for the dose over time and all the input parameters. $D_{m\,0.05}$ is also provided for each time to know what values are statistically significant and which are not. Results reported in this figure do essentially agree (though there are some differences) with the ones reported by FAST: W is the most relevant parameters at intermediate times while $V^{(1)}$ predominates at early and late times, being their effect statistically significant at all times. The rest are essentially irrelevant except during short periods.
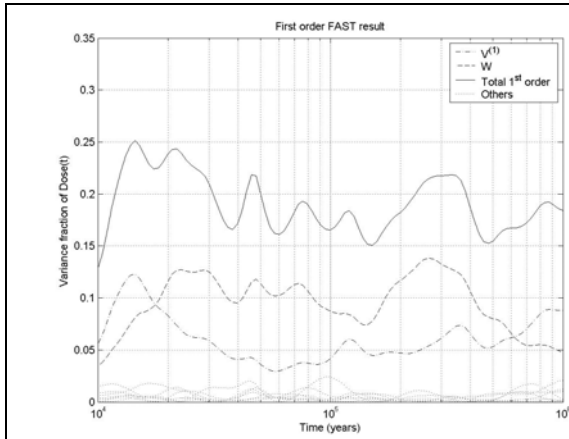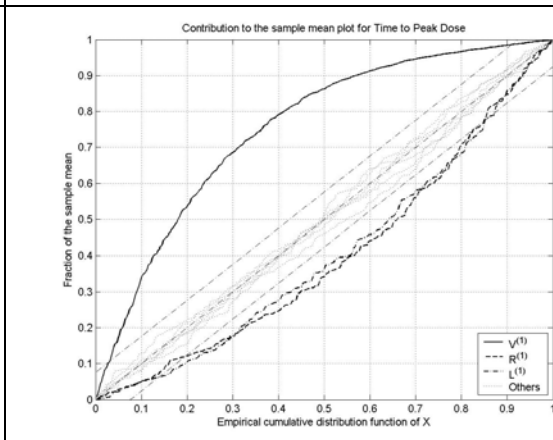

*Figure 5.3.5.2.4.- **Variance based first order sensitivity indices obtained with FAST for the dose over time. Level_E test case.***
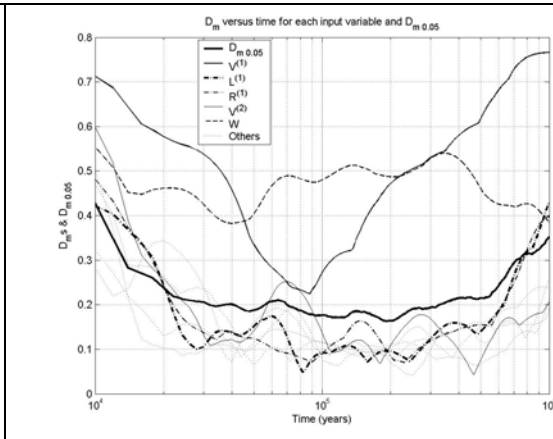
Figure 5.3.5.2.5.- Sensitivity indices obtained with the CSM plot for the dose over time. Level_E test case.
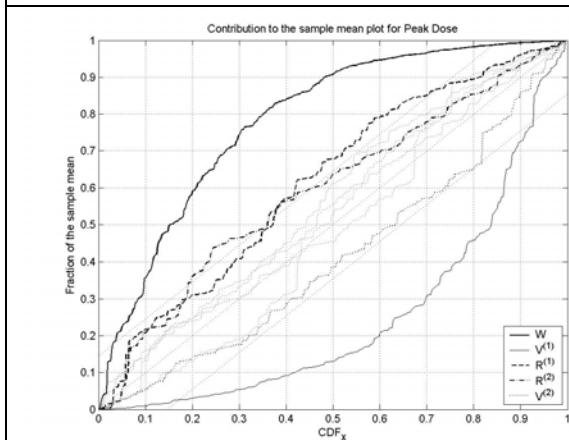
Figure 5.3.5.2.6.- CSM plot for the peak dose with bands set at α=0.05. Level_E test case.

Figure 5.3.5.2.7.- CSM plot for the time to the peak dose with bands set at α=0.05. Level_E test case.

Figures 5.3.5.2.6 and 5.3.5.2.7 show respectively the CSM plots for the peak dose and the time to the peak dose. Tables 5.3.5.2.2 and 5.3.5.2.3 show the FAST results (only first order effects), regression analysis results (R^2 and SRRCs) and CSM results (values of D_m for each input parameter) for the same outputs. The symbol '*' in the CSM results column means statistically significant result with α=0.05. We can see the very good agreement between all the techniques when working on these output variables, at least in the identification of most relevant parameters and their order of importance. It is also remarkable the large fraction of the variability of these outputs that is explained by first order effects (47% for the peak dose and almost 70% for the time to the peak dose).

Table 5.3.5.2.2.- FAST results (first order effects), regression analysis results (R^2 and SRRCs) and CSM results (values of D_m for each input parameter, $\alpha=0.05$) for the peak dose.

Input parameters	Sensitivity measure		
	SRRC	Fraction of σ^2	D_m
T	0.000 (9)	0.001 (8)	0.116 (8)
k	0.003 (8)	0.000 (9)	0.064 (9)
$V^{(1)}$	0.639 (2)	0.167 (2)	*0.407 (2)
$L^{(1)}$	-0.118 (4)	0.006 (6)	0.145 (6)
$R^{(1)}$	-0.188 (3)	0.024 (3)	*0.201 (3)
$V^{(2)}$	0.044 (6)	0.018 (4)	*0.151 (5)
$L^{(2)}$	-0.029 (7)	0.002 (7)	0.133 (7)
$R^{(2)}$	-0.048 (5)	0.009 (5)	*0.195 (4)
W	-0.747 (1)	0.244 (1)	*0.454 (1)
	R^2=0.957	1st order effects total contribution to σ^2=0.471	$D_{m\alpha}$=0.147

Table 5.3.5.2.3.- FAST results (first order effects), regression analysis results (R^2 and SRRCs) and CSM results (values of D_m for each input parameter, $\alpha=0.05$) for the time to peak dose.

Input parameters	Sensitivity measure		
	SRRC	Fraction of σ^2	D_m
T	0.005 (9)	0.000 (7.5)	0.063 (4)
k	-0.008 (7)	0.000 (7.5)	0.046 (5.5)
$V^{(1)}$	-0.885 (1)	0.501 (1)	*0.395 (1)
$L^{(1)}$	0.304 (2)	0.099 (2)	*0.155 (3)
$R^{(1)}$	0.255 (3)	0.082 (3)	*0.172 (2)
$V^{(2)}$	-0.113 (4)	0.001 (5)	0.042 (8.5)
$L^{(2)}$	0.075 (6)	0.000 (7.5)	0.046 (5.5)
$R^{(2)}$	0.090 (5)	0.004 (4)	0.043 (7)
W	-0.006 (8)	0.000 (7.5)	0.042 (8.5)
	R^2=0.955	1st order effects total contribution to σ^2=0.687	$D_{m\alpha}$=0.076

Figure 5.3.5.2.8 shows the CSM plot for the dose at 10^5 years. This plot shows that the impact of W and $V^{(1)}$ on the mean of the output is not the same in all their regions, clearly the lowest values of W contribute more to the mean of the dose than its largest values, while intermediate values of $V^{(1)}$ are the ones that really affect the mean of the dose at that time. This result is in agreement with the results provided by FAST (figure 5.3.5.2.4); both inputs are identified as the only important ones and in the same order (D_m(W)=0.4798, $D_m(V^{(1)})$=0.2715), no other input parameter reaches $D_{m\alpha}$ ($\alpha=0.05$). Additionally, the CSM line for $V^{(1)}$ explains the very low value of R^2 at 10^5 years in figure 5.3.5.2.3; this line shows the clear lack of monotonocity in the relation between this input and the output since the largest values of the output are obtained for intermediate values of $V^{(1)}$ (steepest region of the CSM line in average). Many other CSM plots realised for the dose at different time steps, which are not in this report, showed agreement with the results of FAST provided in figure 5.3.5.2.4.
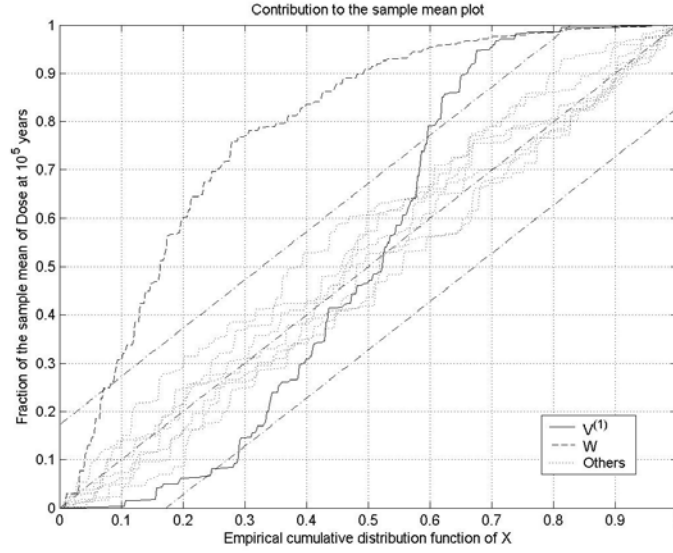
Figure 5.3.5.2.8.- CMS plot for the dose at 10^5 years with bands set at α=0.05. Level_E test case.

Estimation by EFAST method

For the total sensitivity indices, Saltelli et al. (1999) introduced the *extended FAST* (EFAST) method, where the part of variance due to all the variables except X_i is the sum of the squares of the Fourier coefficients due to all the angular frequency $\omega_{\sim i}$ different from ω_i, leading to:

$$S_{T_i} = 1 - \frac{\sum_{k=1}^{\infty}(A_{k\omega_{\sim i}}^2 + B_{k\omega_{\sim i}}^2)}{\sum_{j=1}^{\infty}(A_j^2 + B_j^2)}. \tag{5.3.5.3.1}$$

Another difference from the initial FAST method is that the functions G_i have been chosen such that they are "filling" in a more suitable way the input space:

$$x_i = G_i(\sin(\omega_i s)) = \frac{1}{2} + \frac{1}{\pi}\arcsin(\sin(\omega_i s)) \tag{5.3.5.3.2}$$

$$x_i = G_i(\sin(\omega_i s)) = \frac{1}{2} + \frac{1}{\pi}\arcsin(\sin(\omega_i s + \varphi_i)) \tag{5.3.5.3.3}$$

where φ_i is a random phase chosen uniformly in $[0, 2\pi[$. Moreover, the choice of the angular frequencies ω_i is no longer constrained by the "no interferences up to a certain order" rule. For a given variable X_i, the pair of indices (S_i, S_{Ti}) is computed simultaneously; the only constraint is that the angular frequency ω_i (corresponding to x_i) should be large compared to the ones corresponding to the rest of the variables (for instance ω_i=124, $\omega_{\sim i}$=1).

| (a) | (b) | (c) |
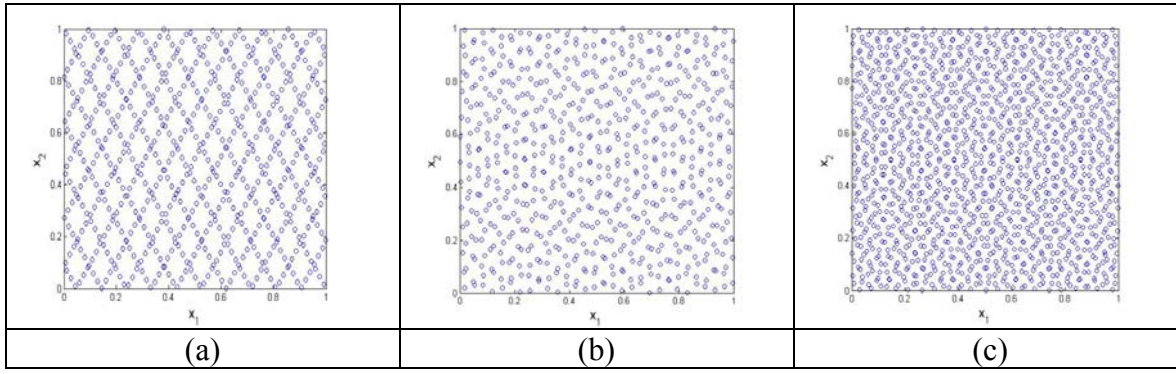
Figure 5.3.5.3.1.- Example of EFAST sampling in 2 dimensions, with a set of frequencies equal to {11, 21} and N_s=691; (a) using formula 5.3.5.3.2; (b) using formula 5.3.5.3.3 with one single random phase; (c) using formula 5.3.5.3.3 with two random phases.

It should be emphasized that when computing sensitivity indices with FAST method, it is not possible to compute tolerance intervals (as it is the case when using Sobol method) because the method is *deterministic*. The number of runs is equal to *n*x*d* for estimating 2*d* sensitivity indices.

Example (the Ishigami function continued)

For the Ishigami function we get, using the package *sensitivity* in R, for $n = 1000 : 3000$ model evaluations for estimation of 6 indices

$$\hat{S}_1 = 0.3077, \hat{S}_2 = 0.442, \hat{S}_3 = 0, \hat{S}_{T_1} = 0.5506, \hat{S}_{T_2} = 0.47, \hat{S}_{T_3} = 0.2391. \tag{5.3.5.3.4}$$
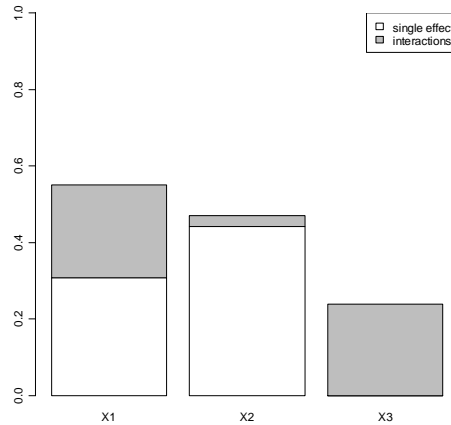
Figure 5.3.5.3.2.- First order and total sensitivity indices for Ishigami function using extended FAST method.

Estimation by random balanced design (RBD)

The RBD method (see Tarantola et al. (2006) or Saltelli et al. (2008)) is similar to FAST or EFAST. It uses the parametrization $x_i = G_i(\sin(\omega_i s))$, $s \in]-\pi, \pi[$ the scalar variable and $\{\omega_i\}$ is the set of integer angular frequencies (the function G may be taken as in expressions 5.3.5.3.2 or 5.3.5.3.3). The scalar variable is then discretized. The main difference with FAST – EFAST is that the input space is explored using the same frequency ω, to avoid the use of a complicated algorithm for choosing the different frequencies. Doing so, the set of discretized input parameters x_i (i.e. the design) is no longer

space-filling. Therefore, random permutations of the coordinates of those points are taken in order to generate a set of scrambled points that cover the input space. An example of such "scrambled" points is shown in figure 5.3.5.4.1. The model is then evaluated at each design point. To compute the first order sensitivity index S_i, the output y is re-ordered in increasing order of the values taken by the factor X_i. The Fourier spectrum of the output is calculated for the frequencies $\{\omega, 2\omega,..., M\omega\}$ to the estimate the sensitivity index S_i.

The procedure is repeated for all the other factors to obtain all the first order sensitivity indices.

The main drawback of this method is that it only computes the first order sensitivity indices.

Its main advantages with respect to (E)FAST is that there is no minimum sample size to avoid interference problems and no special algorithm for providing the free interference set of frequencies. Also, the number of harmonics in the spectrum (i.e. M) may be increased without affecting the size of the sample.
Another advantage is that confidence intervals could be computed for those indices.

The number of runs is equal to n for estimating d sensitivity indices.
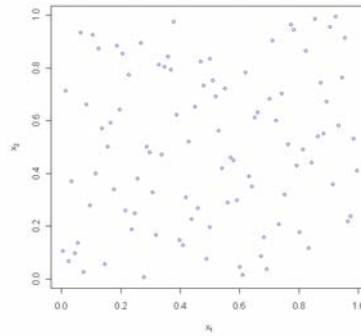
Figure 5.3.5.4.1.- Example of RBD sampling in 2 dimensions, with $\omega = 1$ and Ns=100; (4.3.35) have been used for generating the design .

Example (the Ishigami function continued):

For the Ishigami function we obtain with this method for $n = 1000$ (1000 model evaluations for estimation of 3 indices) $\hat{S}_1 = 0.319, \hat{S}_2 = 0.454, \hat{S}_3 = 0.019$. These results are very similar to the theoretical ones (5.3.4.1) and to the ones obtained using Sobol's or Saltelli's method (5.3.5.1.10) and EFAST method (5.3.5.3.4). The computations have been made using R.

Other variance decomposition based methods

McKay (1997) also gives a method of estimation of the variances $Var(Y)$ and $Var(E[Y \mid X_i])$ based on replicated Latin Hypercube Sampling, which can be used to estimate the first order sensitivity indices. Hofer (1999) uses correlation ratios to estimate first order sensitivity indices. The output sample is divided in subsamples according to a partition of each input sample. The output mean is computed for each subsample and the variance of these means divided by the variance of the output is the first order sensitivity index for that input parameter. Correlation ratios are the square root of first order sensitivity indices computed in this way.

5.4.   Distribution sensitivity methods

Many of the uncertainties that appear in a PA are epistemic (lack of knowledge). The assessment of these uncertainties is done most frequently via expert judgement. In many cases the experts show some reluctance to provide accurate distributions, as is the case of underconfident experts. In other situations they acknowledge that the distributions could be slightly different from the ones they are actually providing. One of the targets of SA is to measure the potential impact of those changes on the distributions of the outputs.

The trivial solution for this problem is to run the code a number of times under the original or main distribution, let us say *n* times, and another number of times under the alternative distribution, let us say *n'* times, and to compare the results (mainly means, distribution functions and success or failure probabilities). In the case of *k* input parameters we need to run *n+kn'* times the code to measure the influence of changing the input distribution of each input parameters. This problem becomes a combinatorial problem as we try to measure the effect of changing simultaneously the distribution of two or more input parameters. Certainly this is not an efficient way to measure the effect of input distribution changes on the output distribution.

In the following pages we will describe two methods available in the statistics literature to measure the influence of input distribution changes in the means and the distribution functions of the output variables. These two methods (the weighting method and the rejection method) were developed by Beckman and McKay (1987). This problem did also arise within the Probabilistic Safety Assessment Code Use Group (PSAG and formerly PSAC), in the PA area. Some of the participants in that group proposed solutions similar to the weighting method, see OECD-NEA (1993 and 1997) and Alonso (1993). In fact, the solution proposed by Alonso is a particular case of the method proposed by Beckman and McKay (restricted only to uniform and log-uniform distributions).

The first method developed by Beckman and McKay is suitable for measuring the effect on the mean of the output and resembles a variance reduction technique, importance sampling. The second method is suitable for measuring the effect on the distribution function and is based on the acceptance/rejection sampling technique to sample from distributions with no analytical inverse cumulative distribution function. The second method is more relevant to the estimation of the change in the success probability of a passive system, though the first one does also provide some additional worthy information.

First we will define the problem, second we will show the foundations of these two methods and we also will write down some ideas about their efficiencies. We will also provide some ideas about their actual implementation. Finally, an application example will be shown.

5.4.1.   The problem

Let us consider a *k* components vector of input parameters X. Let us assume that two different distribution functions $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ may be assigned to that input parameter vector. Let us also assume that the first one is the reference one and the second one is the one we are addressing for sensitivity. For simplicity, let us consider only one output variable Y. Since X is a random vector, Y will also be random and its distribution function will depend on the distribution function of X. Let us call $F_1(y)$ and $F_2(y)$ to the distribution functions of Y when X follows the distributions $f_1(\mathbf{x})$ and $f_2(\mathbf{x})$ respectively.

5.4.2. The weighting method

The weighting method resembles importance sampling. In the case of importance sampling the problem is to estimate the mean of a reference random variable as accurately as possible, and the proposed solution is to find an ancillary random variable with the same mean and a smaller variance than the reference variable. In our case we have both, the reference distribution and the ancillary one, so that we can apply the method for our purposes. This method is only adequate for estimating changes in the mean.

Let us consider the random variable Y' defined as $Y'(\mathbf{x}) = w(\mathbf{x})Y(\mathbf{x}) = (f_2(\mathbf{x})/f_1(\mathbf{x}))Y(\mathbf{x})$. Let us demonstrate that the mean of Y', when sampling $\mathbf{X}$ from $f_1(\mathbf{x})$, is the same as the mean of Y when sampling $\mathbf{X}$ from $f_2(\mathbf{x})$. In other words, let us demonstrate that $E_1(Y'(\mathbf{X}))=E_2(Y(\mathbf{X}))$, where the sub-indices indicate what input vector distribution function we are using to compute the mean. The only requirement we are going to impose is that the support R_2 of $f_2(\mathbf{x})$ is contained in the support R_1 of $f_1(\mathbf{x})$.

$$E_1(Y'(\mathbf{X})) = \int_{R_1} Y'(\mathbf{x})f_1(\mathbf{x})d\mathbf{x} = \int_{R_1} [f_2(\mathbf{x})/f_1(\mathbf{x})]Y(\mathbf{x})f_1(\mathbf{x})d\mathbf{x} = \int_{R_1} Y(\mathbf{x})f_2(\mathbf{x})d\mathbf{x} \ . \qquad (5.4.2.1)$$

Since $R_2 \subset R_1$, and $f_2(\mathbf{x})$ is null outside R_2, the last integral in R_1 and in R_2 are the same so that we can write

$$E_1(Y'(\mathbf{X})) = \int_{R_1} Y(\mathbf{x})f_2(\mathbf{x})d\mathbf{x} = \int_{R_2} Y(\mathbf{x})f_2(\mathbf{x})d\mathbf{x} = E_2(Y(\mathbf{X})) \ . \qquad (5.4.2.2)$$

From a practical point of view, this theoretical result means that a way to estimate the mean of Y under $f_2(\mathbf{x})$ is to get a sample of Y under $f_1(\mathbf{x})$ and to multiply each one of those sampled value of Y under $f_1(\mathbf{x})$ by its corresponding weight $w(\mathbf{x})=f_2(\mathbf{x})/f_1(\mathbf{x})$. The arithmetic mean of those sampled values multiplied by their corresponding weights is an unbiased estimate of $E_2(Y(\mathbf{X}))$. In the following lines there is the procedure to be followed:

- *Step 1*⇨ Obtain a sample of size n of the input random vector under the reference distribution: $\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}$. Their actual values will be $\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}$.
- *Step 2* ⇨ Run the code for those n sets of inputs in order to get the corresponding sample of the output variable: $Y_1, Y_2, \ldots, Y_n$. Their actual values will be $y_1, y_2, \ldots, y_n$.
- *Step 3*⇨ Weight the sample with the corresponding weights, getting for each actually sampled value $y_i=y(\mathbf{x_i})$ the corresponding value $y'(\mathbf{x_i})= y(\mathbf{x_i})w(\mathbf{x_i})= y(\mathbf{x_i})f_2(\mathbf{x_i})/f_1(\mathbf{x_i})$.
- *Step 4*⇨ Estimate $E_2(Y(\mathbf{X}))$ through:

$$\hat{\mu}_2 = \frac{1}{n}\sum_{i=1}^{i=n}\frac{f_2(\mathbf{x_i})}{f_1(\mathbf{x_i})}y(\mathbf{x_i}) \ . \qquad (5.4.2.3)$$

The efficiency of the weighting method

A general problem in statistical estimation is the determination of the accuracy of the estimates generated with a given method. In the general case the accuracy of the estimates is measured with their variance. The larger the variance is, the smaller the accuracy is. In our case we can compare the

accuracy or variance of the estimator of the mean of Y under the reference distribution using a random sample, $\hat{\mu}_1$, with the accuracy of the proposed estimator $\hat{\mu}_2$ (formula 5.4.2.3) for estimating the mean of Y under the sensitivity distribution.

Let us define the efficiency of the second estimator with respect to the first as the quotient of the variance of the first divided by the variance of the second. Since both estimators are simple arithmetic averages of two different magnitudes, Y and Y', this efficiency will be equal to the quotient of the variances of Y and Y'. The consequences of this fact are that, depending on the characteristics of Y', we will get efficiencies larger or smaller than one. In other words, $\hat{\mu}_2$ could be more accurate or less accurate than $\hat{\mu}_1$. This could lead to the surprising result that, though we sampled under the conditions of f_1, our estimate for the mean of Y under f_2 could have less error than the estimate for the mean of Y under f_1.

In order to understand this phenomenon, let us see the following example. Let us assume that we have a very simple model that depends on only one input parameter X. Let us assume that the experts provided as their best estimate for this model an exponential distribution with mean 10. Let us assume that we know the closed solution of our model and its analytical form is exactly the same as the former exponential density function. Let us also consider that our interest is to study the effect of changing the mean of the input distribution to any other value between 2 and 50, keeping the type of distribution (exponential). All these assumptions may be resumed as

$$f_1(x) = \lambda e^{-\lambda x} \qquad \lambda = 0.1$$
$$y(x) = \lambda e^{-\lambda x} \qquad \lambda = 0.1$$
$$f_2(x) = \lambda_2 e^{-\lambda_2 x} \qquad \lambda_2 \in [0.02, 0.5] \ .$$

We can see that in this case $Y'(x) = f_2(x)$. Moreover, under these assumptions it is quite easy to demonstrate that the efficiency of the weighting method proposed by Beckman and Mckay is

$$eff = \frac{Var(\hat{\mu}_1)}{Var(\hat{\mu}_2)} = \frac{Var(Y(x))}{Var(Y'(x))} = \frac{Var(Y(x))}{Var\left(\dfrac{f_2(x)}{f_1(x)} Y(x)\right)} = \left[12\lambda_2^2 \left(\frac{1}{\lambda^2 + 2\lambda\lambda_2} - \frac{1}{(\lambda + \lambda_2)^2} \right) \right]^{-1}$$

(5.4.2.1.1)

Figure 5.4.2.1.1 shows the reference input probability density function f_1 and the response of the computer code Y, the same function in this example (the continuous line $f_1(\mathbf{x}) = Y(\mathbf{x})$), same function in this example; and the two extreme cases for f_2 among the infinite set considered (λ_2 between 0.02 and 0.5). For each one of those infinite alternative distributions f_2, the corresponding function $Y'(x)$ is equal to f_2. Figure 5.4.2.1.2 shows the efficiency of the weighting estimator with respect to the estimator of the mean of Y under f_1. A straightforward conclusion from that plot is that the smaller λ_2 (the larger the mean of X) the larger the efficiency. Efficiencies are larger than 1 for $\lambda_2 < 0.1$ and smaller than 1 for $\lambda_2 > 0.1$. For $\lambda_2 = 0.02$, the efficiency is approximately 100; in that case we need samples 100 times larger to estimate the mean of Y under the reference distribution that to estimate the mean of Y under this alternative distribution with the same accuracy. The most surprising fact of this result is that we are using a sample of f_1!
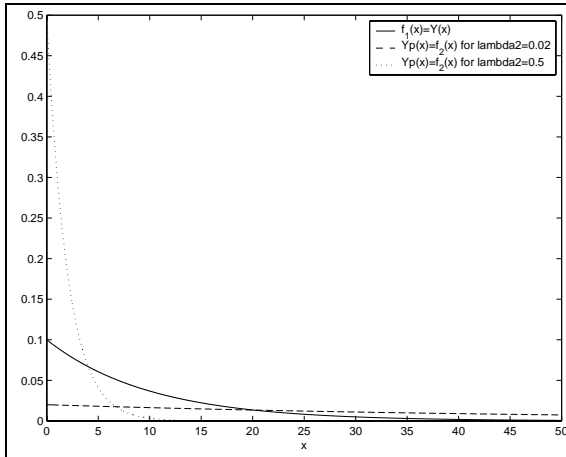
Figure 5.4.2.1.1.- Input reference distribution, model (same curve), and extreme alternative input distributions (equal to the corresponding *Y'* functions).
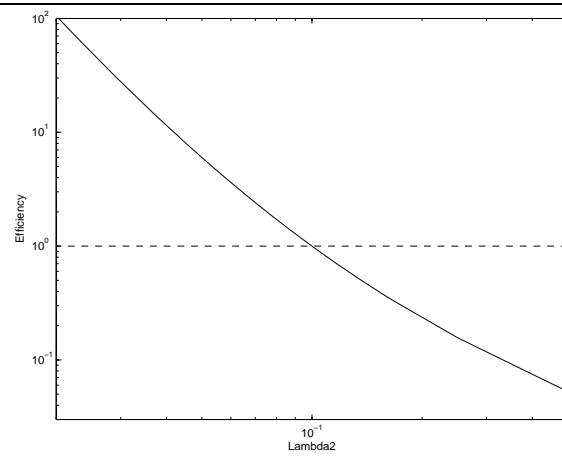
Figure 5.4.2.1.2.- Efficiency of the weighting estimator, for the example with the exponential distributions, as a function of λ_2 (that represents the alternative distribution).

The reason for such a surprising result comes from the fact that, for all the functions *Y'(x)*, *X* follows the same law of probability, but the range of *Y'* (remind that it is equal in this example to the corresponding f_2) decreases dramatically as λ_2 decreases, so that the variance of *Y'* decreases as λ_2 decreases, producing the result shown in figure 5.4.2.1.2. It is quite interesting to check that better results are obtained as the variance of f_2 increases.

Beckman and Mckay (1987) provide further studies about the efficiency of this method for the cases of normal and beta distributions, discussing about the origin of the obtained results.

5.4.3. The rejection method

The rejection method is based on the acceptance/rejection sampling method for random variables with cumulative distribution function with no analytical inverse function, see Johnson (1987) and Fishman (1996).

There are two conditions for the application of this method: First, as in the previous method, the support of $f_2(\mathbf{x})$, R_2, must be contained in the support of $f_1(\mathbf{x})$, R_1; and second, the quotient $f_2(\mathbf{x})/f_1(\mathbf{x})$ must be bounded. Let us assume that the bound is *M*; in other words, $\left(f_2(\mathbf{x})/f_1(\mathbf{x})\right) \le M \quad \forall \mathbf{x} \in R_2$. In the following lines there is the procedure to be followed:

- *Step 1*⇨ Obtain a sample of size *n* of the input random vector under the reference distribution: $\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}$. Their actual values will be $\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}$.
- *Step 2* ⇨ Run the code for those *n* sets of inputs in order to get the corresponding sample of the output variable: $Y_1, Y_2, \ldots, Y_n$. Their actual values will be $y_1, y_2, \ldots, y_n$.
- *Step 3*⇨ For each sample $\mathbf{x_i}$, take a sample of the uniform distribution V_i between *0* and $Mf_1(\mathbf{x_i})$.
- *Step 4*⇨ Retain in the sample the corresponding output value $Y_i = y_i$ if the realisation v_i of V_i is less or equal to $f_2(\mathbf{x_i})$, otherwise reject that value from the sample.

- *Step 5*⇨   Consider the values of Y remaining in the sample as a random sample of Y under $f_2(\mathbf{x})$, and use this sample of size $k \leq n$ to build up an empirical distribution function that estimates the actual distribution function of Y under $f_2(\mathbf{x})$. Each step in that empirical distribution function will have a height $1/k$.

The objective of sampling Y under $f_1(\mathbf{x})$ and under $f_2(\mathbf{x})$ is to get an estimate of the probability of failure of the system under those different circumstances. If we assume that the system fails when the variable Y exceeds the value y_0, our estimate of the probability of failure will be the number of observations of Y that exceed such a value divided by n for the reference case and divided by k in the sensitivity case.

This procedure for estimating the distribution function of Y under $f_2(\mathbf{x})$ produces an unbiased estimator for that function since we are applying strictly the acceptance/rejection method for sampling $\mathbf{X}$ under $f_2(\mathbf{x})$ using as an ancillary function $f_1(\mathbf{x})$. The acceptance/rejection method provides a random sample of $\mathbf{X}$ under $f_2(\mathbf{x})$. This fact guaranties that the transformation of this sample through the model provides a random sample of Y under $f_2(\mathbf{x})$. This sample may be used in the usual way to provide any unbiased estimator related to Y, in particular the empirical distribution function.

The efficiency of the rejection method

In this case Beckman and McKay propose as a measure of efficiency the probability that a realisation of the random vector $\mathbf{X}$ under $f_1(\mathbf{x})$, $\mathbf{x}$, be accepted as a random variate under $f_2(\mathbf{x})$. This probability is $1/M$ since

$$ eff = P(\text{a random } \mathbf{X} \text{ is retained}) = \int_{R_1} P(V \leq f_2(\mathbf{u}) \mid \mathbf{u}) f_1(\mathbf{u}) d\mathbf{u} = 1/M \ . \qquad (5.4.3.1.1) $$

The intuitive justification for this result comes from the fact that the quotient between the hypervolume under $Mf_1(\mathbf{x})$ and the hypervolume under $f_2(\mathbf{x})$ is M, so that, in the average, according to the acceptance criterion, only a fraction $1/M$ of the sample obtained under $f_1(\mathbf{x})$ will remain as a sample under $f_2(\mathbf{x})$. A detailed demonstration may be found in Beckman and McKay (1987).

Let us revisit the example of the exponential functions shown in section 5.4.2.1. If we try to apply the rejection method to that case, the first thing we find is that the method may not be applied to any alternative distribution with $\lambda_2 < 0.1$ since the quotient $f_2(x)/f_1(x)$ must be bounded and that is not the case under these conditions. For all the other cases ($\lambda_2 > 0.1$), it is quite easy to show that the efficiency is

$$ eff = \lambda/\lambda_2 \ . \qquad (5.4.3.1.2) $$

Let us consider now the alternative exponential distribution function $f_2(x)$ with $\lambda_2 = 0.2$. We have sampled 50 observations from $f_1(x)$ and we have applied the rejection method. Figure 5.4.3.1.1 shows the three essential functions in this method for the example case: $f_1(x)$, $2 f_1(x)$ and $f_2(x)$. It is convenient to remember that in this example $f_1(x)$ and $Y(x)$ are identical functions. The 50 values sampled from $f_1(x)$ are the x component of the points in figure 5.4.3.1.1. The y components of those points are the corresponding realisations of the uniform random variables V_i. In agreement with the method, only those x values corresponding to points below $f_2(x)$ (dotted line) are retained as valid x values under $f_2(x)$. The values of Y for those x values are those that will be considered to build up the distribution

function for *Y*. Figure 5.4.3.1.2 shows the empirical distribution function for *Y* under f_1(x) (solid line) and the empirical distribution function for *Y* under f_2(x) (void line).
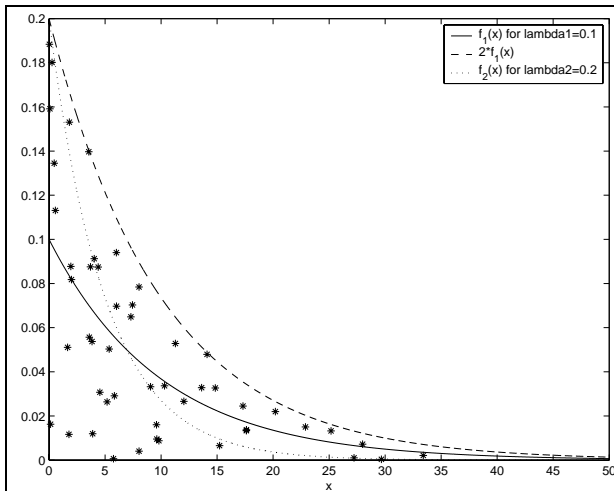
Figure 5.4.3.1.1.- f_1(x), f_2(x) and 2f_1(x). The output variable of this model coincides with f_1(x).
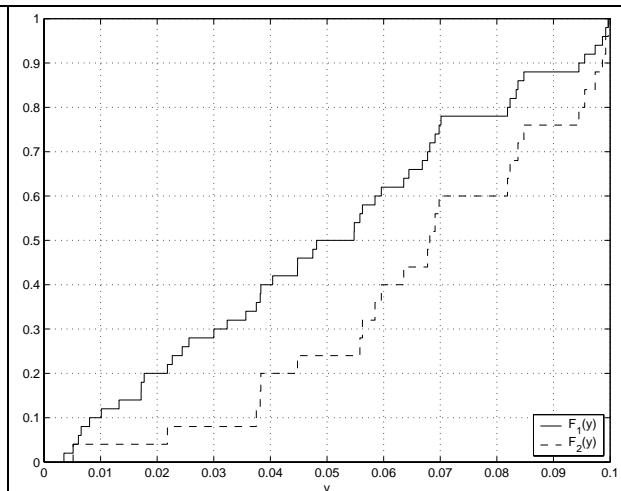
Figure 5.4.3.1.2.- Empirical distribution function for *Y* under f_1(x) and empirical distribution function for *Y* under f_1(x), using the sample obtained under f_1(x).

A careful look at figure 5.4.3.1.1 shows that in this sample 25 points are above f_1(x) and the rest are below it. This sample efficiency is exactly the same as the predicted efficiency, though it could be different in another sample. As a consequence of this fact, the empirical distribution function for *Y* under f_2(x) in figure 5.4.3.1.2 will have only 25 steps, each one with height 1/25. If we consider that the system fails as soon as *Y* is larger than 0.09, by inspection of figure 5.4.3.1.2 we easily see that the estimate for the probability of failure under the reference distribution is 6/50=0.12, while the estimate for the probability of failure under the alternative distribution is 6/25=0.24. The estimate of that probability increases by a factor 2. This result could be expected since f_1(x) puts more weight on the small values and less weight on the large values of *X* than f_2(x). Nevertheless, *Y*(*X*), the model itself, is monotonically decreasing, so that a shift towards smaller *X* values implies a shift towards larger *Y* values. This example is for a model with only one input parameter, but its application to a multi-parameter model is straightforward.

Both methods are suitable for measuring the sensitivity to the change in one, several or all the input parameters, though with some restrictions (if a set of the input parameters are mutually dependent, the sensitivity to a change in one subset may not be addressed separately).

An extension of the rejection method

As we have seen in the previous section, the main problem of the rejection method is its potential low efficiency due to discarding many observations from the sample under some circumstances. A way to increase this efficiency is repeating many times the process described in section 5.4.3 and averaging. If we do so, we will arrive at an output estimated distribution function under the alternative input distribution (f_2(x)) that attributes the following probability to each output value
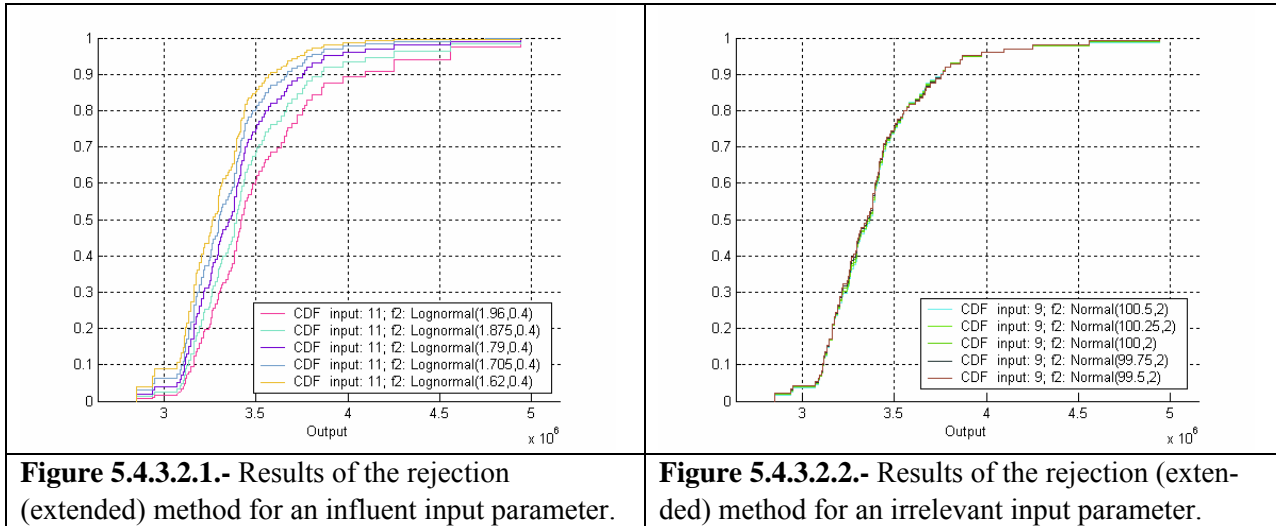
$$P(Y(\mathbf{x}_i)) = \frac{\dfrac{f_2(\mathbf{x}_i)}{f_1(\mathbf{x}_i)}}{\displaystyle\sum_{i=1}^{n}\dfrac{f_2(\mathbf{x}_i)}{f_1(\mathbf{x}_i)}} \qquad (5.4.3.2.1)$$

Application example of the rejection method (extended)

The rejection method (extended according to section 5.4.3.2) was applied to assess the changes in the reliability of a passive safety system in an advanced nuclear power reactor. Several input parameters were affected by epistemic uncertain and their uncertainty was characterised via probability density functions. All input distributions were allowed to vary their means up to 15% up and down. So, if the mean of a given uncertain parameter was 10, the intention of the study was to see what were the consequences on the output (pressure in the primary system) of changing the mean of the input between 8.5 and 11.5.

Figures 5.4.3.2.1 and 5.4.3.2.2 show the results corresponding to two input parameters: different cumulative distributions of the pressure under different input distributions. The system was supposed to fail when a pressure of 4 Mpa was exceeded (value 4 in the x-axis). Figure 5.4.3.2.1 shows the results corresponding to the most influent parameter (input parameter 11). We can see the shift towards larger pressures when the mean of the input parameter diminishes (orange →blue →purple →green →red). The output distribution under the original input distribution is the purple line. Under that hypothesis, the probability of failure of the system was roughly 4%. When analysing the spread of that probability under different alternative input distributions we can see that it may vary between roughly 2% (orange line) and 11% (red line). Figure 5.4.3.2.2

Shows the results for a completely irrelevant parameter (input parameter 9); it is practically impossible to distinguish the different output distributions. Changing the mean of this input parameter has no impact on the output distribution.

Figure 5.4.3.2.1.- Results of the rejection (extended) method for an influent input parameter.	**Figure 5.4.3.2.2.-** Results of the rejection (extended) method for an irrelevant input parameter.

6. Response surface based

The most widely used response surface model is regression, see Iooss et al. (2006), and sections 5.2.1.3 – 5.2.1.7 in this report. Among the other response surface models, the polynomial chaos

expansions are quite effective for the sensitivity analysis, because once the coefficients of the expansion are estimated, the computation of the Sobol sensitivity indices is straightforward.

6.1. Polynomial chaos expansions

Polynomial chaos expansions of random functionals are based on the mathematical theory developed by Wiener (1938), Cameron and Martin (1947). Their use for uncertainty and sensitivity purposes started with the work of Ghanem and Spanos (1991) on the stochastic finite element method and ever since they have gained in popularity, especially in the case when the physical system under study is computationally expensive, making Monte Carlo simulations impossible to use.

Polynomial chaos consist in expanding the output on an orthogonal basis of polynomial chaos denoted by $\{\psi_k\}$:

$$y(\boldsymbol{x}) = \sum_{k=0}^{\infty} \beta_k \psi_k(\boldsymbol{x}).$$
(6.1.1)

The orthogonality is associated to the joint probability density function (pdf($\boldsymbol{x}$)) of the random vector $\boldsymbol{x}$ (the input), i.e. $\langle \psi_k(\boldsymbol{x}), \psi_l(\boldsymbol{x}) \rangle = \int \psi_k(\boldsymbol{x}) \psi_l(\boldsymbol{x}) pdf(\boldsymbol{x}) d\boldsymbol{x} = \|\psi_k(\boldsymbol{x})\|^2 \delta_{kl}$. As an example, for a normally distributed 1-dimensional input, the basis of polynomial chaos is formed by the Hermite polynomials

$$\psi_0 = 1, \qquad \psi_1 = x, \qquad \psi_2 = x^2 - 1, \qquad \psi_3 = x^3 - 3x, \dots$$

The response surface is obtained by approximating the expansion (6.1.1) by a finite sum

$$y(\boldsymbol{x}) \approx \sum_{k=0}^{M} \beta_k \psi_k(\boldsymbol{x}).$$
(6.1.2)

The coefficients β_k are computed as $\beta_k = \frac{1}{\|\psi_k\|^2} \int y(\boldsymbol{x}) \psi_k(\boldsymbol{x}) pdf(\boldsymbol{x}) d\boldsymbol{x}$. Finally, in order to obtain the estimations of these coefficients, a quadrature formula is used. The choice of the quadrature method will lead to the choice of the design of experiments, i.e. the values of the input vector where the computations with the original model have to be done; it will also give the weights w_j to be used:

$$\beta_k \approx \frac{1}{\|\psi_k\|^2} \sum_j y(\boldsymbol{x}_j) \psi_k(\boldsymbol{x}_j) w_j.$$
(6.1.3)

Due to the orthogonality being associated to the joint probability density function (pdf($\boldsymbol{x}$)) of the input, straightforward formulae for the total (V) and *partial* (V_u) variances are deduced:

$$V = Var(Y) \approx \sum_{k=1}^{M} \beta_k^2 \|\psi_k\|^2$$
(6.1.4)

$$V_u \approx \sum_{k \in U(u)} \beta_k^2 \|\psi_k\|^2 ; U(u) = \{k, \psi_k(x) = \psi_k(x_u)\}, \qquad (6.1.5)$$

where $U(u)$ is a set of indices.

The Sobol sensitivity indices can then be computed as the ratio between V_u and V. An important remark is that with this method we can compute sensitivity indices up to any order we need to, without any computation effort. This allows deciding whether higher order interactions between the inputs are significant or not.

Example of transport of a radionuclide in a nuclear waste repository (continued)

For the example of the transport of a radionuclide (^{129}I) in a nuclear waste repository (section5.2.1.5), a deterministic design of experience with 737 points (in 6 dimensions) has been used for the quadrature method. Sensitivity indices up to the fourth order have been computed using the software Petras (http://www-public.tu-bs.de:8080/~petras/software.html). We present in table 6.1.1 the values for the total sensitivity indices.

Table 6.1.1.- Polynomial chaos expansion sensitivity results for the example of the transport of a radionuclide.

Variable name	Sobol total sensitivity indices	Order of variable importance
Kh1	S_{T1}= 3.51e–01	1
Kv1	S_{T2}= 3.48e–01	2
K2	S_{T3}= 2.45e–01	5
K3	S_{T4}= 2.55e–01	4
poro	S_{T5}= 3.00e–01	3
de	S_{T6}= 1.82e–01	6

There is one significant difference between those results and the ones obtained for the regression methods previously used, which is the fact that the input variable *Kh1* appears as the most important one. However, *Kv1* and *poro* which were the most influent ones in the different regression methods are the next important ones. Another significant difference is the fact is that the initial computational effort was quite large for the polynomial chaos expansions: a *deterministic* design of experiments with 737 points has been used (i.e. 737 runs of the numerical code), while a *random* design of experiments (latin hypercube) with only 60 points have been used for the regression methods.

6.2. Kriging

Kriging was developed initially by geostatisticians in the 60's. It's use in the context of computer experiments started with the work of Sacks et al. (1989a). A detailed description of kriging may be found in Santner et al. (2003). Kriging is an interpolating method. The kriging model can be written in the form

$$y(\boldsymbol{x}) = f(\boldsymbol{x})\beta + Z(\boldsymbol{x}), \qquad (6.2.1)$$

where $f(x)\beta$ is the deterministic part (called the trend) and $Z(x)$ is the random part (a centred, stationary Gaussian process). The trend takes into account the large scale variations of the output, while the random part takes into account its small scale variations. The Gaussian process is entirely characterized by its covariance function. The covariance function determines the smoothness of the response surface and it depends on $k+1$ parameters; its form has to be chosen a priori (out of a list of possible covariance functions, see Santner et al. (2003)).

The parameters that have to be estimated from the data are the coefficients β of the trend and the $k+1$ parameters of the covariance function. The estimation is done by the maximum likelihood method.

As an example, the Gaussian covariance function is defined by:

$$C(h) = \sigma_Z^2 \exp\left(- \sum_{i=1}^{d} (h_i/\theta_i)^2\right) \quad \text{for any } h \in IR^d \tag{6.2.2}$$

where σ_Z^2 and θ_i, $i=1,\ldots,d$ represent the variance and the scale parameters of the Gaussian process, have to be estimated from the experiments by maximum likelihood.

One of the main advantages of kriging is the fact the predictor is an interpolator whose smoothness depends on the data (via the covariance function) and yet not imposed a priori as in a regression method.

The surface response obtained by kriging can be used to compute Sobol sensitivity indices.

Example of transport of a radionuclide in a nuclear waste repository (continued)

For the example of the transport of one radio nuclide (^{129}I) in a nuclear waste repository, the latin hypercube design with 60 points has been used to estimate the parameters of a kriging model with a linear trend. This means that 7 coefficients (denoted $\beta_i, i = 0,\ldots 6$) had to be estimated for the trend and 7 parameters (σ_Z^2 and θ_i, $i=1,\ldots,6$) for the Gaussian process. Sobol total sensitivity indices have been computed. We present in table 6.2.1 the sensitivity results obtained.

Table 6.2.1.- Kriging (with linear trend) sensitivity results for the example of the transport of a radionuclide.

Variable name	Sobol total sensitivity indices	Order of variable importance
Kh1	S_{T1}= 2.37e–06	6
Kv1	S_{T2}= 9.04e–01	1
K2	S_{T3}= 3.72e–03	4
K3	S_{T4}= 4.58e–02	3
poro	S_{T5}= 8.68e–02	2
de	S_{T6}= 9.47e–04	5

Again, like in the regression examples, *Kv1* and *poro* are the most influent input variables.

7. Conclusions

A review of most interesting and useful SA techniques in the context of a PA has been done, concentrating efforts on screening methods and global methods. Screening methods focus on identifying strong functional relations between inputs and outputs, while global methods focus on how input uncertainty maps on the output space.

Within screening methods we have focused our attention on classical full factorial and fractional factorial methods, Morris' method and sequential bifurcation. We have found full factorial and fractional factorial methods as powerful tools when the number on input parameters is moderate, but its applicability cannot be recommended when the number of input factors is very large; in those cases methods like Morris' and sequential bifurcation are more appropriate.

In this study, global methods have been classified as graphic methods, Monte Carlo based methods, variance decomposition based methods and distribution sensitivity methods. This classification is a bit arbitrary since there are many overlaps among these methods (graphic tools may be used with data obtained via Monte Carlo simulation, but they may also be used with data obtained under different sampling schemes, as for example the traditional FAST sampling), but we have found it useful.

Monte Carlo based methods (regression based and Monte Carlo filtering) are quite well known in the scientific and technical community. They are simple to use and provide easily interpretable results. The main shortcoming of regression-based techniques is the specification, a priori, of a given structure for the model under study, which makes less powerful the results. Monte Carlo filtering, which allows identifying relations between different regions of inputs and outputs, is not affected by this problem. An important advantage of these methods is that they allow the simultaneous use of the same sample (input and output) to perform uncertainty and sensitivity analysis, not needing specific additional code runs for each specific analysis. This fact is a strong reason in favour of these methods. An important area of research for the next future is the adaptation of specific efficient techniques to allow computing variance based sensitivity indices using Monte Carlo samples.

Variance based methods provide information about what input factors and what interactions among input factors introduce more variability in the output, which made them very powerful tools to understand the behaviour of PA models. The main problem with many of these techniques is the need of using specific sampling schemes, not appropriate to perform simultaneously uncertainty analysis. A large improvement has been achieved during the last years to make these methods cheaper in computational terms, though there is still room for improvement.

Graphical methods (scatter plots, cobweb plots and contribution to the sample mean plots –CSM plots-) are strongly recommended. They provide a lot of information in support of numeric sensitivity techniques and illustrate many model features that are not shown by pure numeric measures. Additionally, one of them, CSM plots, provides a numeric measure that is itself a measure of importance linked to variance based sensitivity indices. This method identifies what region(s) of each input variable has/have the strongest impact on the output mean and allows the representation, in the same graphic, of may inputs, which facilitates comparing the effect of different inputs. The use of cobweb plots in support of Monte Carlo filtering techniques is strongly recommended. These techniques do also allow representing the relation between one output and several inputs.

Distribution sensitivity techniques have been identified as the mean to check what could be the effect on output distributions of changes in the distributions of the inputs. The use of these techniques could be very helpful to avoid expensive experiments and expert judgement processes. This would be the case of input parameters whose likely alternative distributions do not show an important impact on the output distribution.

The whole set of methods described in this report allow PA modellers to study and get information about their model from different perspectives, which allows them to understand correctly their models.

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Annex 1: Level E test model description.

The model under study reproduces the behaviour of a high-level radioactive waste repository and the contaminant disposed of. The repository is considered without any geometric complexity, as just a point. Engineered barriers are modelled through a containment time during which there is no release. After the containment period, the contaminant starts releasing at a fractional constant rate. Only one radionuclide is considered in this study, ^{129}I. This radionuclide was selected because of its relevance in many safety assessments already performed worldwide. The contaminant is carried by groundwater through two consecutive geosphere layers to the biosphere, where it makes its way into a water stream from which exposed population take drinking water. This model has 15 inputs, nine of which are affected by uncertainty. These model inputs are the initial inventory of ^{129}I (M_0), its decay rate (λ), the dose conversion factor (β), and all the other inputs that characterize the physical-chemical properties of the near field, both geosphere layers and the biosphere.

There are three components in this system model, which will be described in the following subsections: the source term model, geosphere models and the biosphere model.

7.1. A.1.- Source term model

The source term model consists of a simple delay in the release, after which a fractional constant release begins (the release being proportional to the remaining quantity of contaminant). During the whole period, the inventory also decreases due to radioactive decay. Therefore, during the containment period, the inventory of ^{129}I decreases according to the following ordinary differential equation (ODE):

$$\frac{dM(t)}{dt} = -\lambda M(t) \qquad t \leq T \,, \tag{A.1}$$

while, after the containment period, the inventory of ^{129}I decreases according to the following ODE:

$$\frac{dM(t)}{dt} = -\lambda M(t) - k M(t) \qquad t > T \,. \tag{A.2}$$

The initial condition is $M(0)=M_0$. The flow of contaminant escaping from the facility to the first geosphere layer is given by

$$S(t) = k M(t) \,. \tag{A.3}$$

Both containment time (T) and release rate (k) are considered to be uncertain.

7.2. A.2.- Geosphere model

The transport of contaminant through both geosphere layers is simulated in one dimension (*1-D*). Each geosphere layer is characterized by its length ($L^{(i)}$, where i stands for the layers; $i=1$ corresponds to the first layer and $i=2$ to the second). The transport equation is

$$R^{(i)} \frac{\partial C^{(i)}}{\partial t} + V^{(i)} \frac{\partial C^{(i)}}{\partial x} - d^{(i)} V^{(i)} \frac{\partial^2 C^{(i)}}{\partial x^2} = -\lambda R^{(i)} C^{(i)} \qquad (A.4)$$

where $R^{(i)}$, $V^{(i)}$ and $d^{(i)}$ stand, respectively, for the retardation coefficient, the groundwater velocity and the dispersion length in the corresponding geosphere layer, which is indicated by i. $C^{(i)}$ stands for the concentration of contaminant in any position x at time t, so that formally it should be considered $C^{(i)}(x,t)$. Velocities of groundwater, retardation coefficients and lengths of both layers are considered +to be uncertain model inputs, whereas dispersion lengths are known inputs. Null concentration of contaminant in both layers is considered for the initial condition. For the specification of the boundary conditions, it is assumed that the contaminant flow rate into the first layer is the flow coming from the facility. Moreover, the flow rate into the second layer is equal to the flow rate from the first layer; similarly, the flow rate into the biosphere is equal to the flow rate from the second geosphere layer.

7.3.   A.3.- The biosphere model

The biosphere model is very simple. It is assumed that the contaminant coming from the second biosphere layer gets into a stream used for drinking water. Therefore, the dose is a function of the proportion of water drunk by individuals. Mathematically it can be formulated as

$$D(t) = \beta \frac{w}{W} G^{(2)}(t) \qquad (5)$$

where $G^{(2)}(t)$ is the flow rate coming from the second geosphere layer into the biosphere, β is the dose conversion factor, w is the individual's annual water consumption rate and W is the flow rate of the biosphere water stream.

Table A.1.- Model inputs in the problem under study (U = uniform distribution, LU = logarithmic-uniform distribution; in both cases values shown in brackets denote lower and upper bounds).

PARAMETER	TYPE	VALUE/DISTRIBUTION	UNITS
M_0	Constant	10^2	Mol
Λ	Constant	$4.41 \cdot 10^8$	y^{-1}
T	Random/uncertain	$U[10^2, 10^3]$	Y
K	Random/uncertain	$LU[10^{-3}, 10^{-2}]$	y^{-1}
$V^{(1)}$	Random/uncertain	$LU[10^{-3}, 10^{-1}]$	$m \cdot y^{-1}$
$L^{(1)}$	Random/uncertain	$U[10^2, 5 \cdot 10^2]$	M
$d^{(1)}$	Constant	10	M
$R^{(1)}$	Random/uncertain	$U[1,5]$	Dimensionless
$V^{(2)}$	Random/uncertain	$LU[10^{-2}, 10^{-1}]$	$m \cdot y^{-1}$
$L^{(2)}$	Random/uncertain	$U[5 \cdot 10^1, 2 \cdot 10^2]$	m
$d^{(2)}$	Constant	5	m
$R^{(2)}$	Random/uncertain	$U[1,5]$	Dimensionless
W	constant	0.73	$m^3 \cdot y^{-1}$
W	Random/uncertain	$LU[10^5, 10^7]$	$m^3 \cdot y^{-1}$
B	constant	56	$Sv \cdot mol^{-1}$

Abstract
This reports gives an overview of sensitivity methods (screening, global and response surface based) that are suitable for safety analysis of a repository for radioactive waste or spent nuclear fuel. The theoretical background of the methods, their limitations and suitability for different analyses are discussed and illustrated by examples.

The mission of the JRC is to provide customer-driven scientific and technical support for the conception, development, implementation and monitoring of EU policies. As a service of the European Commission, the JRC functions as a reference centre of science and technology for the Union. Close to the policy-making process, it serves the common interest of the Member States, while being independent of special interests, whether private or national.