Second-Order Effects in Model Sensitivity Analyses and the Role of Graph Theory

F. Campolongo and R. Braddock
Environmental Sciences
Griffith University

Abstract Sensitivity analysis is an important component of model building. Sensitivity of the model outputs to variations in the parameter and initial values of variables may affect the method of solution which is selected, may reduce confidence in the model and its predictions, and may be an important indicator as to which parameters and initial values need to be measured accurately. This paper extends the current first-order sensitivity techniques and methods to consider second-order effects on the sensitivity of models. This obviously includes non-linear effects which are not fully quantifiable by methods based on first-order techniques. The efficient calculation of the sampling of the parameter space leads to graph theory and the 'handcuffed-prisoner problem'. Solutions to the optimal sampling problem are obtained and applied to test problems. The techniques are readily applicable to estimating third and higher order effects.

1. INTRODUCTION

Sensitivity testing is an important component of building mathematical and simulation models. The values of model parameters and the initial (input) values of variables are subject to many sources of uncertainty. An understanding of the sensitivity of the model outputs to the uncertainty in the values of the input variables and parameters is necessary to developing confidence in the model and its predictions.

Sensitivity analysis (SA) experiments may be performed on mathematical and computational models to determine the relative contribution of input variables and parameter values to the observed variations in model outputs. These computational experiments can determine, within reasonable limits, which parameters or initial variable values may have effects on the model outputs which are negligible, significant, linear or non-linear.

Box *et al.* [1978] discuss and define the main effects (first order), as well as the higher order effects (second order, third order, etc.), and relate these effects to the Taylor series expansion of the response (or output) function of the model. In particular, the first-derivative terms in the Taylor series correspond to the main effects (i.e. the effect on the response function due to perturbation of a single variable); the second-derivative terms correspond to two-factor interactions (including the quadratic effects which are two-factor interactions of a factor with itself); and so on.

Several sensitivity techniques are available in the literature to estimate main and higher order effects (for a review, see Helton [1993]). Different methods have been developed to address the estimation of higher order effects [Baker and Bargman, 1985]. As a drawback, those methods generally have a relatively high computational cost. Fractional factorial designs of resolution V and higher, or the central composite design [Baker and Bargman, 1985], do permit the detection of two-factor interaction effects, but are expensive in terms of the number of model evaluations required. Even a two-level resolution V fractional factorial design requires 2^{k-p} model evaluations, where $1/(2^p)$ is the degree of fractionation [Box *et al.*, 1978]. Any eventual increase in the degree of fractionation (to decrease the computational cost) would lower the resolution of the best fraction, so increasing confounding between effects of various orders.

In dealing with models which are computationally expensive to evaluate and which have a large number of input parameters, it is very important to adopt methods which are "economic", or which require a relatively small number of model evaluations. These computationally efficient sensitivity analysis techniques include the 'one-factor-at-a-time', or OAT, screening designs [Morris, 1991], which assess the impact on the output of changing one parameter value at a time. These methods aim to isolate the most important factors from amongst a large number that may affect a particular response, and have been used to consider first-order effects.

The OAT screening method [Morris, 1991] requires O(k) model evaluations, where k is the number of model input factors. In practical applications, the range of values taken by a particular model parameter may be discretised into a number of discrete values or levels. In the Morris method, increasing the number of levels does not increase the computational cost.

The current Morris method provides sensitivity estimates of total effects (i.e. the sum of first and higher order effects due to a single parameter), and an 'overall' sensitivity measure of curvature and interactions between factors. It does not distinguish non-linear from interaction effects. The 'overall' measure of the interactions of a particular factor or parameter value with the rest of the model is given by the Morris method, but it does not give specific

information as to which part of the rest of the model is interacting. Distinct sensitivity measures for each possible two-factor, three-factor or higher interactions are not given.

The obvious problem is to develop or extend an existing method which is computationally efficient in terms of model evaluations, yet provides more information on the higher order interactions. This paper shows how the Morris method can be extended to develop information on two-factor interactions, whilst still retaining its computational efficiency.

2. BACKGROUND

Assume that the model output $y = y(\mathbf{x})$ is a scalar function of the vector $\mathbf{x}$ of input factors. The vector $\mathbf{x} = (x_1, x_2, ..., x_k)$ has k components x_i, each of which can assume integer values or levels in the set $\{0,...,p-1\}$. This assumes that the range of any parameter or initial value has been scaled to the set of levels $\{0,...,p-1\}$, and takes only integer values over this range. This represents a scaling and discretisation of the parameter space which is denoted by Ω.

For a given $\mathbf{x} \in \Omega$, the *elementary effect* for the i^{th} input factor (Morris, 1991) is defined as:

$$E_i(\mathbf{x}) = [y(\mathbf{x} + \mathbf{e}_i\Delta_i) - y(\mathbf{x})]/\Delta_i \,, \qquad (1)$$

where $\mathbf{e}_i$ is a vector of zeros but with a unit as its i^{th} component, and $\underset{\sim}{\Delta} = (\Delta_1, ..., \Delta_k)$ is a vector whose components are preselected integer step lengths so that $(\mathbf{x} + \mathbf{e}_i\Delta_i)$ is still in Ω for each index $i = 1,...,k$. The value of $\mathbf{x}$ can be varied for each input factor so as to generate a finite distribution of elementary effects, F_i, containing $p^{(k-1)}(p-\Delta)$ elements.

Sensitivity analysis requires each distribution F_i to be sampled by selecting sampling points for the input vector $\mathbf{x}$ [Morris, 1991; Campolongo and Gabric, 1996; Campolongo and Saltelli, 1997]. Subsequent analysis of the sampled data assesses the relative importance of the input factors on the output.

In its simplest form, randomly selecting a value from F_i requires the evaluation of the output y at two points, $\mathbf{x}$ and $(\mathbf{x} + \mathbf{e}_i\Delta_i)$. The total computational cost is then $n = 2rk$ model executions, where r is the selected sample size. A more economical design, requiring $n = r(k+1)$ model executions, has been suggested by Morris [1991] and implemented by Campolongo and Gabric [1996]. This method carries out the random sampling by

- randomly selecting a "base" point $\mathbf{x}^0$ in Ω;
- using $\mathbf{x}^0$ to generate a trajectory consisting of the points $\mathbf{x}^g$, $g = 1,...,k+1$ (note that $\mathbf{x}^0$ is not included in the trajectory). The $\mathbf{x}^g$ are selected so that either $\mathbf{x}^{g+1} = \mathbf{x}^g + \mathbf{e}_i\Delta_i$ or $\mathbf{x}^g = \mathbf{x}^{g+1} + \mathbf{e}_i\Delta_i$ is in Ω, thus producing a trajectory which consists of 'one at a time' steps parallel to the k co-ordinate axes in Ω;
- the elementary effects $E_i(\mathbf{x}^g)$ can be estimated along this trajectory, yielding one sample value for each of the k examined factors;
- further starting points can be used to generate r trajectories and obtain r samples of each of the elementary effects.

The above algorithm generates r "One-factor-At-a-Time" (OAT) trajectories in Ω. Morris [1991] shows that the construction of such a trajectory is equivalent to the construction of a (k+1)-by-k sampling matrix $\mathbf{B}$, called an *orientation matrix*, such that the following properties hold:

(P1) the elements of $\mathbf{B}$ are either 0 or 1;
(P2) for each value of $i = 1,2,...,k$, there are two rows of $\mathbf{B}$ that differ only in the i^{th} entries.

In the Morris experiment, data analysis is carried out by examining the distributions F_i of elementary effects relative to each of the input factors. In particular, the estimated mean μ and standard deviation σ of F_i, are two sensitivity measures indicating respectively the "overall" effect of the i^{th} input on the output, and the "overall" non-linear or interactions effects.

For a given value of the input vector $\mathbf{x}$, selected in the parameter space Ω, we define the *elementary effect* EE_{ij} $(1 \le i \le j \le k)$, attributable to the pair of i^{th} and j^{th} factors, as

$$EE_{ij}(\mathbf{x}) = [y(\mathbf{x} + \mathbf{e}_i\Delta_j + \mathbf{e}_j\Delta_j) - y(\mathbf{x})]/\Delta_i\Delta_j \,, \qquad (2)$$

where $\underset{\sim}{\Delta} = (\Delta_1, ..., \Delta_k)$ is a predetermined vector such that the transformed $(\mathbf{x} + \mathbf{e}_i\Delta_i + \mathbf{e}_j\Delta_j)$ is still in Ω. The distribution of EE_{ij}'s is denoted by FF_{ij}.

The quantities EE_{ij} can be used in order to provide a measure of the effect on the output due to the interaction between the i^{th} and the j^{th} input factors. The effect on the output y due to the interaction of factors i and j can be measured by computing the partial derivative of the output function y with respect to its input variables x_i and x_j. An approximation for this derivative is given by

$$\frac{\partial^2(y)}{\partial \mathbf{x}_i \partial \mathbf{x}_j} \cong \frac{y(\mathbf{x}) + \mathbf{e}_i\Delta_i + \mathbf{e}_j\Delta_j) - y(\mathbf{x} + \mathbf{e}_i\Delta_i) - y(\mathbf{x} + \mathbf{e}_j\Delta_j) + y(\mathbf{x})}{\Delta_i\Delta_j}, \qquad (3)$$

or by adding and subtracting $y(\mathbf{x})$, subtracting the quantity $y(\mathbf{x})$ as

$$\frac{\partial^2 y}{\partial x_i \partial x_j} \cong EE_{ij} - \frac{1}{\Delta_i} E_i - \frac{1}{\Delta_j} E_j \,. \qquad (4)$$

A local measure of the magnitude of the effects due to the interaction between the i^{th} and j^{th} input factors is given by

$$TFE_{ij} = \left| EE_{ij} - \frac{1}{\Delta_i} E_i - \frac{1}{\Delta_j} E_j \right| . \qquad (5)$$

Denote by T_{ij} the distribution of the TFE_{ij}'s obtained by varying the point $\mathbf{x}$ in the parameter space. The estimated mean $\lambda_{i,j}$ of the distribution T_{ij} are global sensitivity measures of the two-factor interactions.

3. THE SAMPLING STRATEGY

Note that, for a model containing k input factors, the number of distributions $T_{i,j}$ equal to the number of two-factor interactions is

$$\binom{k}{2} = \frac{k(k-1)}{2} .$$

Also note that the computation of each TFE_{ij} in (5) necessitates the computation of three different quantities, E_i, E_j and EE_{ij}. Thus the model has to be evaluated at four different points of the parameter space:

A: $\mathbf{x} = (x_1, ..., x_k)$; B: $(\mathbf{x} + \mathbf{e}_i\Delta_i)$;
C: $(\mathbf{x} + \mathbf{e}_j\Delta_j)$; D: $(\mathbf{x} + \mathbf{e}_i\Delta_i + \mathbf{e}_j\Delta_j)$.

The goal of the experimental design is to extract from each distribution T_{ij}, a sample of r elements, $TFE_{ij}^1, ..., TFE_{ij}^r$, in order to estimate the distribution mean.

The sampling strategy proposed below aims to provide the model evaluations needed to compute the quantities E_i (for $i = 1, ..., k$) and EE_{ij} (for $1 \le i \le j \le k$). The computation of the E_j's is carried out in a second phase of the experimental plan.

In analogy with the sampling plan described by Morris, the basic idea is to construct a *multiple trajectory* (MT) in the parameter space Ω which allows the computation of one EE_{ij} per distribution FF_{ij}. A *multiple trajectory* (MT) is constructed by joining together a number of simple trajectories, all having the same starting point. The MT needs to maintain the properties required by Morris so that at least one elementary effect E_i per input can still be estimated. Attention has then to be restricted to those single trajectories for which properties P1 and P2 hold.

As in the Morris method, each single trajectory in Ω corresponds to an orientation matrix. Here an MT corresponds to the junction of several orientation matrices. Thus, if each single orientation matrix B_i has dimension m_i-by-k, the MT will correspond to a *multiple orientation matrix* M_B (or simply, *multiple matrix*),

$$\mathbf{M}_B = \begin{bmatrix} \mathbf{B}_1 \\ \mathbf{B}_2 \\ \\ \mathbf{B}_n \end{bmatrix},$$

of dimension $\left(\sum_{i=1}^{n} m_i\right)$-by-k .

In Section 2, it has been pointed out how a (k+1)-by-k sampling matrix $\mathbf{B}$ would allow the estimation of (k-1) distinct EE_{ij}'s (i.e. belonging to different distributions). Using a *multiple trajectory* to estimate a total number $k(k-1)/2$ of EE_{ij}'s (i.e. one EE_{ij} per distribution FF_{ij}), the minimum number of orientation matrices that have to be joined to provide an MT is respectively k/2, if k is even and (k+1)/2 if k is odd. This minimum will be obtained provided that the following property holds.

(P3) for any pair of orientation matrices $\mathbf{B}_i$, $\mathbf{B}_j$, $i \neq j$, being part of the same MT, the EE_{ij}'s produced by $\mathbf{B}_i$ and $\mathbf{B}_j$ are distinct.

To simplify the notation, let

- (i,j) denote an EE_{ij} relative to the i and j factors;
- given k factors identified by the integers (1, ..., k), then $\Gamma = \{(i,j), i < j\}$, and this will be used to identify the set of EE_{ij};
- the path $\{(i_0,i_1),(i_1,i_2),...,(i_{n-1},i_n)\}$, $i_j \in \{1,...,k\}$ is denoted $\langle i_0,i_1,...,i_n \rangle$ [Berge, 1973].

The implementation of the experimental design calls for the construction of multiple trajectories, or equivalently the construction *multiple matrices*, which are made up of *single orientation matrices* such that: (i) each single matrix allows the estimation of (k-1) distinct EE_{ij}'s; (ii) each single matrix satisfies properties P1 and P2.

In Appendix A, it is shown how, given a block of (k-1) distinct EE_{ij}'s, the construction of a (k+1)-by-k sampling matrix $\mathbf{B}^*$ (single matrix) satisfying (i) and (ii), is possible if the pairs contained in the block are *handcuffed*, i.e. they form a path $\langle i_1,i_2,...,i_k \rangle$. In order to build an experimental design which estimates all the total and interaction effects, the set $\Gamma = \{(i,j)\ i < j\}$, containing the

$$\binom{k}{2} = \frac{k!}{2!(k-2)!} ,$$

EE_{ij}'s is to be "covered" by subsets of (k-1) elements which are handcuffed pairs (for each of those subsets, a single matrix $\mathbf{B}^*$ can then be constructed as shown in Appendix A).

In particular, the optimal experimental design (in terms of computational cost), will be the one in which the number of sets utilised in the experimental plan to cover the whole of Γ, is a minimum.

4. CONSTRUCTING MULTIPLE TRAJECTORIES

The cases in which the number of input factors k is even or odd are treated separately.

If $k = 2s$, the minimum number of (k-1)-subsets needed to cover the whole set Γ is k/2. The most economical experimental plan is the one in which each multiple

orientation matrix is formed by exactly k/2 single orientation matrices of dimension (k+1)-by-k.

This reduces to

Problem I: "Find a partition of Γ made of k/2 subsets composed of (k-1) handcuffed pairs each".

The (k-1) handcuffed pairs, $\{(i_0,i_1),(i_1,i_2),\ldots,(i_{k-2},i_{k-1})\}$, represent a path or trajectory, and Problem I relates to the theory of block designs on graphs.

Following the notation of Hung and Mendelshon [1977], a handcuffed design with parameters v, k, ω, denoted by H(v,k,ω), consists of a system of ordered k-subsets of a v-set called handcuffed blocks. In a block $\langle i_0,i_1,\ldots,i_k-1\rangle$, each element is assumed to be handcuffed to its neighbours and the block contains (k-1) handcuffed pairs.

In order for a handcuffed design to exist, the following conditions have to hold [Hell and Rosa, 1972]:

(1) each element of the v-set appears amongst the blocks the same number of times;

(2) each pair of distinct elements of the v-set are handcuffed in exactly ω blocks.

A solution for Problem I is equivalent to proving the existence of a handcuffed design H(k,k,1).

A sufficient condition for the existence of such design is Hell and Rosa [1972]:

(3) H(k,k,ω) exists if and only if k or ω is even.

Since k = 2s, Condition (3) is satisfied.

An example of the solution of Problem I is described in Hung and Mendelshon [1977]. The elements of the k-set (where k = 2s), identified by the numbers $\{0,\ldots,2s-1\}$ with s = 4, are displayed as edges on a graph as shown in Figure 1.

The construction of the first path, called the beginning path, is represented in Figure 1 and is identified by ⟨6,7,5,0, 4,1,3,2⟩, starting at node 6.

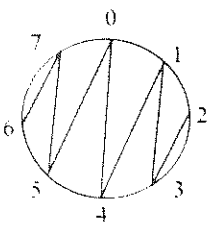

Figure 1: A multiple trajectory path for k even

A second path can then be obtained by simply shifting the starting node from node 6 to node 7, i.e. moving the full path clockwise by one node to obtain the path ⟨7,0,6,1,5,2,4,3⟩.

In the same way, shifting the second path by one node, a third path ⟨0,1,7,2,6,3,5,4⟩ is found. Once the beginning block has been found, all the other blocks are completed by adding one to each element of the previous block and reducing it mod 2s.

A set of s blocks thus obtained, which decompose the graph into s paths of length (k-1), is called a *selection*.

If k = 2s+1, the minimum number of (k-1)-subsets needed to cover the whole set Γ is (s+1), i.e. the most economical experimental plan is the one in which each multiple orientation matrix is formed by exactly (s+1) single orientation matrices of dimension (k+1)-by-k. Indeed, as shown below, not all the rows of the $(s+1)^{th}$ single orientation matrix are needed. Of those (k+1) rows, only the first (s+2) are actually employed as input strings for the model.

In analogy with the case of k even, and on the basis of the proof given in Appendix A, the problem reduces to

Problem II: "Find a partition of Γ made of s = (k-1)/2 subsets composed of (k-1) handcuffed pairs each, plus a subset composed of s handcuffed pairs.

Again, Problem II can be solved using the classical construction of Hamilton cycles in a graph.

First of all, the elements of the k-set (where k = 2s+1), identified by the numbers $(0,\ldots,2s-1,2s\}$, are displayed on a graph, as shown in Figure 2, for s = 3.

A 'beginning' Hamilton cycle is found, having as starting/ ending node the edge placed in the middle of the graph, i.e. 2s. For example, if k = 7, the beginning Hamilton cycle can be taken as H1 = ⟨6,0,1,5,2,4,3,6⟩ (see Figure 2).

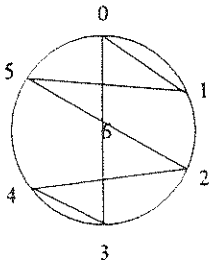

Figure 2: A multiple trajectory for k odd

Each of the subsequent cycles is constructed by shifting the previous one clockwise by one node. In the example where k = 7, the second and third cycles are H2 = ⟨6,1,2,0, 3,5,4,6⟩ and H3 = ⟨6,2,3,1,4,0,5,6⟩.

From the s cycles constructed above, s paths can be derived by cutting one of the construction lines. In particular, the line that has to be cut is the one joining two adjacent edges, i.e. edges represented by two consecutive indices i and (i+1).

In the above example, with k = 7, the lines to eliminate in H1, H2 and H3 are respectively: the one joining (0,1), the one joining (1,2), and the one joining (2,3). Cutting those lines, the edges 0 and 1 become the extremes of the path PH1 (derived from H1), the edges 1 and 2 become the extremes of the path PH2 (derived from H2), and, finally, the edges 2 and 3 become the extremes of the path PH3 (derived from H3). Thus, the three paths P1, P2 and P3 are identified respectively by the blocks: PH1 = ⟨0,6,3,4,2,5,1⟩, PH2 = ⟨1,6,4,5,3,0,2⟩, and PH3 = ⟨2,6,5,0,4,1,3⟩.

To complete the solution of Problem II, the last step is now the construction of a shortest path of length (s+1), containing the s handcuffed pairs missing to cover the whole set Γ. It can be easily seen that, for k = 7, the missing path is the one represented by the block ⟨0,1,2,3⟩.

In general, the last block missing would be the one given by ⟨0,1,2,...,s⟩. From this final block, an orientation matrix of dimension (s+2)-by-k can be constructed following the rules given in Appendix A. Note that, in order to simplify notation, such matrix will be completed to a (k+1)-by-k matrix in which the last (k+1)-(s-2) rows are made of 0's. Obviously, those rows will not be utilised in the experimental design.

5. THE COMPUTATIONAL COST

Once an MT has been constructed in Ω, the trajectories are used to perform model runs at each node and to evaluate each E_i and EE_{ij}.

In particular, each single matrix of the MT permits the estimation of one E_i per input and (k-1) EE_{ij}. In order to be able to compute (k-1) TFE_{ij} for each single matrix, the missing (k-1) E_j's need to be estimated. For a given pair of factors (i,j), the values of E_i and EE_{ij} were obtained by evaluating the model at the points A, B and D, identified earlier.

The model also needs to be evaluated at the point C: $(\mathbf{x} + \mathbf{e}_j\Delta_j)$, and a further (k-1) model evaluations have to be added on the side of each single matrix, one for each TFE_{ij} computed.

The computation of a TFE_{ij} requires four model evaluations. Thus, randomly selecting a value from each distribution T_{ij}, (i.e. computing one TFE_{ij} per pair (i,j) of input), would require

$$4 \times \frac{k(k-1)}{2},$$

model evaluations.

The sampling strategy proposed here is more economical. To calculate its computational cost, consider the two cases.

(i) k is even

The cost of randomly selecting a value from each distribution T_{ij} (i.e. computing one TFE_{ij} per pair (i,j) of input) is equal to the number of points covered in the parameter space by an MT. If k is even, the number of single trajectories contained in an MT is ν = k/2.

Thus, in a first approach, the cost of computing one TFE_{ij} per pair (i,j) of input is given by {[(k+1)+(k-1)]*k/2}. (Note that the (k+1) evaluations are needed to compute the EE_i's and the EE_{ij}'s, while the (k-1) are needed to compute the EE_j's).

In practice, each single trajectory contained in the same MT has the same starting and ending points. Thus, if an MT is made by the single trajectories, $ST_1, ST_2, ..., ST_{k/2}$, once the model has been evaluated at the (k+1) points corresponding to each ST_1, the number of evaluations required for each ST_i, i = 2,...,k/2 is (k-1). It follows that the total number of model evaluations corresponding to each MT is given by

$$\begin{aligned} \mathbf{C}_{even} &= \{(k+1) + [(k-1)\times(k/2-1)]\} + (k-1)\times k/2 \\ &= k^2 - k + 2 \ . \end{aligned} \tag{6}$$

If r is the selected size of the sample to be extracted from each T_{ij}, the total computational cost of the design is $r*\mathbf{C}_{even}$ model simulations.

(ii) k is odd

If k is odd, the number of single trajectories forming an MT is ν = s+1, where s = (k-1)/2. Each of the first s single trajectories contains (k+1) points, while the $(s+1)^{th}$ contains (s+2) points.

To calculate the total number of model simulations for k odd, it is sufficient to add to (6) the evaluations needed to cover the points contained in the $(s+1)^{th}$ trajectory. Since the $(s+1)^{th}$ trajectory has the same starting point as the others, but a different finishing point, then (s+1) = (k+1)/2 model evaluations have to be added. The total cost of computing one TFE_{ij} per pair of input leads to

$$\begin{aligned} \mathbf{C}_{odd} &= \{(k+1) + [(k-1)\times(k/2-1)]\} + (k-1)\times k/2 + (k+1)/2 \\ &= k^2 - \frac{k}{2} + \frac{5}{2} \ . \end{aligned} \tag{7}$$

and the total cost of the experimental design is $r*\mathbf{C}_{odd}$ model simulations.

6. TESTING THE METHOD

The analytical function f_1, defined on the four-dimensional cube,

$$f_1 = \sum_{i=1}^{4} b_i w_i + \sum_{i<j} b_{ij} w_i w_j \ , \tag{8}$$

where $w_i = 2 \times (x_i - ½)$ has been constructed to test the method. The coefficients b_i and b_{ij} are: $b_3 = 10$; $b_{22} = 30$; $b_{12} = 80$; $b_{13} = 60$; $b_{14} = 40$. All the other coefficients are randomly generated from a normal distribution with zero mean and unit standard deviation.

The SA experiment described above has been applied to the analytical function f_1 with a sampling step $\Delta^* = ⅓$, $\Delta_i = \Delta^*$, $i = 1,...,4$, and a sample size $r = 10$. Results of the experiment, given in Tables 1 and 2 for the Morris [1991] sensitivity measures $\mu(F_i)$ and $\sigma(F_i)$, $i = 1,2,3,4$, and are attributing an order of importance to the four variables of the function f_1, which is in good agreement with the values assigned to the coefficients.

Values of the sensitivity measures $\lambda_{i,j}$, relative to the effects on the output due to the interaction between the i^{th} and j^{th} parameters, are in excellent agreement with the values that one would expect given the values of b_{ij}. According to the $\lambda_{i,j}$'s, the only parameter which has a significant effect because of interactions with other parameters is x_1 (the values of $\lambda_{i,j}$ with $i \neq 1$ and $j \neq 1$ are negligible with respect to the others); the ranking attributed by the $\lambda_{1,j}$'s for $j = 2,3,4$ agrees with the ranking of the $b_{1,j}$'s for $j = 2,3,4$.

Note that the new measures $\lambda_{i,j}$ complement the information provided by μ and σ. For instance, the high value of σ obtained in the example for x_1 can be explained as due to the interaction of this variable with the others. In contrast, a variable such as x_2, having a high value of σ, and only one high value out of the three $\lambda_{2,j}$'s, $j = 1,3,4$, is suspected to be a variable whose effects involve either curvature or interaction of third or higher order.

Stronger evidence of this has been obtained by repeating the experiment on the analytical function f_2, which is f with the value of b_{12}, changed from $b_{12} = 80$ to $b_{12} = 0.8$ (so that all the two-term interaction effects involving x_2 are expected to be negligible). Results of the analysis on f_2 are given in Tables 2 and 3, where the same sensitivity measures μ, σ and λ are used. These results show that the value obtained for σ is still high, while all the $\lambda_{2,j}$'s, $j = 1,3,4$ are low. This confirms that the comparison of the σ with the $\lambda_{i,j}$ values helps in the identification of effects due either to curvature or third and higher order interactions.

In general, a high value of $\lambda_{i,j}$ indicates a pair of input factors largely affecting the output through their mutual interaction. Conversely, a value of $\lambda_{i,j}$ which is close to zero indicates that the i^{th} and j^{th} input factors are acting independently on the output.

The three sensitivity measures, λ, μ and σ, provide a high level of information about the relative importance of the input factors, and also the nature of their effects on the output. The values of μ and σ indicate which inputs are important, and distinguish the ones having strong additive effects from the ones either involved in curvature or interaction effects. The additional information provided by λ not only establishes an order of importance of the two-term interaction effects, but also, considered together with σ, may be helpful in distinguishing curvature effects from second-order interactions.

Table 1: First-order effects for f_1 (see (8))

Variable	Total effects (measured by $\mu(F_i)$)	Higher order effects (measured by $\sigma(F_i)$)
x1	122.0	147.0
x2	66.7	124.1
x3	124.4	64.6
x4	16.2	51.31

Table 2: Second-order effects for f_1 and f_2

Variable	Interaction effects for f_1 (measured by $\lambda_{i,j}$)	Interaction effects for f_2 (measured by $\lambda_{i,j}$)
x1, x2	318.3	0.318
x1, x3	240.9	240.9
x1, x4	160.6	160.6
x2, x3	2.001	2.001
x2, x4	0.200	0.199
x3, x4	0.808	0.808

Table 3: First-order effects for f_2

Variable	Total effects (measured by $\mu(F_i)$)	Higher order effects (measured by $\sigma(F_i)$)
x1	48.17	74.97
x2	15.68	71.54
x3	124.4	64.40
x4	16.22	51.31

Table 4: Means of first-order effects on f_1 for various values of Δ^* and r

Variable	$\mu(F_i)$	$\mu(F_i)$
	$\Delta^* = ⅓$, r = 10	$\Delta^* = ⅓$, r = 30
x1	223.0	229.5
x2	186.8	192.4
x3	97.39	98.39
x4	4.407	2.733
	$\Delta^* = ⅕$, r = 10	$\Delta^* = ⅕$, r = 30
x1	258.5	249.1
x2	206.2	199.1
x3	97.67	97.93
x4	7.57	2.91
	$\Delta^* = ⅐$, r = 10	$\Delta^* = ⅐$, r = 30
x1	244.7	237.5
x2	199.1	192.9
x3	91.08	90.87
x4	9.65	6.24

The experiment on the analytic function f, using the standard parameter values, has been replicated for different values of the sample sizes r, and the sampling step Δ^*. The results are given for the means of the first-order effects

(Table 4) and second-order effects (Table 5). These results indicate that the method is relatively independent of r and Δ^*. In fact, any change in $\mu(F_i)$ due to variations in r or Δ^* does not affect the ranking of the variables in terms of sensitivity of the output.

The results for pair-wise interactions are similar in nature. For all values of Δ^*, the order of importance is the same for Orders 1 to 4. For $\Delta^* = 1/7$, the ordering of the interactions x_2 with x_3, and x_3 with x_4, is reversed. These are the least important of the interactions and they are small compared with the major interaction effects. In general, the differences in value of the lowest two interaction effects are relatively small.

Table 5: Means of second-order effects on f_1 for various values of Δ^* and r

Variable	$\mu(T_{ij})$		$\mu(T_{ij})$	
	$\Delta^* = 1/3$, r = 10		$\Delta^* = 1/3$, r = 30	
x1, x2	1	1474	1	1529
x1, x3	3	741.7	3	778.1
x1, x4	4	471.6	4	481.3
x2, x3	6	162.3	6	171.4
x2, x4	2	1056	2	1094
x3, x4	5	186.2	5	191.6
	$\Delta^* = 1/5$, r = 10		$\Delta^* = 1/5$, r = 30	
x1, x2	1	3312	1	3151
x1, x3	3	1871	3	1747
x1, x4	4	1023	4	1005
x2, x3	6	414.2	6	384.7
x2, x4	2	2262	2	2160
x3, x4	5	421.3	5	403.7
	$\Delta^* = 1/7$, r = 10		$\Delta^* = 1/7$, r = 30	
x1, x2	1	4568	1	4364
x1, x3	3	2594	3	2436
x1, x4	4	1431	4	1409
x2, x3	⑤	627.7	⑤	591.3
x2, x4	2	3055	2	2917
x3, x4	⑥	604.5	⑥	583.1

8. SUMMARY AND CONCLUSIONS

The SA method proposed here is a development of the OAT screening method proposed by Morris [1991]. The new method, in addition to the sensitivity measures already provided by the traditional Morris, offers estimates of the effects due to the interactions between any pair of input factors. Many of the already existing screening methods do not take into account those effects, but assume instead that the input variables act additively. This assumption, although undesirable, is needed in order to simplify the problem and keep low the computational cost of the experiment. Methods rejecting such an assumption, and computing higher order effects (i.e. the class of the factorial designs) are computationally expensive, and their computational cost increases with the number of levels across which the model input variables are varied.

The method illustrated here requires a number of model evaluations of the $O(k^2)$, where k is the number of model input factors. By comparison with other methods available in the literature, and given the information that this method produces, this cost is 'reasonable'. Also, the computational cost does depend on the number of 'levels' selected for each parameter.

The strategy adopted for sampling in the parameter space is based on notions deriving from the graph theory. The method can be extended to handle third and higher order effects. It can be shown that the optimal design leads to the handcuffed-triplet-prisoner problem, and a constructive solution has not yet been found. Extensions to higher order interaction effects lead to similar handcuffed-prisoner problems.

REFERENCES

Baker, F.D., and R.E. Bargmann, Orthogonal central composite designs of third order in the evaluation of sensitivity and plant growth models, *Journal of the American Statistical Association, 80*, 574-579, 1985.

Berge, C., *Graphs and Hypergraphs*, North-Holland, Amsterdam, 1973.

Box, G.E.P., W.G. Hunter, and J.S. Hunter, *Statistics for Experimenters*, Wiley and Sons, New York, 1978.

Campolongo, F., and A.J. Gabric, The parametric sensitivity of the sea-to-air flux of dimethylsulfide in the Southern Ocean, *Journal of Statistical Computation and Simulation, 57*(1-4), 337-352, 1997.

Campolongo, F., and A. Saltelli, Sensitivity analysis of an environmental model: an application of different analysis methods, *Reliability Engineering and System Safety, 52*, 1997.

Hell, P., and A. Rosa, Graph decomposition, handcuffed prisoners and balanced p-designs, *Discrete Mathematics, 2*, 229-252, 1972.

Helton, J.C., Uncertainty and sensitivity analysis techniques for use in performance assessment for radioactive waste disposal, *Reliability Engineering and System Safety, 42*, 327-367, 1993.

Hung, S.H.Y., and N.S. Mendelshon, Handcuffed designs, *Discrete Mathematics, 18*, 23-33, 1977.

Morris, M.D., Factorial sampling plans for preliminary computational experiments, *Technometrics, 33*(2), 161-174, 1991.

APPENDIX A

Given a block of (k-1) distinct EE_{ij}'s that form a path $\langle i_1, i_2, ..., i_k \rangle$, construct a (k+1)-by-k sampling matrix **B**, whose elements are 0's and 1's, such that:

(i) **B** allows the estimation of (k-1) distinct EE_{ij}'s;
(ii) for each value of i = 1,2,...,k, there are two rows of **B** that differ only in their i^{th} entries.

The construction of the matrix $\mathbf{B}(i,j)$, $i = 1,...,k+1$, $j = 1,...,k$ starts by initialising each element to zero. Then the following steps are taken:

Step 1: Let (i_1, i_2) be the first of the EE_{ij}'s that have to be estimated by $\mathbf{B}$. The construction of $\mathbf{B}$ starts from the third row, where the elements $\mathbf{B}(3, i_1)$ and $\mathbf{B}(3, i_2)$ are changed into 1's. Then the step is completed by filling down the columns i_1 and i_2 with 1's, i.e. all the elements $\mathbf{B}(i, i_1)$, $i \geq 4$ and $\mathbf{B}(i, i_2)$, $i \geq 4$ are changed into 1's.

Step 2: Let (i_2, i_3) be the second of the EE_{ij}'s that have to be estimated by $\mathbf{B}$. The fourth row of $\mathbf{B}$ is constructed by changing the element $\mathbf{B}(4, i_3)$ into 1. Again, this step is completed by filling down the column i_3 with 1's.

Step 3: On the basis of the previous two steps, the second column of $\mathbf{B}$ can be modified by changing the element $\mathbf{B}(2, i_2)$ into 1.

Step 4: If (i_3, i_4) is the third EE_{ij} to be estimated, the fifth row of $\mathbf{B}$ is completed by changing the element $\mathbf{B}(5, i_4)$ into 1. Consequently, all the elements $\mathbf{B}(i, i_4)$, $i \geq 6$ are changed into 1's.

Step n: Step 4 is repeated till the matrix is exhausted.

In the final k^{th} step, the only element of the $(k+1)^{th}$ row of $\mathbf{B}$ which has not been modified in any of the previous steps (and so is still a 0) is turned into a 1. The $(k+1)^{th}$ row of $\mathbf{B}$ is then reduced to a row of all 1's.