Chemometrics and Intelligent Laboratory Systems 113 (2012) 52–57

Contents lists available at SciVerse ScienceDirect

Chemometrics and Intelligent Laboratory Systems

journal homepage: www.elsevier.com/locate/chemolab

Improved sensitivity through Morris extension

J. Santiago [a,b], B. Corre [b], M. Claeys-Bruno [a,*], M. Sergent [a]

[a] Institut des Sciences Moléculaires de Marseille, AD²EM, Université Paul Cézanne Aix-Marseille III, 13397 Marseille Cedex 20, France
[b] TOTAL, CSTJF, Avenue Larribau, 64018 PAU Cedex, France

ARTICLE INFO

Article history:
Received 31 January 2011
Received in revised form 6 September 2011
Accepted 3 October 2011
Available online 15 October 2011

Keywords:
Sensitivity study
Space-filling design
Morris's screening method
Computer experiment

ABSTRACT

This paper presents a new sensitivity analysis method called ISTHME based on the principles of Morris's method without the construction of randomized one-at-time (OAT) design. The presented method can be applied on any experimental design and more particularly on space filling designs. This specificity is very interesting in terms of time and calculation economy. Indeed, we can use a universal design, which is adapted to sensitivity analysis as well as optimization without any supplementary simulation.

1. Introduction

In the last decade, industrial phenomena (oil industry, nuclear, etc.) are often studied using numerical simulation [1]. These simulation models are increasingly complex with a large number of input parameters and consequently a long time of calculation. Therefore, it becomes essential to determine the most important factors to include in a metamodel, simpler but realistic, by using screening [2] or sensitivity analysis. The classical screening methods such as Plackett and Burman designs [3], supersaturated designs [4,5] or sequential bifurcation [6,7] are not adapted when the variation domains are very large since the points are located close to the extreme limits of the domain. Specific sensitivity analysis are now required as Morris's method [8–12] which is better adapted and often applied when a large number of simulations can be performed (more than $5k$ simulations, where k is the number of inputs) to identify the few important factors among a lot in models. Nevertheless, this method which allows the determination of the main effects and gives indication on nonlinearities or interactions requires many simulations without the possibility of using the simulations for a subsequent study.

The method ISTHME presented in this article is based on classical Morris's method but uses any set of points spread in the interior of the experimental volume. This set is often a uniform design allowing different studies in a second time as response surface [13–15] or/and kriging [16–19].

* Corresponding author. Tel.: +33 491288186.
E-mail address: m.claeys-bruno@univ-cezanne.fr (M. Claeys-Bruno).

0169-7439/$ – see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.chemolab.2011.10.006

2. Presentation of the Morris method

2.1. Classical Morris's OAT method

The method proposed by Morris [11] provides a global sensitivity measure to identify the factors with (1) negligible effects, (2) linear and additive effects or (3) nonlinear or interaction effects. For that, a design composed of individual randomized one-at-a-time (OAT) designs is built in order to determine, for each factor X_j, the elementary effects $d_j(y)$.

$$d_j(y) = \frac{y(x_1,\ldots,x_{j-1},x_j+\Delta_j,x_{j+1},\ldots,x_J)-y(x)}{\Delta_j}$$

where Δ_j is a value in $\{1/(p-1), \ldots, 1-1/(p-1)\}$, with p as the number of levels (Fig. 1).

Considering L different trajectories, a statistical analysis of these elementary effects provides the mean $\mu_j(y)$ which assesses the global influence of the factor X_j.

$$\mu_j(y) = \frac{1}{L}\sum_{\ell=1}^{L} d_j^{\ell}(y)$$

As elementary effects with opposite signs cancel each other, the mean of the absolute value $\mu_j^*(y)$ is also considered [9].

$$\mu_j^*(y) = \frac{1}{L}\sum_{\ell=1}^{L}\left|d_j^{\ell}(y)\right|$$

The third considered statistic is the standard deviation $\sigma_j(y)$ which indicates the presence of higher order effects and measures

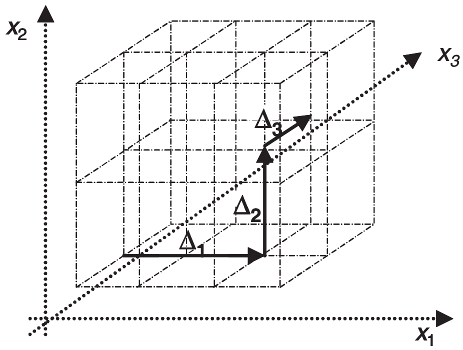

Fig. 1. Morris's OAT design in a 3 dimensional space.

the non-linearities or the interactions of the j^{th} factor with others factors.

$$\sigma_j(y) = \sqrt{\frac{1}{L}\sum_{\ell=1}^{L}\left(d_j^{\ell}(y) - \mu_j(y)\right)^2}$$

According to the values of $\mu_j^*(y)$ and $\sigma_j(y)$, Morris shows that studied factors can be classed into three groups as follows: factors having (1) negligible effects, (2) linear and additive effects or (3) nonlinear or interaction effects. Nevertheless, this method does not allow the discrimination between non-linearities and interactions. For an easier interpretation, the values of $\mu_j^*(y)$ and $\sigma_j(y)$ can be plotted as shown on Fig. 2.

Factors with negligible effects are characterized by low values of $\mu_j^*(y)$ and $\sigma_j(y)$, factors with linear effects present a high value of $\mu_j^*(y)$ and a low value of $\sigma_j(y)$, and for factors with nonlinear or interaction effects, $\mu_j^*(y)$ and $\sigma_j(y)$ present high values.

2.2. Improved sensitivity through Morris extension method

Contrary to classical Morris's method, this method (ISTHME) is based on any set of points and more particularly a uniform design.

The first step is the construction of constellations from this set of points. In 2 dimensional space, the constellations are constructed with 3 points, in 3 dimensional space, the constellations are defined using 4 points and in k dimensional space, $k+1$ points are necessary (a same point can belong to different constellations). For this construction, we defined the following two parameters as shown Fig. 3:

- the length l of the segments of the constellations.
- the angle α between two segments of a constellation

All these constellations are chosen in order to obtain quasi orthogonal dihedron (with a fixed length l of segments) and it is obvious

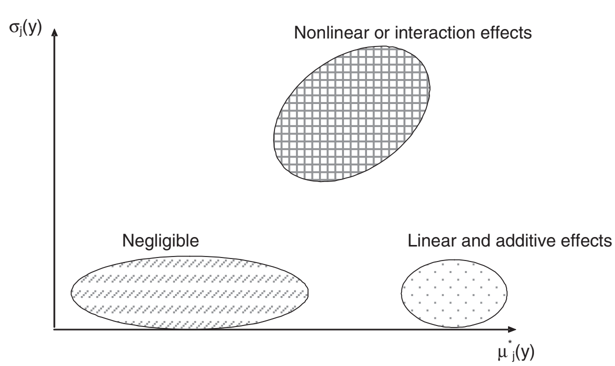

Fig. 2. Theoretical disposition of means $\mu^*_j(y)$ and standard deviations $\sigma_j(y)$ of the effects distribution.

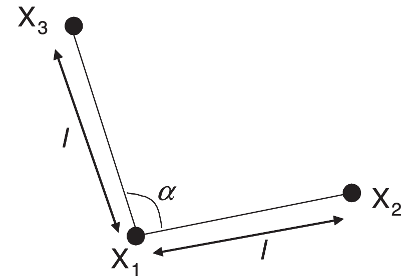

Fig. 3. Parameters of construction for the constellations: the length l of the segments and the angle α between two segments.

that the variation of l and α induces a variation of the number of constellations (Fig. 4). Consequently, a preliminary study of these parameters is required to define values providing a sufficient number of constellations for the calculations of step 2.

In a second time, elementary effects $d_j(y)$ are calculated for each constellation and then, the sensitivity indices $\mu_j^*(y)$ and $\sigma_j(y)$ are calculated as follows (in a 2 dimensional space).

Let a function of two variables x_1 and x_2 varying respectively in a domain $[n_1, m_1]$ and $[n_2, m_2]$, linear with interaction in a bidimensional space.

$$f(x_1, x_2) = ax_1 + bx_2 + cx_1x_2 \quad \text{with} : x_1 \in [n_1, m_1] \text{ and} x_2 \in [n_2, m_2]$$

In order to separate the effects, we have to establish a decomposition of f as follows:

$$f(x_1, x_2) = f_0 + f_1(x_1) + f_2(x_2) + f_{12}(x_1, x_2)$$

where

f_0 represents the mean effect
$f_1(x_1)$ corresponds to the principal effect of x_1
$f_2(x_2)$ corresponds to the principal effect of x_2
$f_{12}(x_1, x_2)$ corresponds to the interaction effect between x_1 and x_2.

The mean effect f_0 is provided by the mean of f which is

$$\begin{aligned} f_0 &= \frac{1}{(m_1 - n_1)(m_2 - n_2)} \int_{n_2}^{m_2}\int_{n_1}^{m_1} f(x_1, x_2)\,dx_1\,dx_2 \\ &= \frac{1}{(m_1 - n_1)(m_2 - n_2)} \int_{n_2}^{m_2}\left[\int_{n_1}^{m_1} f(x_1, x_2)\,dx_1\right]dx_2 \end{aligned}$$

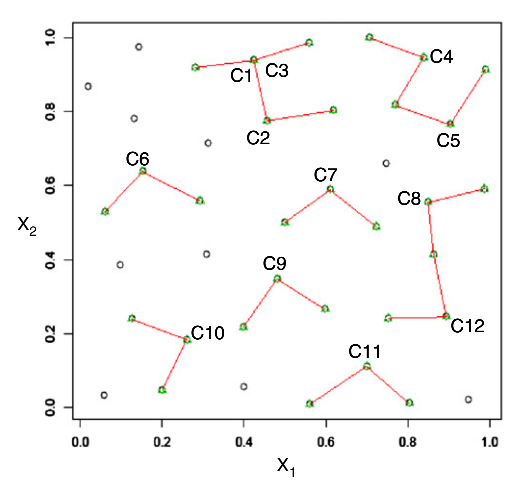

Fig. 4. Example of 12 constellations (C1, C2,..., C12) in a 2 dimensional space with $N=40$ points for fixed length of segments and angle α.

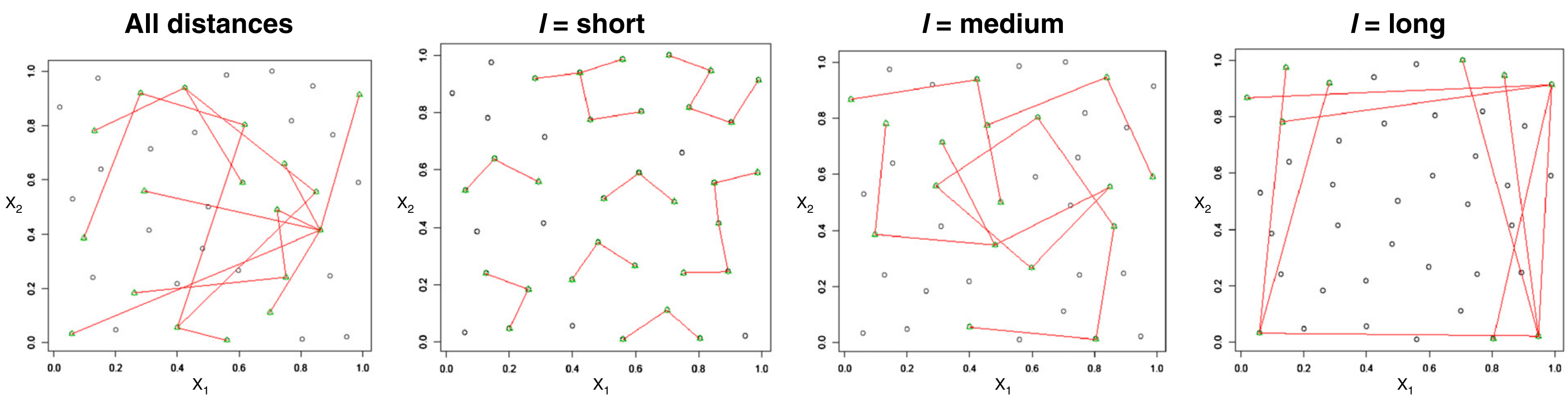

Fig. 5. Constellations obtained for different length *l* of segments.

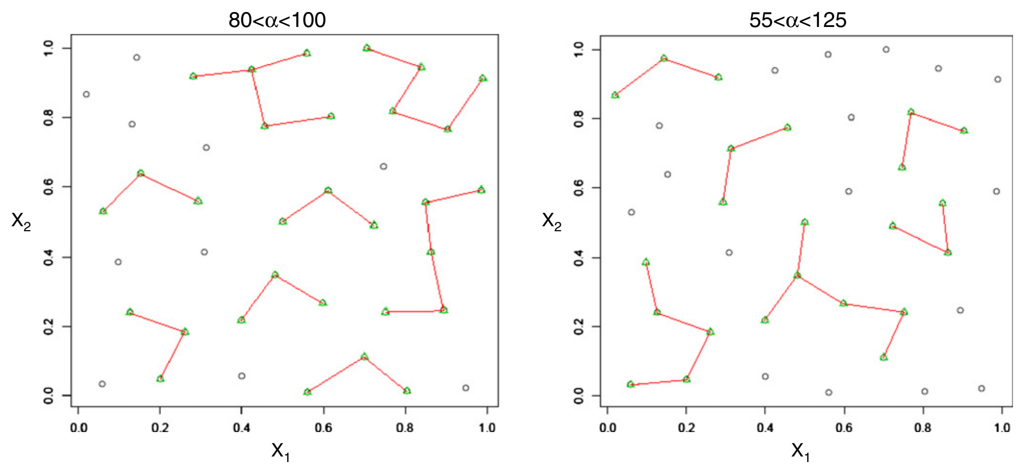

Fig. 6. Constellations obtained for variable angle α.

The principal effect of x_1 is obtained by subtracting from $f(x_1, x_2)$, the mean effect f_0 and by integrating the function obtained on x_2, which cancels the effect of this variable.

Thus

$$f_1(x_1) = \frac{1}{(m_2 - n_2)} \int_{n_2}^{m_2} (f(x_1, x_2) - f_0) dx_2$$

and $f_2(x_2) = \frac{1}{(m_1 - n_1)} \int_{n_1}^{m_1} (f(x_1, x_2) - f_0) dx_1$

For each constellation, an elementary effect $d_j(y)$ per factor j can be computed by interpolating a first order polynomial equation

$$Y = d_0 + \sum_{j=1}^{p} d_j X_j$$

The elementary effects are provided by the coefficients d_j. Thus, there will be as many elementary effects as constellations and the sensitivity indices $\mu_j^*(y)$ and $\sigma_j(y)$ are calculated according to Morris's method presented above where the mean and the standard deviation are computed on the whole population of constellations. The same procedure is generalized for any dimension.

Table 1
Number of constellations in function of α and all segment lengths l.

α (°)	Number of constellations
90	0
85–95	0
82–98	26
80–100	433
75–105	4324
70–110	32,129

Table 2
Number of constellations in function of α and for l varying between 0.60 and 0.90.

α (°)	Number of constellations
90	0
85–95	0
82–98	2
80–100	42
75–105	408
70–110	2140

Table 3
Details of calculations of $\mu_j^*(y)$ and $\sigma_j(y)$ for the simulation model Y_1 with 408 constellations. For each factor (X_1,…,X_5) and for each constellation (C1–C408), elementary effects $d_j(y)$ are calculated and reported in the second column. The values $\mu_j^*(y)$ and $\sigma_j(y)$ obtained for each factor are reported in columns 3 and 4.

Factor	Elementary effects $d_j(y)$	$\mu_j^*(y) = \frac{1}{L}\sum_{\ell=1}^{L}\left\|d_j^\ell(y)\right\|$	$\sigma_j^*(y) = \frac{1}{L}\sum_{\ell=1}^{L}\left\|d_j^\ell(y)\right\|$
X_1	27.899, 27.899, 27.900, 27.900, ,…., 27.900, 27.899, 27.900, 27.901.	27.8999	0.0009
X_2	2.300,2.301, 2.298, 2.297, ,…., 2.300, 2;300, 2.300, 2.299	2.2992	0.0009
X_3	6.500, 6.500, 6.500, 6.500, ,…., 6.498, 6.498, 6;500, 6;501	6.4997	0.0011
X_4	52.400, 52.400, 52.400, 52.399, ,…., 52.400, 52.400, 52.397, 52.398	52.3992	0.0009
X_5	16.598, 16.601, 16.602, 16.602, ,…., 16.599, 16.600, 16.599, 16.600	16.6000	0.0009

3. Results and discussion

3.1. Study of the constellations: length l of segments and angle α of dihedrons in a 2 dimensional space

In our method, the first step consists in the construction of constellations using points of a space filling design. The number of these constellations depends on two parameters l (length of the segments) and α (the angle between two segments).

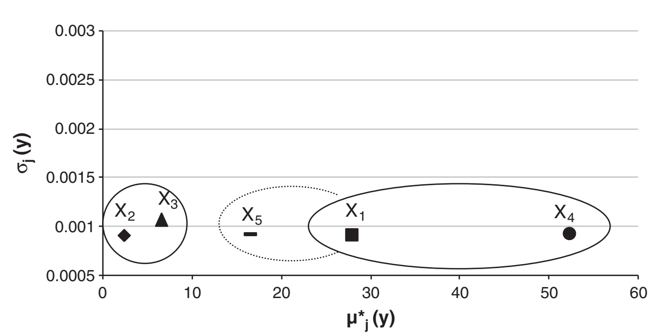

Fig. 7. Sensitivity measures $\mu_j^*(y)$ and $\sigma_j(y)$ for the model Y_1.

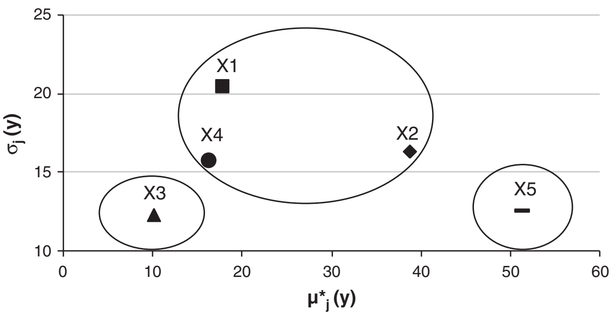

Fig. 8. Sensitivity measures $\mu^*_j(y)$ and $\sigma_j(y)$ for the model Y_2.

Fig. 5 shows constellations obtained with different length l of the segments.

A systematic study of the constellations was achieved and has clearly shown that the number of constellations decreases when the segment length l increases and we know that a high number of constellations is needed in order to have representative values of $\mu^*_j(y)$ and $\sigma_j(y)$. Moreover, long segments appear as not pertinent since the non-linearities and interactions effects could be hidden and averaged. Therefore, we will only keep constellations with short lengths.

In the same way, the number of constellations depends on the angle α, theoretically fixed to 90°. Fig. 6 shows two different cases of constellations obtained with variable angle α.

We can observe that the number of constellations varies with the variation of the segment length l and the angle α. In order to perform statistical study of the two parameters $\mu^*_j(y)$ et $\sigma_j(y)$, we considered only short lengths and angle varying from 70° to 110°.

3.2. Study in a five dimensional space

In order to test the ISTHME method, different cases are proposed in a five dimensional space.

In a first step, we draw up constellations from a WSP space filling design [20] with 100 points. The segment lengths l and the angle α are studied and Table 1 reports the number of constellations detected in function of the angle α considering all segment lengths l.

As explained above, it would be preferable to only consider short segment lengths, but, with the number of constellations decreasing quickly, a greater variation of the angle α is needed in order to obtain significant and sufficient information. Table 2 reports the variation of the number of constellations considering only short segment lengths ($0.60<l<0.90$).

Different studies were generated from simulated results, in three cases with different significant effects. To calculate $\mu^*_j(y)$ and $\sigma_j(y)$, 408 constellations were used with segment length varying from 0.60 to 0.90 and α from 75° to 105°. The scales of the plots are adjusted in order to make an easier interpretation.

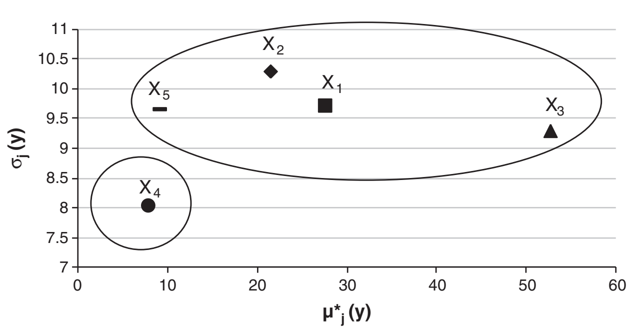

Fig. 9. Sensitivity measures $\mu^*_j(y)$ and $\sigma_j(y)$ for the model Y_3.

3.2.1. Simulation model Y_1

In the first case, only some linear effects are simulated as significant. From the 408 constellations, the elementary effects of the 5 factors were calculated (Table 3) and the values of the sensitivity measures $\mu^*_j(y)$ and $\sigma_j(y)$ are reported on Fig. 7.

Fig. 7 shows that factors X_1 and X_4 are well separated from the other factors because of both high values of $\mu^*_j(y)$ and low values of $\sigma_j(y)$. Factor X_5 presents a high value of $\mu^*_j(y)$ and a low value of $\sigma_j(y)$ but to a lesser extent. So we can conclude that X_1, X_4 and X_5 have significant linear effect and X_2 and X_3 are relatively unimportant in this model.

A global interpretation of the plot leads to the following conclusions:

X_1	linear effect
X_2	negligible effect
X_3	negligible effect
X_4	linear effect
X_5	low linear effect

to compare to the reference model Y_1, which is

$$Y_1 = 240.4 + 27.9\ X_1 + 3.0\ X_2 - 6.5\ X_3 - 52.4\ X_4 + 16.6\ X_5$$

The ranking provided by the ISTHME method is in accordance with the coefficients values of the reference model. The linear effects are accurately identified.

3.2.2. Simulation model Y_2

In the second case, linear and interaction effects were considered and simulated in the model Y_2 in order to check their differentiation on the plot.

The results are reported on Fig. 8. The factor X_5 presents a high value of $\mu^*_j(y)$ and a low value of $\sigma_j(y)$ corresponding to a significant linear effect for this factor in the considered model. The factors X_1, X_2, and X_4 present high values of $\mu^*_j(y)$ and high values of $\sigma_j(y)$, so we can conclude that these factors, well separated from the linear or negligible effects, have non linear or interaction effects.

The complete interpretation of Fig. 8 leads to the following conclusions:

X_1	nonlinear or interaction effect
X_2	nonlinear or interaction effect
X_3	negligible effect
X_4	nonlinear or interaction effect interaction
X_5	linear effect

This analysis is consistent with the reference model Y_2 whose coefficients are

$$Y_2 = 278.5 + 10.7\ X_1 + 41.4\ X_2 + 3.7\ X_3 + 10.4\ X_4 - 52.9X_5 + 38.7\ X_1X_2 - 31.9X_1X_4$$

3.2.3. Simulation model Y_3

In the third reference model, we added quadratic and cubic effects in order to visualize their respective position on the plot.

Fig. 9 clearly shows the following 2 groups of factors: the factors X_1, X_2, X_3, X_5 with high values of $\mu^*_j(y)$ and $\sigma_j(y)$ corresponding to non-linear or interaction effect and the factor X_4 with low values of $\mu^*_j(y)$ and $\sigma_j(y)$ corresponding to an unimportant factor.

The interpretation of Fig. 9 provides conclusion as

X_1	has nonlinear or interaction effect
X_2	has nonlinear or interaction effect
X_3	has nonlinear or interaction effect

X_4 has negligible effect
X_5 has nonlinear or interaction effect

which is in accordance with the reference model

$$Y_3 = 112 + 4.2\ X_1 – 5.3\ X_2 + 21.7\ X_3 – 4.1\ X_4 + 20.6\ X_5 – 31.3\ X_1{}^2 + 29.8\ X_3{}^3 – 31.2\ X_2X_5$$

The plot does not show any difference between interactions, quadratic or cubic effects but separates the non influential factors which is the aim of a sensitivity analysis.

In the three presented cases, all the effects are clearly identified: the conclusions are true compared to the “true” reference model.

4. Conclusion

The different presented cases show that this new approach, ISTHME, leads to promising results for sensitivity analysis. It allows the identification of non influential factors without hypothesis on effects contrary to classical screening strategies such as Plackett and Burman designs which are not adapted for simulation problems. In such designs, the effects are supposed to be independent and the presence of interaction effects could distort the interpretation and generate false positive or false negative. In the ISTHME method, even if the non linear and interaction effects are not distinguished, negligible factors are safely identified and could be subsequently removed in the final model. More complicated models (with high number of parameters and nonlinear complex effects) for industrial problems are now in progress.

These results are identical to those obtained with classical Morris method, but the construction of the design is very different since it is based on any experimental design and more particularly space filling design for which points are uniformly spread in the experimental volume . This specificity is, in our opinion, very interesting in terms of time and calculation economy because we can re-use runs. Moreover, we could consider a universal design which is adapted to sensitivity analysis as well as optimization with no supplementary simulations.

References

[1] T.J. Santner, B.J. Williams, W.I. Notz, The Design and Analysis of Computer Experiments, Springer, New York, 2003.
[2] R. Cela, M. Claeys-Bruno, R. Phan-Tan-Luu, Comprehensive Chemometrics, Oxford, 2009.
[3] R.L. Plackett, J.P. Burman, Design of Optimum Multifactorial Experiments, Biometrika 33 (1946) 305–325.
[4] M. Claeys-Bruno, M. Dobrijevic, R. Cela, R. Phan-Tan-Luu, M. Sergent, Supersaturated designs for computer experiments: Comparison of construction methods and new methods of treatment adapted to the high dimensional problem, Chemometrics and Intelligent Laboratory 105 (2011) 137–146.
[5] M. Claeys-Bruno, M. Dobrijevic, R. Phan-Tan-Luu, M. Sergent, A new class of supersaturated design: Application to a sensitivity study of a photochemical model, Chemometrics and Intelligent Laboratory Systems 95 (2009) 86–93.
[6] B. Bettonvil, Detection of important factors by sequential bifurcation. Tilburg, 1990.
[7] B. Bettonvil, J.P.C. Kleijnen, Searching for important factors in simulation models with many factors: Sequential bifurcation, European Journal of Operational Research 96 (1997) 180–194.
[8] F.M. Alam, K.R. McNaught, T.J. Ringrose, Using Morris' randomized OAT design as a factor screening method for developing simulation metamodels, Proceedings of the 2004 winter simulation conference, 2004.
[9] F. Campolongo, J. Cariboni, A. Saltelli, An effective screening design for sensivity analysis of large models, Environmental Modelling and Software 22 (2007) 1509–1518.
[10] A. Saltelli, S. Tarantola, F. Campolongo, M. Ratto, Sensitivity Analysis in Practice: A Guide to Assessing Scientific Models, John Wiley and Sons Publishers, 2004.
[11] M.D. Morris, Factorial sampling plans for preliminary computational experiments, Technometrics 33 (1991) 161–174.
[12] G. Pujol, Simplex-based screening designs for estimating metamodels, Reliability Engineering and System Safety 94 (2009) 1156–1160.
[13] G.E.P. Box, N.R. Draper, A basis for the selection of a response surface basis, Journal of the American Statistical Association 54 (1959) 622–654.
[14] G.E.P. Box, N.R. Draper, Empirical Model-Building and Response Surfaces New York, 1987.
[15] D.C. Montgomery, Design and Analysis of experiments, (5th ed.), 2001.
[16] N. Cressie, The origins of kriging, Mathematical Geology 22 (1990) 239–252.
[17] D. Krige, A statistical approach to some basic mine valuation problems on the Witwatersrand, Journal of the Chemical, Metallurgical and Mining Society 52 (1951) 119–139.
[18] G. Matheron, Principles of Geostatistics, Economic Geology 58 (1963) 1246–1266.
[19] H. Wackernagel, Multivariate Geostatistics: An Introduction with Applications. Berlin, 2003.
[20] J. Santiago, M. Claeys-Bruno and M. Sergent, Construction of space-filling designs using WSP algorithm for high dimensional spaces. Journal of Chemometrics and Intelligent Laboratory in press.