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

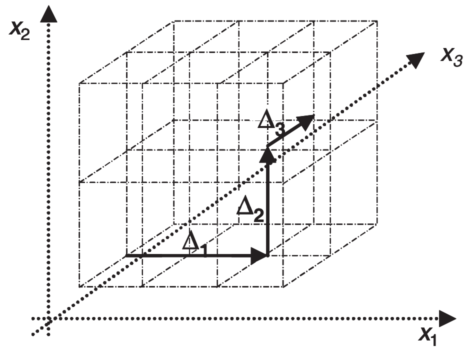

Fig. 1. Morris's OAT design in a 3 dimensional space.

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

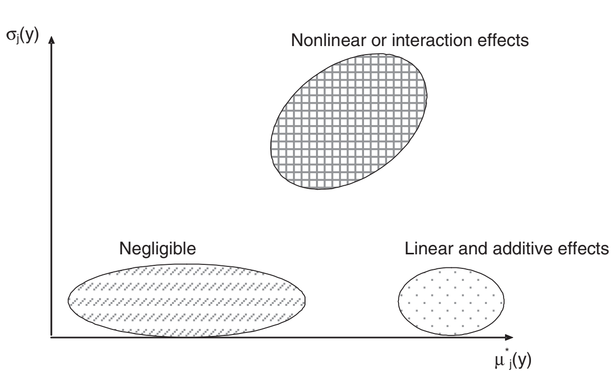

Fig. 2. Theoretical disposition of means $\mu^*_j(y)$ and standard deviations $\sigma_j(y)$ of the effects distribution.

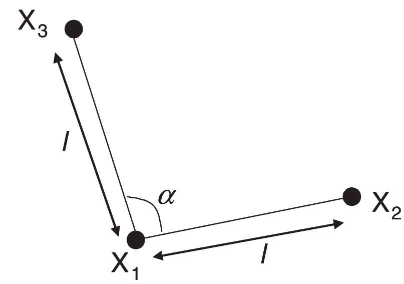

Fig. 3. Parameters of construction for the constellations: the length l of the segments and the angle α between two segments.

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

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

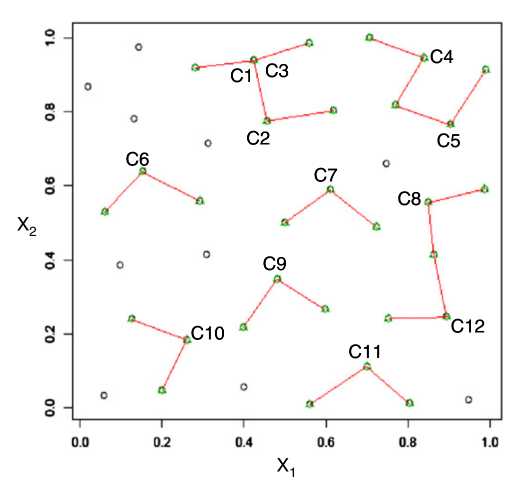

Fig. 4. Example of 12 constellations (C1, C2,..., C12) in a 2 dimensional space with $N=40$ points for fixed length of segments and angle α.