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Simplex-based screening designs for estimating metamodels

Gilles Pujol *

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Abstract

The screening method proposed by Morris in 1991 allows to identify the important factors of a model, including those involved in interactions. This method, known as the elementary effects method, relies on a “one-factor-at-a-time” (OAT) design of experiments, i.e. two successive points differ only by one factor. In this article, we introduce a non-OAT simplex-based design for the elementary effects method. Its main advantage, compared to Morris’s OAT design, is that the sample size doesn’t collapse when the design is projected on sub-spaces spanned by groups of factors. The use of this design to estimate a metamodel depending only on the (screened) important factors is discussed.

Key words: computer experiments, sensitivity analysis, factor screening, elementary effect, simplex design

1 Introduction

The framework of this article is experimentation with deterministic computer codes (simulation models), as presented for example by Santner et al. [1]. Computational models are used when the direct investigation of some real phenomena is expensive, dangerous, or even impossible. However, there are three main obstacles to the study of a computational model: the computation time, the number of inputs, and the size of the input space. Increasingly, the purpose of computer experiments is to study the model over a large range of inputs, rather than around some specific values; see for example Jones et al. [2].

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In such situations, reducing the input dimensionality is a necessity. For this purpose, screening methods aim at identifying the non-important input parameters at a low computational cost. The screening design proposed by Morris [3] may be effective because it doesn't rely on a strong prior assumption about the model. In a recent work, Alam et al. [4] use this design for developing a metamodel, i.e. an approximation of the model. The procedure has two steps: a first design (Morris's OAT) for the screening, and a second design (latin hypercube design in the subspace spanned by the important inputs, while the non-important inputs are fixed) for estimating the metamodel.

In this article, we propose a screening design that can be reused for the estimation of the metamodel, thereby improving the economy of the second set of simulations. Indeed, Morris's design is not well-suited for metamodel estimation: there is an important loss of points when this design is projected into the subspace formed by ignoring some inputs (here, the non-important inputs), so-called collapsing of the design.

Section 2 recalls Morris's screening method with the last improvements by Campolongo et al. [5]. Using this method in the framework of metamodel estimation is discussed in section 3. Section 4 introduces the new design, and its efficiency is illustrated through an example.

2 Morris's Elementary Effects Method

[Fig. 1 about here.]

The starting point of Morris [3] is that traditional screening methods, based on the theory of designs of experiments (Fisher [6]), rely on strong assumptions, such as monotonicity of outputs with respect to inputs, or adequacy of a low-order polynomial approximation. In contrast, the method he proposed doesn't rely on such assumptions. His method is referred to as the elementary effects method, and is more and more popular thanks to its moderate computational cost and its graphical aspects (as we shall see).

Let the function $f : \mathbf{x} \in \Omega \rightarrow y \in \mathbf{R}$ denote the computational model. The input space Ω is a subset of \mathbf{R}^p ; in most cases it is a hypercube: $\Omega = \prod_{i=1}^p [a_i, b_i]$. The p input parameters $\mathbf{x} = (x_1, \dots, x_p)$ are called the *factors*, and the scalar output y is called the *response*. In practice, however, simulation models have multiple outputs. Assuming that the response is scalar isn't restrictive in this article since we only consider initial designs, and not adaptive ones; therefore, the screening can be done separately for each response based on the same design.

The objective of screening is to split the factors into two subsets $\mathbf{x} = (\mathbf{u}, \mathbf{v})$, where \mathbf{u} (resp. \mathbf{v}) is the vector of the important (resp. non-important) factors. “Non-important” means that these factors can be fixed, while having little impact on the model response (see for example Alam et al. [4]). In section 3, we present an alternative approach to factor fixing, based on regression.

2.1 The design of experiments

Morris’s design has the following characteristics; also see figure 1(a):

- (1) the design belongs to the family of fractional factorial designs, i.e. the points are sampled from a p -dimensional regular grid;
- (2) the design is structured in groups of points, called *trajectories*; these trajectories are random, but follow a specific scheme:
 - (a) the trajectories are one-factor-at-a-time (OAT), i.e., two successive points differ by one factor only;
 - (b) this occurs exactly once for each factor and for each trajectory.

To illustrate the construction of a trajectory, a base point \mathbf{x}_0 is randomly chosen on the grid, and each coordinate is increased or decreased in turn: $\mathbf{x}_i = \mathbf{x}_{i-1} + \Delta_i \mathbf{e}_i$ for $i = 1 \dots p$, where Δ_i is a multiple of the grid spacing in the i th direction, $e_{ii} = 1$, and $e_{ij} = 0$ if $i \neq j$. In practice, the trajectories aren’t generated with this scheme, but in one step with a matrix approach (see Morris [3]).

Composed of R trajectories of $p+1$ points each, the design has $R(p+1)$ points; for example in figure 1(a), $R = 10$ and $p = 3$. Then, the number of points of the design is linear with respect to the number of factors. The number of trajectories R should be large enough to compute statistics such as means and standard deviations (see section 2.2). In the following, $\mathbf{x}_i^{(r)}$ denotes the i th point of the r th trajectory ($i = 0, \dots, p, \quad r = 1, \dots, R$).

A randomly generated design can have a poor coverage of the space, especially if the number of points is low with respect to the input space dimension. Space-filling-designs (SFD) were introduced to assure a better spread of the points over the input space (see for example Santner et al. [1]). Following these principles, Campolongo et al. [5] improved Morris’s design by maximizing the distances between the trajectories.

2.2 The screening method

The structure of the design allows to calculate, for each trajectory $r = 1, \dots, R$, one *elementary effect* per factor, i.e. the increase or the decrease of the response when the considered factor is disturbed, while the other factors are fixed:

$$d_i^{(r)} = \frac{f(\mathbf{x}_i^{(r)}) - f(\mathbf{x}_{i-1}^{(r)})}{\Delta_i}, \quad i = 1 \dots p \quad (1)$$

(recall that $\mathbf{x}_i^{(r)} = \mathbf{x}_{i-1}^{(r)} + \Delta_i \mathbf{e}_i$).

The elementary effects are then post-processed into statistics expressing the sensitivities of the factors. The first statistic is the mean $\hat{\mu}_i$,

$$\hat{\mu}_i = \frac{1}{R} \sum_{r=1}^R d_i^{(r)}, \quad i = 1 \dots p. \quad (2)$$

$\hat{\mu}_i$ is a measure of the i th factor's importance. Noting that elementary effects with opposite signs cancel each other, Campolongo et al. [5] suggest to consider instead the mean of the absolute value:

$$\hat{\mu}_i^* = \frac{1}{R} \sum_{r=1}^R |d_i^{(r)}|, \quad i = 1 \dots p. \quad (3)$$

Empirical studies [5] tend to show that $\hat{\mu}_i^*$ proxies the so-called “total sensitivity index”, denoted S_{T_i} (Homma and Saltelli [7]). The third statistic is the standard deviation $\hat{\sigma}_i$,

$$\hat{\sigma}_i = \sqrt{\frac{1}{R-1} \sum_{r=1}^R (d_i^{(r)} - \hat{\mu}_i)^2}, \quad i = 1 \dots p. \quad (4)$$

$\hat{\sigma}_i$ is either a measure of the non-linearities with respect to the i th factor, or a measure of the interactions involved with the i th factor, or both. Morris highlights that his method doesn't allow to distinguish between non-linearities and interactions, remarking however that data analysis could give insight into these phenomena.

To screen the factors, the statistics $\hat{\mu}_i$, $\hat{\mu}_i^*$ and $\hat{\sigma}_i$ are simultaneously considered. In practice, a graph representing $\hat{\sigma}_i$ versus $\hat{\mu}_i^*$ for $i = 1, \dots, p$ is sufficient to distinguish between three groups of factors:

- (1) negligible factors (low $\hat{\mu}_i^*$);
- (2) factors with linear effects without interactions (high $\hat{\mu}_i^*$ and low $\hat{\sigma}_i$);
- (3) factors with non-linear effects and/or interactions (high $\hat{\mu}_i^*$ and $\hat{\sigma}_i$).

See, for example, figure B.3 (discussed later in the paper).

3 Using the Elementary Effects Method with metamodeling

Alam et al. [4] present the elementary effects method as a tool to reduce the dimensionality, when estimating complex metamodels such as neural networks, support vector machines, kriging, etc. Indeed, these metamodels are used when the relationship between the inputs and the output cannot be represented by simple models, such as polynomial approximations; in this case, the screening procedure should not rely on a strong assumption about the form of the simulation model. That is why the elementary effects method is one of the rare screening methods that can be used in that context.

After the screening phase, the common practice is to use a second design for the regression where the non-important factors are fixed at their nominal values. This implies that more simulations must be run. However, even if the computational cost of the elementary effect method can be considered as moderate (linear with respect to the number of factors), it often reaches the maximally allowed number of simulations. Then, there is no other choice than estimating the regression metamodel from the screening design points only.

We recall that $\mathbf{x} = (\mathbf{u}, \mathbf{v})$ denotes the splitting between important and non-important factors, according to the screening results (i.e. the values of the statistics $\hat{\mu}_i^*$ and $\hat{\sigma}_i$). The objective is to build a metamodel \tilde{f} that depends only on important factors:

$$y = f(\mathbf{u}, \mathbf{v}) = \tilde{f}(\mathbf{u}) + \varepsilon(\mathbf{u}, \mathbf{v}) , \quad (5)$$

where ε is a residual random variable representing the gap between the simulation model and the metamodel; we assume that $\tilde{f}(\mathbf{u})$ and $\varepsilon(\mathbf{u}, \mathbf{v})$ are non-correlated, and that $E(\varepsilon(\mathbf{u}, \mathbf{v})|\mathbf{u}) = 0$. The variance of ε gives information about the quality of the screening. Indeed,

$$\frac{\text{var}(\varepsilon)}{\text{var}(y)} = 1 - \frac{\text{var}(\tilde{f}(\mathbf{u}))}{\text{var}(y)} \quad (6)$$

$$= 1 - \frac{\text{var}(E(y|\mathbf{u}))}{\text{var}(y)} \quad (7)$$

$$= \frac{E(\text{var}(y|\mathbf{u}))}{\text{var}(y)} , \quad (8)$$

where (8) follows from (7) by the total variance law. Hence, $\text{var}(\varepsilon)/\text{var}(y)$ is the so-called “total sensitivity index” with respect to the non-important factors, denoted S_{T_v} (Homma et Saltelli [7]). Here, the non-important factors \mathbf{v} are considered as noise in the model, and the index S_{T_v} is a measure of this noise over the response y (as in Iooss and Ribatet [8]). A low value confirms that the dropped factors are really non-important. In this sense, the regression model

provides a post-validation of the screening results. It must be noted that, when fixing the non-important factors, this post-validation cannot be provided: the practitioner has to trust the screening results.

To estimate a metamodel depending only on the important factors (\mathbf{u}), the orthogonal projections of the points of the design onto the subspace formed by the \mathbf{u} -coordinates are considered. In Morris’s OAT design, the aligned points collapse through the projections, leading to a loss of points¹. For example, figure 1(a) represents such a design in $p = 3$ dimensions with $R = 10$ trajectories (altogether 40 points), and figure 1(b) shows the projection of this design onto the (x_1, x_2) -plane (27 remaining points), and onto the x_1 -axis (7 remaining points). The loss of points can be explained by the OAT structure (one point lost per eliminated dimension and per trajectory), but also by the grid structure of the design. To illustrate, if $\alpha\%$ of the factors are important, the loss of points is greater than $(1 - \alpha)\%$ for the regression. This can be dramatic in high dimensions, because α is expected to be lower than 20%: the loss of points is then greater than 80%. Therefore, we develop simplex-based designs.

4 Simplex designs for computing the elementary effects

[Fig. 2 about here.]

To avoid the loss of points, the idea is to allow a better flexibility in the way the trajectories are done. In our new design, the trajectories are assumed to be simplexes. A simplex is the p -dimensional analogue of a triangle in two dimensions. Specifically, a simplex is the convex hull of a set of $p + 1$ linearly independent points. In this article, the term “simplex” is referring only to the nodes, i.e. a sequence of $p + 1$ points $\mathbf{x}_i = (x_{i1}, \dots, x_{ip})$, $i = 0 \dots p$. To illustrate, figure 2(a) represents such a design in three dimensions.

The design is composed of R different random simplexes in the domain. The simplexes are successively generated, and the space filling improvement referred to in section 2.1 (Campolongo et al. [5]) can also be applied. The simplexes can be of any shape. Technical details about simplex generation are discussed in appendix A.

Figure 2(b) shows the projections of the design of figure 2(a). As expected, most of the points don’t collapse through the successive projections.

¹ Although this is commonly referred to as a “loss of points” (see for example Morris [3]), this is in fact a loss of information: all the points will be used for the regression, but one projected point could match several points of the original design, and so, several values of the response.

The simplex-based designs enable the computation of the elementary effects. Fitting a first-order polynomial to each simplex,

$$y_i^{(r)} = c_0^{(r)} + \sum_{j=1}^p c_j^{(r)} x_{ij}^{(r)}, \quad r = 1 \dots R, \quad i = 0 \dots p, \quad (9)$$

implies the assumption that the model is without interactions. The coefficients $c_i^{(r)}$ are then proxies of the elementary effects $d_i^{(r)}$. Hence, the statistics $\hat{\mu}_i$, $\hat{\mu}_i^*$ and $\hat{\sigma}_i$ can be computed by (2)–(4).

It is important to notice that the size of the simplexes must be chosen properly. Small simplexes imply that the model has to be linear (in the factors \mathbf{x}) without interactions at a local scale, whereas with simplexes that spread over the input space each, the model is assumed to be globally linear without interactions.

4.1 Example

[Fig. 3 about here.]

We illustrate the elementary effects method with a simplex-based design through the function introduced by Morris [3]:

$$\begin{aligned} y &= f(x_1, \dots, x_{20}) \\ &= \beta_0 + \sum_{i=1}^{20} \beta_i w_i + \sum_{i<j}^{20} \beta_{ij} w_i w_j + \sum_{i<j<l}^{20} \beta_{ijl} w_i w_j w_l \\ &\quad + \sum_{i<j<l<s}^{20} \beta_{ijls} w_i w_j w_l w_s, \end{aligned} \quad (10)$$

where $\Omega = [0, 1]^{20}$, $w_i = 2(x_i - 1/2)$ except for $i = 3, 5, 7$, where $w_i = 2(1.1x_i/(x_i + 0.1) - 1/2)$. Coefficients of relatively large value are assigned as: $\beta_i = 20$, $i = 1, \dots, 10$; $\beta_{ij} = -15$, $i, j = 1, \dots, 6$; $\beta_{ijl} = -10$, $i, j, l = 1, \dots, 5$; $\beta_{ijls} = 5$, $i, j, l, s = 1, \dots, 4$. The remaining first and second order coefficients are generated independently from a standard normal distribution $\mathcal{N}(0, 1)$, and the remaining third and fourth order coefficients are set to zero.

The non-important factors are x_{11}, \dots, x_{20} . Concerning the important factors, their effects are linear, except for x_3 , x_5 and x_7 which are non-linear; factors involved in interactions are x_1, \dots, x_4 (second, third and fourth-order interactions), x_5 (second and third-order interactions) and x_6 (second-order interactions). Hence, the expected result for the elementary effects method is

- (1) non-important factors: x_{11}, \dots, x_{20} ;

- (2) factors with linear effects without interactions: x_8 , x_9 and x_{10} ;
- (3) factors with non-linear effects and/or interactions: x_1, \dots, x_7 .

We applied the elementary effects method with a simplex-based design and compare it with Morris’s OAT design. In both cases, the number of OAT trajectories/simplexes is $R = 10$; for the OAT design, the grid spacing is $1/4$ (5 levels for each factor); for the simplex design, the simplexes are orthonormal, with an homothety parameter of $1/4$ (see appendix A); hence, the simplexes are random rotations of OAT trajectories. The OAT trajectories/simplexes were generated at random (no space filling improvement). Both methods were repeated 100 times. The results are presented in figure B.3. In both cases, the results are as expected. Moreover, the 100 replicates allow to see that:

- the estimation of the statistics based on the elementary effects has a large variability, due to the small size of the samples ($R = 10$);
- with the simplex-based design, the effects of the factors of the third group (interactions and/or non-linear effects) are underestimated; indeed, for these factors, the model isn’t linear at the scale of a simplex (here $1/4$); however, although underestimated, these effects are properly identified as interactions or non-linearities.

5 Conclusion

In this article, we have proposed simplex-based designs as an alternative to Morris’s OAT designs for the elementary effects screening method. Contrary to Morris’s designs where no explicit assumption is made, the simulation model is now supposed to be linear without interactions at the scale of a simplex; however, if the simplexes are small enough, this assumption isn’t too restrictive. The advantage of simplex-based designs over Morris’s designs is that they keep most of their points (non-collapsing) after the projections on the subspaces formed by groups of factors (typically, important factors), so they are well-suited for metamodel estimation.

The methodology presented in this article – screening followed by regression – may be compared with the forward (stepwise) variable selection procedures where the screening is incorporated into the metamodel estimation procedure. Although these methods are efficient when the assumptions underlying the metamodel fit the problem, it may be difficult to choose, a priori, a kind of metamodel. For example, Welch et al. [9] assume that the model can be approximated through a kriging metamodel, and their screening procedure relies on this assumption. With the methodology presented in this article, the metamodel can be chosen after the screening. Then, several metamodels (regression, kriging, etc.) can be estimated, in order to choose the best one.

The two following issues may be investigated in future research.

The first issue concerns the quality of the design through the different projections. With the space filling algorithm proposed by Campolongo et al. [5], the design is optimized to cover the space over the p dimensions, but it doesn't imply that the subspaces of dimensions lower than p would be correctly filled (i.e. have a nearly uniform distribution). Moreover, it seems impossible to control the quality of the design through all the projections. One possibility could be to optimize the design only in the subspaces formed by single factors, in order to obtain something like a latin hypercube design (following for example Griensven et al. [10]). Another possibility could be to use a priori knowledge of the experimenter, who says that a specific group of factors must be important, and to optimize the design in the subspace formed by these factors.

The second issue concerns the extraction of simplex-based designs from any given design. In particular, this would permit to apply the elementary effects method on existing databases of simulations that don't have the required structure. Two methods have been tested. The first was to sketch an ideal simplex-based design, and then to take the simplexes defined by the nearest points of the real design. The second was to build the Delaunay tessellation of the design (see for example Watson [11]). However, these two approaches seem to be computationally expensive in high dimensions.

A Generating a random simplex in the input space

A random simplex is generated by applying two random transformations to a reference simplex: a rotation to orient it, and a translation to place it in the input space. In the following, we detail how to construct the reference simplex, and how to rotate it.

The reference simplex is represented by a $(p + 1) \times p$ matrix

$$S_{ref} = \begin{pmatrix} x_{01} & \dots & x_{0p} \\ \vdots & \ddots & \vdots \\ x_{p1} & \dots & x_{pp} \end{pmatrix}. \quad (\text{A.1})$$

The reference simplex can be of any shape. The two common shapes are:

- (1) the orthonormal simplex, given by: $\mathbf{x}_0 = (0, \dots, 0)$, $\mathbf{x}_i = \mathbf{e}_i$, $i = 1 \dots p$.
- (2) the isometric simplex, given by: $\mathbf{x}_0 = (0, \dots, 0)$, $\mathbf{x}_1 = \mathbf{e}_1$, and for $i \geq 2$, $x_{ij} = \frac{1}{n} \sum_{k < i} x_{kj}$ if $j < i$, $x_{ii} = \sqrt{1 - \sum_{k < i} x_{ik}^2}$ and $x_{ij} = 0$ if $j > i$.

A homothety must be applied to the reference simplex, in order to scale it

according to the assumed linearity of the model (see section 4).

The rotation is represented by a $p \times p$ matrix belonging to the special orthogonal group $SO(p)$, i.e. having determinant = +1. Let $R_{ij}(\theta_{ij})$ denote the element of $SO(p)$ which rotates the basis vector \mathbf{e}_i through an angle θ_{ij} towards the basis vector \mathbf{e}_j inside the $(\mathbf{e}_i, \mathbf{e}_j)$ -plane, leaving the complementary coordinates fixed. $R_{ij}(\theta_{ij})$ is a $p \times p$ diagonal matrix having 1 on its diagonal, where the 2×2 sub-matrix indexed by $(i, j) \times (i, j)$ is the plane rotation of angle θ_{ij} . The full rotation matrix is the product of all the matrices $R_{ij}(\theta_{ij})$, and the angles θ_{ij} are referred to as “Euler angles”; there are $(p^2 - p)/2$ Euler angles (the number of coordinate-planes in \mathbf{R}^p); see for example Arnold [12].

B Software

The programs used in this article were written in R[13]. The elementary effects method, either with Morris’s OAT and simplex-based designs, is implemented in the R package `sensitivity`, available at <http://cran.R-project.org>.

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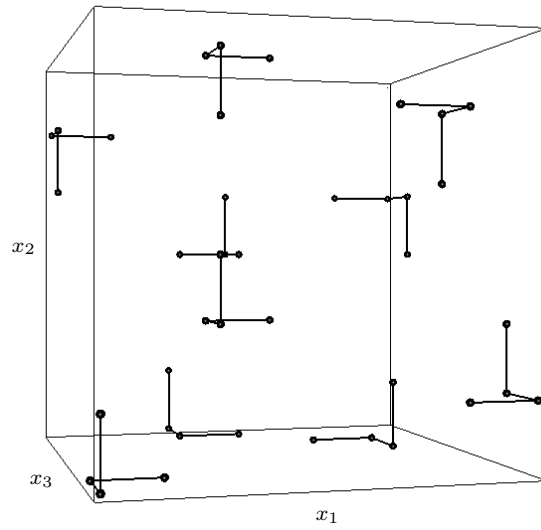
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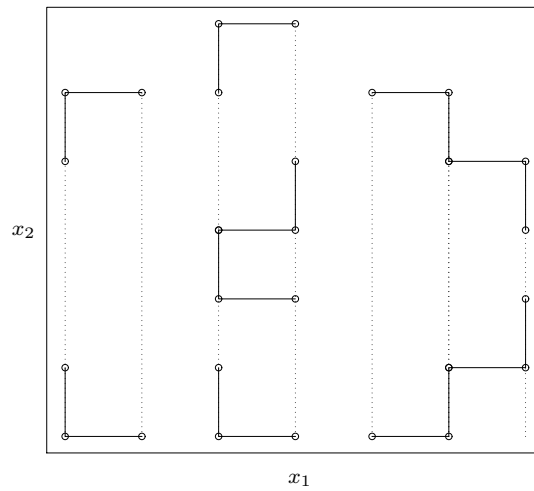
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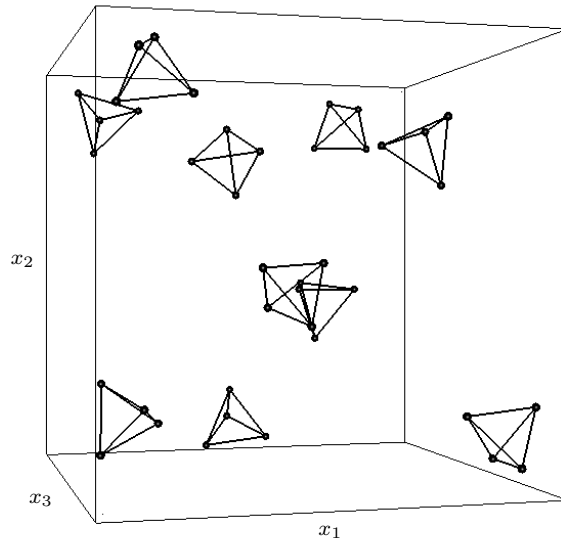


(a)

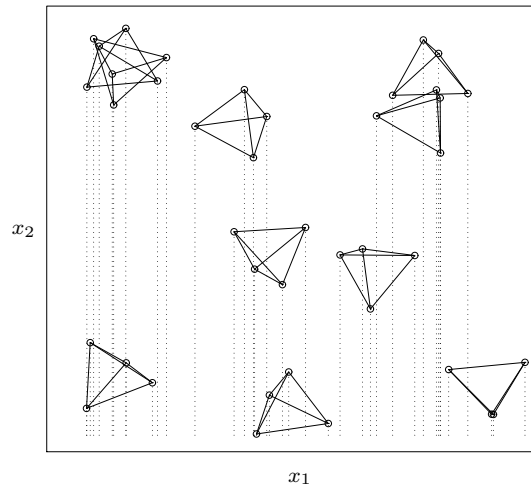


(b)

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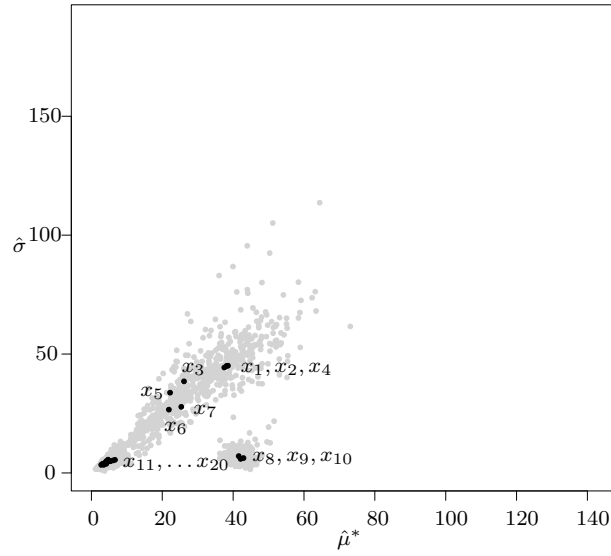


(a)

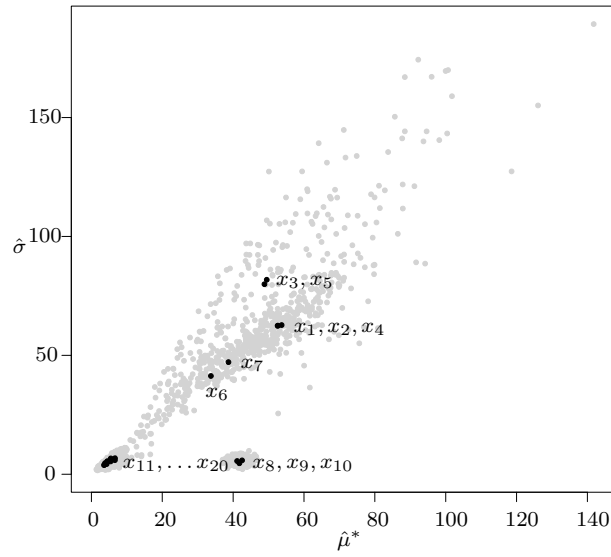


(b)

Fig. B.2. (a) Simplex-based design in $p = 3$ dimensions with $R = 10$ simplexes. (b) Projection of the points of the design on the (x_1, x_2) -plane, and, in dotted lines, on the x_1 -axis.



(a) simplex



(b) OAT

Fig. B.3. Elementary effects sensitivity test with (a) a simplex-based design and (b) a Morris's OAT design, on Morris's function at the computation cost of $N = 210$ ($p = 20$, $R = 10$). Plots of $\hat{\sigma}$ versus $\hat{\mu}^*$. In the background, the superimposition of 100 independent studies. In the foreground, the means over the 100 replicates.