Construction of replicated designs based on Sobol' sequences

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Abstract

In the perspective of estimating main effects of model inputs, two approaches are studied to construct replicated designs based on Sobol' sequences. *To cite this article: L. Gilquin, Ll. A. Jiménez Rugama, E. Arnaud, F. J. Hickernell, H. Monod, C. Prieur, C. R. Acad. Sci. Paris, Ser. I 340 (2005).*

Résumé

Construction de plans répliqués à partir de séquences de Sobol'. Dans le contexte d'estimer les effets principaux des paramètres d'un modèle, nous proposons d'étudier deux approches pour construire des plans répliqués à partir de séquences de Sobol'. *Pour citer cet article : L. Gilquin, Ll. A. Jiménez Rugama, E. Arnaud, F. J. Hickernell, H. Monod, C. Prieur, C. R. Acad. Sci. Paris, Ser. I 340 (2005).*

1. Introduction

Mathematical models often involve a substantial number of poorly known parameters. The effect of these parameters to the output of the model can be assessed through sensitivity analysis. Global sensitivity analysis methods are useful tools to identify the parameters having the most influence on the output. A well known approach is the variance based method introduced by Sobol' in [9]. This method estimates sensitivity indices called Sobol' indices that summarize the influence of each model input. In particular, one can distinguish first-order indices that estimate the main effect of each input.

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The procedure proposed by Sobol' to estimate first-order Sobol' indices and its improvements (see Saltelli [7] for an exhaustive survey) all suffer from a prohibitive cost of model evaluations that grows with respect to the input space dimension. An elegant solution to reduce this cost relies on the construction of particular design of experiments called replicated designs. The notion of replicated designs was first introduced by McKay through its introduction of replicated Latin Hypercubes in [3]. Below we define replicated designs in a wider framework:

Définition 1.1 *Denote by $\boldsymbol{x} \in [0,1)^s$ a point with components $x_1, \ldots, x_s$ and $\mathcal{D} = \{1, \ldots, s\}$. Let $\mathcal{P} = \{\boldsymbol{x}_i\}_{i=0}^{n-1}$ and $\mathcal{P}' = \{\boldsymbol{x}'_i\}_{i=0}^{n-1}$ be two point sets in $[0,1)^s$. Let $\mathcal{P}^u = \{\boldsymbol{x}_{i,u}\}_{i=0}^{n-1}$ (resp. $\mathcal{P}'^u$), $u \subsetneq \mathcal{D}$, denote the subset of dimensions of $\mathcal{P}$ (resp. $\mathcal{P}'$) indexed by u. We say that $\mathcal{P}$ and $\mathcal{P}'$ are two replicated designs of order a if $\forall\ u \subsetneq \mathcal{D}$ of cardinality $|u| = a$, $\mathcal{P}^u$ and $\mathcal{P}'^u$ are the same point set in $[0,1)^a$.*

The replication procedure introduced in [2,11] allows to estimate all first-order Sobol' indices with only two replicated designs of order 1. This procedure has the major advantage of reducing the estimation cost as the number of model evaluations (one design $\mathcal{P}$ of size n and its replication $\mathcal{P}'$) becomes independent of the input space dimension. However, Sobol' indices estimates may still not be accurate enough if the input space is not properly explored.

In this note, we propose the construction of two replicated point sets based on Sobol' sequences that identify as two space-filling replicated designs of order 1. These two designs ensure that the input space is properly explored and can be used within the replication procedure to estimate all main-effects of a numerical model. We first provide a brief introduction on digital sequences and then present two iterative approaches to construct the two replicated point sets.

2. Digital sequences background

2.1. *Preliminaries*

Digital nets and sequences were first introduced by Niederreiter [4] in the numerical integration framework to define good uniformly distributed points in $[0,1)^s$. They can also appear in the literature as digital (t,m,s)-nets and digital (t,s)-sequences, or simply (t,m,s)-nets and (t,s)-sequences. Sobol' and Niederreiter-Xing sequences are two examples of digital sequences detailed in [8] and [5].

The quality of any (t,m,s)-net or (t,s)-sequence is measured by t, called the t-value. The t-value is introduced in the (t,m,s)-net definition as follows:

Définition 2.1 *Let $\mathcal{A}$ be the set of all elementary intervals $A \in [0,1)^s$ where $A = \prod_{j=1}^s [\alpha_j b^{-\gamma_j}, (\alpha_j + 1)b^{-\gamma_j})$, with integers $s \geq 1$, $b \geq 2$, $\gamma_j \geq 0$, and $b^{\gamma_j} > \alpha_j \geq 0$. For $m \geq t \geq 0$, the point set $\mathcal{P} \in [0,1)^s$ with b^m points is a $(t,m,s)-net$ in base b if every A with volume b^{t-m} contains b^t points of $\mathcal{P}$.*

Thus, a (t,m,s)-net is defined such that all elementary intervals of volume at least b^{t-m} will enclose a proportional number of points of $\mathcal{P}$, namely $b^{t-m}|\mathcal{P}|$ points. The most evenly spread nets are $(0,m,s)$-nets, since each elementary interval of the smallest volume possible, b^{-m}, contains exactly one point.

By increasing m, we increase the number of points of the (t,m,s)-net. In the limit case where $m \to \infty$, we can define (t,s)-sequences as:

Définition 2.2 *For integers $s \geq 1$, $b \geq 2$, and $t \geq 0$, the sequence $\{\boldsymbol{x}_i\}_{i \in \mathbb{N}_0}$ is a (t,s)-sequence in base b, if for every set $\mathcal{P}_{\ell,m} = \{\boldsymbol{x}_i\}_{i=\ell b^m}^{(\ell+1)b^m-1}$ with $\ell \geq 0$ and $m \geq t$, $\mathcal{P}_{\ell,m}$ is a (t,m,s)-net in base b.*

Replicated design properties can apply to digital sequences. Therefore, we introduce the definition,

Définition 2.3 *Two digital sequences $\{\boldsymbol{x}_i\}_{i \in \mathbb{N}_0}$ and $\{\boldsymbol{x}'_i\}_{i \in \mathbb{N}_0}$ are* digitally replicated *of order a if for all $m \geq 0$, $\{\boldsymbol{x}_i\}_{i=0}^{b^m-1}$ and $\{\boldsymbol{x}'_i\}_{i=0}^{b^m-1}$ are two replicated designs of order a.*

2.2. *Sobol' sequences*

s-dimensional Sobol' sequences are digital sequences designed in base $b = 2$ and can be computed using the *generating matrices*, a set of s full rank infinite dimensional upper triangular matrices over $\mathbb{F}_2 := \{0, 1\}$. We will denote by $\oplus$ the addition in $\mathbb{F}_2$. These generating matrices are recursively constructed through primitive polynomials and initial directional numbers. In [1], Kuo and Joe detail this construction and also suggest a particular choice for these matrices that optimize the 2 dimensional projection t-values.

Consider the generating matrices $C_1, \dots, C_s$, and $C_1^m, \dots, C_s^m$ their upper left corner blocks of size $m \times m$. Although $C_1, \dots, C_s$ are of infinite size, one only requires the knowledge of $C_1^m, \dots, C_s^m$ to construct the first 2^m points: for each $i = 0, \dots, 2^m - 1$, the point $\boldsymbol{x}_i = (x_{i,1}, \dots, x_{i,s})^\intercal$ of the sequence is obtained dimension-wise by:

$$(x_{i,j,1}, \dots, x_{i,j,m})^\intercal = C_j^m \boldsymbol{i}, \qquad j = 1, \dots, s\,, \tag{1}$$

where $x_{i,j} = \sum_{k \geq 1} x_{i,j,k} 2^{-k}$ and $\boldsymbol{i} = (i_0, \dots, i_{m-1})^\intercal$ are the binary decompositions of $x_{i,j}$ and i, and matrix operations are performed in $\mathbb{F}_2$. Below we provide an example on how to compute $x_{11,1} = 0.8125$ and $x_{9,2} = 0.4375$,

$$\begin{pmatrix} x_{11,1,1} \\ x_{11,1,2} \\ x_{11,1,3} \\ x_{11,1,4} \end{pmatrix} = \overbrace{\begin{pmatrix} 1&0&0&0 \\ 0&1&0&0 \\ 0&0&1&0 \\ 0&0&0&1 \end{pmatrix}}^{C_1^4} \overbrace{\begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}}^{\mathbf{11}} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \qquad \begin{pmatrix} x_{9,2,1} \\ x_{9,2,2} \\ x_{9,2,3} \\ x_{9,2,4} \end{pmatrix} = \overbrace{\begin{pmatrix} 1&1&1&1 \\ 0&1&0&1 \\ 0&0&1&1 \\ 0&0&0&1 \end{pmatrix}}^{C_2^4} \overbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}}^{\mathbf{9}} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

To compute the next 2^m points of the sequence, one can infer from equation (1) that $(x_{i+2^m,j,1}, \dots, x_{i+2^m,j,m+1})^\intercal = (x_{i,j,1}, \dots, x_{i+2^m,j,m}, 0)^\intercal \oplus (c_j^{m+1})^\intercal$, where c_j^{m+1} is the last column of C_j^{m+1}.

Lemma 2.1 *All Sobol' sequences are digitally replicated of order 1.*

Proof. Consider any two s-dimensional Sobol' sequences generated by $C_1, \dots, C_s$ and $C'_1, \dots, C'_s$ respectively. Since any two matrices C_j^m and ${C'}_j^m$ are square and full rank, the operations $C_j^m \boldsymbol{i}$ and ${C'}_j^m \boldsymbol{i}$ are one-to one and onto for all $i = 0, \dots, 2^m - 1$. Therefore, they generate the same point sets.

3. Iterative constructions of extensible replicated point sets

In this section we propose two different approaches to construct extensible replicated point sets, $\mathcal{P}_m$ and $\mathcal{P}'_m$, based on Sobol' sequences. These two constructions are iteratively extended according to:

$$\mathcal{P}_m = B_0 \cup \dots \cup B_m\,,$$

$$\mathcal{P}'_m = {B'}_0 \cup \dots \cup {B'}_m\,,$$

where B_m and B'_m, $m \geq 0$, are new sets of points added at step m to refine $\mathcal{P}_{m-1}$ and $\mathcal{P}'_{m-1}$. For all m, $\mathcal{P}_m$ and $\mathcal{P}'_m$ are two replicated designs of order 1.

The first approach is called multiplicative because $|P_m| = 2^m$ while the second one with $|P_m| = m|B_0|$ is called additive. In the multiplicative case, we will directly use 2 s-dimensional sequences as a result from Lemma 2.1. However, for the additive case, we will consider an initial set of Sobol' points and apply different scramblings and digital shifts to extend the point sets. Additionally, in both cases one can randomize the points with Owen's scrambling [6] as long as equal dimensions between $\mathcal{P}_m$ and $\mathcal{P}'_m$ share the same scrambling.

3.1. *Multiplicative approach*

Two replicated point sets of order 1 $\mathcal{P}_m$ and $\mathcal{P}'_m$ can be constructed using two s-dimensional Sobol' sequences. We note $C_1, \dots, C_s$ the generating matrices used to generate $\mathcal{P}_m$ and $C'_1, \dots, C'_s$ those used to generate $\mathcal{P}'_m$. All these matrices need to be different.

In order to iteratively construct designs $\mathcal{P}_m$ and $\mathcal{P}'_m$, one just needs to compute $B_\ell = \{\boldsymbol{x}_{2^{\ell-1}}, \dots, \boldsymbol{x}_{2^\ell-1}\}$ and $B'_\ell = \{\boldsymbol{x}'_{2^{\ell-1}}, \dots, \boldsymbol{x}'_{2^\ell-1}\}$ for all $\ell = 1, \dots, m$, with $B_0 = B'_0 = \{\boldsymbol{0}\}$. Each set B_ℓ can be obtained applying equation (1) to $C_1, \dots, C_s$ and likewise for B'_ℓ using $C'_1, \dots, C'_s$.

As a direct consequence of Lemma 2.1, at each step ℓ designs $\mathcal{P}_\ell$ and $\mathcal{P}'_\ell$ are two replicated designs of order 1. Furthermore, they both inherit the space-filling properties of (t, ℓ, s)-nets.

3.2. *Additive Approach*

With the multiplicative approach, the size of designs $\mathcal{P}_m$ and $\mathcal{P}'_m$ is multiplied by 2 each time m is increased by one. This growth rate may be inadequate for some applications. The additive approach presented in this section is attractive due to a slower size growth. Given a particular choice of $r \geq 1$, only $|B_0| = 2^r$ points are added to both designs at each step. However, the main drawback is that $\mathcal{P}_m$ and $\mathcal{P}'_m$ do not possess the structure of a Sobol' sequence when $m \geq 1$.

The two replicated point sets $\mathcal{P}_m$ and $\mathcal{P}'_m$ constructed with the additive approach are iteratively refined with B_{m+1} and B'_{m+1}. Each B_{m+1} and B'_{m+1} are (t, r, s)-nets.

First, $B_0 = \{\boldsymbol{x}_i^{(0)}\}_{i=0}^{2^r-1}$ is set to be the first 2^r Sobol' points of a s-dimensional sequence. Then, B'_0, B_ℓ and B'_ℓ, for $\ell \geq 1$, are obtained from B_0 by carrying out digital shifts and scrambling operations. These operations guarantee that both B_ℓ and B'_ℓ inherit the (t, r, s)-net structure of the initial set B_0. We detail below the construction of B_ℓ and B'_ℓ.

At step ℓ, $\ell \geq 1$, $B_\ell = \{\boldsymbol{x}_i^{(\ell)}\}_{i=0}^{2^r-1}$ is generated by applying a digital shift to B_0:

for each $i = 0, \dots, 2^r - 1$, points $\boldsymbol{x}_i^{(\ell)} = (x_{i,1}^{(\ell)}, \dots, x_{i,s}^{(\ell)})^\intercal$ are obtained by:

$$(x_{i,j,1}^{(\ell)}, \dots, x_{i,j,r}^{(\ell)})^\intercal = (x_{i,j,1}^{(0)}, \dots, x_{i,j,r}^{(0)})^\intercal \oplus \boldsymbol{e}_j, \qquad j = 1, \dots, s\,, \tag{2}$$

where $x_{i,j}^{(\ell)} = \sum_{k=1}^r x_{i,j,k}^{(\ell)} 2^{-k}$ and $\boldsymbol{e}_j = (e_{j,0}, \dots, e_{j,r-1})^\intercal \in \mathbb{F}_2^r$.

Then, $B'_\ell = \{\boldsymbol{x'}_i^{(\ell)}\}_{i=0}^{2^r-1}$ is obtained from B_ℓ by applying Tezuka's i-binomial scrambling [10]. This scrambling operation writes as follows:

for each $i = 0, \dots, 2^r - 1$, points $\boldsymbol{x'}_i^{(\ell)} = (x'^{(\ell)}_{i,1}, \dots, x'^{(\ell)}_{i,s})^\intercal$ are obtained by:

$$(x'^{(\ell)}_{i,j,1}, \dots, x'^{(\ell)}_{i,j,r})^\intercal = L_j^r (x_{i,j,1}^{(\ell)}, \dots, x_{i,j,r}^{(\ell)})^\intercal, \tag{3}$$

where $x'^{(\ell)}_{i,j} = \sum_{k=1}^r x'^{(\ell)}_{i,j,k} 2^{-k}$ and each L_j^r is a full rank lower triangular matrix of size $r \times r$ over $\mathbb{F}_2$.

Lemma 3.1 *Using the additive construction, $\mathcal{P}_m$ and $\mathcal{P}'_m$ are two replicated designs of order* 1 *for* $m \geq 0$.

Proof. For each $\ell \geq 1$, digital shift and scrambling operations carried out in equations (2) and (3) are bijections from $\mathbb{F}_2^r$ to $\mathbb{F}_2^r$. Hence, equal dimensions of B_ℓ and B'_ℓ will contain the same set of 2^r values.

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