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# Iterative construction of replicated designs based on Sobol' sequences



## Construction de plans répliqués à partir de séquences de Sobol'

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### ABSTRACT

In the perspective of estimating main effects of model inputs, two approaches are studied to iteratively construct replicated designs based on Sobol' sequences. Space-filling properties of the resulting designs are studied based on two criteria.

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### RÉSUMÉ

Dans l'objectif d'estimer les effets principaux des paramètres d'un modèle, nous proposons d'étudier deux approches pour construire itérativement des plans répliqués à partir de séquences de Sobol'. Les propriétés de remplissage de l'espace des plans construits sont étudiées sur la base de deux critères.

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## 1. Introduction

Mathematical models often involve a substantial number of poorly known parameters. The effect of these parameters on 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 [11]. This method estimates sensitivity indices called Sobol' indices that summarize the influence of each model input. Among all Sobol' indices, one can distinguish the first-order indices that estimate the main effect of each input.

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The procedure to estimate first-order Sobol' indices proposed by Sobol' and its improvements (see Saltelli [9] for an exhaustive survey) all suffer from a prohibitive number of model evaluations that grows with respect to the input space dimension. An elegant solution to reduce this number relies on the construction of particular designs of experiments called replicated designs. The notion of replicated designs was first introduced by McKay through its definition of replicated Latin Hypercubes in [4]. Below we provide this definition in a more general framework:

**Definition 1.1.** Consider  $\mathbf{x} \in [0, 1]^s$ , and  $\mathbf{x}_u \in [0, 1]^{|u|}$  the subset of elements of  $\mathbf{x}$  given by  $u \subsetneq \{1, \dots, s\}$ , where  $|u|$  is the cardinality of  $u$ . Let  $\mathcal{P} = \{\mathbf{x}_i\}_{i=0}^{n-1}$  and  $\mathcal{P}' = \{\mathbf{x}'_i\}_{i=0}^{n-1}$  be two point sets in  $[0, 1]^s$ , and denote by  $\mathcal{P}^u = \{\mathbf{x}_{i,u}\}_{i=0}^{n-1}$  (resp.  $\mathcal{P}'^u$ ) the subset of elements of points in  $\mathcal{P}$  (resp.  $\mathcal{P}'$ ) indexed by  $u$ . We say that  $\mathcal{P}$  and  $\mathcal{P}'$  are two replicated designs of order  $a = 1, \dots, s-1$ , if for any  $u \subsetneq \{1, \dots, s\}$  with  $|u| = a$ ,  $\mathcal{P}^u$  and  $\mathcal{P}'^u$  are the same point set in  $[0, 1]^a$ , perhaps in a different order.

The replication procedure described in [2,12] allows the estimation of all first-order Sobol' indices with only two replicated designs of order 1. This procedure has the major advantage of reducing the number of model evaluations, evaluating only on designs  $\mathcal{P}$  and  $\mathcal{P}'$  regardless of the input space dimension. However, Sobol' indices estimates may still not be accurate enough if designs  $\mathcal{P}$  and  $\mathcal{P}'$  do not explore the input space properly.

In this note, we propose two different constructions of replicated designs of order 1 based on Sobol' sequences. Both constructions ensure that the input space is properly explored and can be used within the replication procedure to estimate all first-order Sobol' indices. The definition of these constructions is recursive, therefore one can iteratively refine each replicated design by adding the corresponding new set of points. We first provide a brief introduction on digital sequences and then present two iterative approaches to construct the two replicated point sets. We end this note by analyzing the space-filling properties of the two designs constructed.

## 2. Digital sequences background

### 2.1. Preliminaries

Digital nets and sequences were first introduced by Niederreiter [6] 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 [10] and [7].

**Definition 2.1.** Let  $\mathcal{A}$  be the set of all elementary intervals  $A \subset [0, 1]^s$  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  $b^{t-m}$  will enclose the same proportion 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. The quality of any  $(t, m, s)$ -net is therefore measured by the parameter  $t$ , called  $t$ -value.

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

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

The replicated design properties can also apply to digital sequences. Hence, we introduce the following definition,

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

### 2.2. Sobol' sequences

Sobol' sequences in dimension  $s$  are digital sequences in base  $b = 2$  that can be computed using the *generating matrices*, a set of  $s$  full-rank infinite dimensional upper triangular matrices over the Galois field  $\mathbb{F}_2 := \{0, 1\}$ . These generating matrices are recursively constructed given some 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  $2^m$  Sobol' points: for each  $i = 0, \dots, 2^m - 1$ , the point  $\mathbf{x}_i = (x_{i,1}, \dots, x_{i,s})^\top$  of the sequence is obtained dimension-wise by:

$$(x_{i,j,1}, \dots, x_{i,j,m})^\top = C_j^m \mathbf{i}, \quad j = 1, \dots, s, \quad (1)$$

where  $x_{i,j} = \sum_{k \geq 1} x_{i,j,k} 2^{-k}$  is the binary expansion of  $x_{i,j}$  and  $\mathbf{i} = (i_0, \dots, i_{m-1})^\top$  is the vector obtained from the binary expansion of  $i = \sum_{k \geq 0} i_k 2^k$ . All matrix operations are performed in  $\mathbb{F}_2$ . Below we provide an example of how to compute  $x_{11,1} = 0.8125$  and  $x_{9,2} = 0.4375$ ,

$$\begin{pmatrix} x_{11,1,1} \\ x_{11,1,2} \\ x_{11,1,3} \\ x_{11,1,4} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{C_1^4} \underbrace{\begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}}_{\mathbf{11}} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} x_{9,2,1} \\ x_{9,2,2} \\ x_{9,2,3} \\ x_{9,2,4} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{C_2^4} \underbrace{\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}}_{\mathbf{9}} = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}.$$

To compute the next  $2^m$  points of the sequence, one can infer from (1) that

$$(x_{i+2^m,j,1}, \dots, x_{i+2^m,j,m+1})^\top = (x_{i,j,1}, \dots, x_{i,j,m}, 0)^\top \oplus (c_j^{m+1})^\top, \quad i = 0, \dots, 2^m - 1, \quad (2)$$

where  $c_j^{m+1}$  is the last column of  $C_j^{m+1}$  and  $\oplus$  is the addition in  $\mathbb{F}_2$ .

In addition, Sobol' sequences have good group structure properties. For any  $m \geq 1$ , the first  $2^m$  points of the sequence form an Abelian group under  $\oplus$ :

$$\begin{aligned} \mathbf{x} &= \left( \sum_{k=1}^m x_{1,k} 2^{-k}, \dots, \sum_{k=1}^m x_{s,k} 2^{-k} \right)^\top, & \mathbf{z} &= \left( \sum_{k=1}^m z_{1,k} 2^{-k}, \dots, \sum_{k=1}^m z_{s,k} 2^{-k} \right)^\top, \\ \mathbf{x} \oplus \mathbf{z} &:= \left( \sum_{k=1}^m (x_{1,k} + z_{1,k} \bmod 2) 2^{-k}, \dots, \sum_{k=1}^m (x_{s,k} + z_{s,k} \bmod 2) 2^{-k} \right)^\top. \end{aligned} \quad (3)$$

From equation (1) above, one may see that the first  $2^m$  points of the sequence are elements of  $(\mathbb{F}_2^m)^s$ .

**Lemma 2.4.** *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  $\mathbf{i} \mapsto C_j^m \mathbf{i}$  and  $\mathbf{i} \mapsto C_j'^m \mathbf{i}$  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 replicated point sets

In this section, we propose two different approaches to iteratively construct two replicated point sets,  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$ , based on Sobol' sequences. These two constructions are carried out according to the following recursive scheme:

$$\begin{cases} \mathcal{P}_0 = B_0 \\ \mathcal{P}_\ell = \mathcal{P}_{\ell-1} \cup B_\ell \end{cases} \quad \begin{cases} \mathcal{P}'_0 = B'_0 \\ \mathcal{P}'_\ell = \mathcal{P}'_{\ell-1} \cup B'_\ell \end{cases}, \quad \ell \geq 1,$$

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

The first approach is called multiplicative because  $|\mathcal{P}_\ell| = 2^\ell$ , while the second one is called additive and  $|\mathcal{P}_\ell| = \ell|B_0|$ . In the multiplicative case, we will directly use 2  $s$ -dimensional sequences as a result from Lemma 2.4. 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 using Owen's scrambling [8] as long as same coordinates of  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  share the same scrambling.

#### 3.1. Multiplicative approach

Two replicated point sets of order 1,  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$ , can be constructed using two  $s$ -dimensional Sobol' sequences. We note  $C_1, \dots, C_s$  the generating matrices used to generate  $\mathcal{P}_\ell$ , and  $C'_1, \dots, C'_s$  those used to generate  $\mathcal{P}'_\ell$ . To ensure that  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  are as uniform as possible, these generating matrices need to be different from each other. We choose  $C_1, \dots, C_s, C'_1, \dots, C'_s$  to be the first  $2s$  generating matrices suggested by Joe and Kuo in [1], not necessarily in this order. In [1], Joe and Kuo minimized the  $t$ -value for all 2-dimensional projections.

In order to iteratively extend designs  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$ , one just needs to compute  $B_\ell = \{\mathbf{x}_{2^{\ell-1}}, \dots, \mathbf{x}_{2^\ell-1}\}$  and  $B'_\ell = \{\mathbf{x}'_{2^{\ell-1}}, \dots, \mathbf{x}'_{2^\ell-1}\}$ , starting with  $B_0 = B'_0 = \{\mathbf{0}\}$ , with  $\mathbf{0}$  the null vector. Each set  $B_\ell$  and  $B'_\ell$  can be constructed using (2) applied to  $\mathcal{P}_{\ell-1}$  and  $\mathcal{P}'_{\ell-1}$ .

As a direct consequence of Lemma 2.4, at each step  $\ell$  designs  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  are two replicated designs of order 1. Furthermore, they both inherit the space-filling properties of  $(t, \ell, s)$ -nets.

### 3.2. Additive approach

With the multiplicative approach, the size of designs  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  is multiplied by 2 each time  $\ell$  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 an initial choice of  $r \geq 1$  that specifies the size of  $B_0$  and  $B'_0$ , only  $|B_0| = 2^r$  points are added to both designs at each step. The main drawback of this approach is that  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  do not inherit the structure of a Sobol' sequence when  $\ell \geq 1$ . Nevertheless, both designs display good space-filling properties, as it will be shown in the next section.

Analogously to the multiplicative case, the two replicated point sets  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  constructed with the additive approach are iteratively refined with  $B_\ell$  and  $B'_\ell$ . First  $\{\mathbf{x}_i\}_{i=0}^{2^r-1}$  and  $\{\mathbf{x}'_i\}_{i=0}^{2^r-1}$  are set to be the first  $2^r$  points of two  $s$ -dimensional Sobol' sequences. The generating matrices of these two sequences are selected as in the multiplicative approach. Then,  $B_\ell$  (resp.  $B'_\ell$ ), for  $\ell \geq 0$ , is obtained from  $\{\mathbf{x}_i\}_{i=0}^{2^r-1}$  (resp.  $\{\mathbf{x}'_i\}_{i=0}^{2^r-1}$ ) by carrying out digital shifts and scrambling operations. Therefore, both  $B_\ell$  and  $B'_\ell$  inherit the  $(t, r, s)$ -net structure of these initial sets.

At step  $\ell = 0$ ,  $B_0 = \{\mathbf{x}_i^{(0)}\}_{i=0}^{2^r-1}$  and  $B'_0 = \{\mathbf{x}'_i^{(0)}\}_{i=0}^{2^r-1}$  are generated as follows: for each  $i = 0, \dots, 2^r - 1$ , points  $\mathbf{x}_i^{(0)} = (x_{i,1}^{(0)}, \dots, x_{i,s}^{(0)})^\top$  and  $\mathbf{x}'_i^{(0)} = (x'_{i,1}^{(0)}, \dots, x'_{i,s}^{(0)})^\top$  are obtained by linearly transforming  $\mathbf{x}_i$ ,

$$\begin{aligned} (x_{i,j,1}^{(0)}, \dots, x_{i,j,r}^{(0)})^\top &= L(x_{i,j,1}, \dots, x_{i,j,r})^\top, & j = 1, \dots, s, \\ (x'_{i,j,1}^{(0)}, \dots, x'_{i,j,r}^{(0)})^\top &= L'(x_{i,j,1}, \dots, x_{i,j,r})^\top, & j = 1, \dots, s, \end{aligned} \quad (4)$$

where  $x_{i,j}^{(0)} = \sum_{k=1}^r x_{i,j,k}^{(0)} 2^{-k}$ ,  $x'_{i,j}^{(0)} = \sum_{k=1}^r x'_{i,j,k}^{(0)} 2^{-k}$  and  $L, L'$  are two distinct full-rank lower triangular matrices of size  $r \times r$  over  $\mathbb{F}_2$ . Left multiplications by  $L$  and  $L'$  in (4) are called linear scramblings [3].

At step  $\ell \geq 1$ , using addition as defined in (3), we construct:

$$B_\ell = \{\mathbf{x}_i^{(0)} \oplus \mathbf{e}_\ell\}_{i=0}^{2^r-1}, \quad B'_\ell = \{\mathbf{x}'_i^{(0)} \oplus \mathbf{e}'_\ell\}_{i=0}^{2^r-1}, \quad (5)$$

where  $\mathbf{e}_\ell \in (\mathbb{F}_2^r)^s \setminus \mathcal{P}_{\ell-1}$  and  $\mathbf{e}'_\ell \in (\mathbb{F}_2^r)^s \setminus \mathcal{P}'_{\ell-1}$ . Indeed,  $B_0$  is a subgroup of  $(\mathbb{F}_2^r)^s$ . Therefore, we construct  $B_\ell = B_0 \oplus \mathbf{e}_\ell$  as a coset of  $B_0$  under the right choice of  $\mathbf{e}_\ell$ . The same reasoning applies to  $B'_0$ . Additions by vectors  $\mathbf{e}_j$  and  $\mathbf{e}'_j$  in (5) are referred to as digital shifts.

There are exactly  $2^{rs}$  different choices of  $\mathbf{e}_\ell$  and  $\mathbf{e}'_\ell$  in  $(\mathbb{F}_2^r)^s$ , and  $2^{r(r-1)/2}$  choices of  $L$  and  $L'$ . The maximum number of iterations  $\ell$  that can be performed equals the number of cosets,  $2^{r(s-1)}$ . If this maximum is reached, designs  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  both correspond to a full grid design of  $2^{rs}$  points with  $2^r$  distinct values per input.

**Lemma 3.1.** *Under the additive construction  $\mathcal{P}_\ell$  and  $\mathcal{P}'_\ell$  are two replicated designs of order 1,  $\ell \geq 0$ .*

**Proof.** For each  $\ell \geq 1$ , digital shift and scrambling operations carried out in (4) and (5) are bijections from  $\mathbb{F}_2^r$  and  $(\mathbb{F}_2^r)^s$ . Hence, the same coordinates of  $B_\ell$  and  $B'_\ell$  will contain the same set of  $2^r$  values.

## 4. Space-filling properties

To analyze the space-filling properties of both approaches, we will use two criteria. The first one is the  $L_2$  star discrepancy that measures the uniformity of a point set. This criterion can be easily computed through an analytical expression provided by [5]. The lower the criterion, the more uniform the point set is. Sobol' sequences were originally constructed to be low discrepancy sequences and therefore, behave well under this criterion. The second criterion is called maximin distance and measures the regularity of a point set. It returns the minimum of all Euclidean distances between pairs of points in the set. The higher the criterion, the more spread the point set is.

We name by design  $M$  (resp.  $A$ ) one of the two replicated designs constructed with the multiplicative (resp. additive) approach, and set the input space dimension  $s$  to 6. For design  $M$ , we study the properties of  $\mathcal{P}_8, \dots, \mathcal{P}_{12}$ , and for design  $A$ , we set the initial value to  $r = 8$  and study the properties of  $\mathcal{P}_0, \dots, \mathcal{P}_{15}$ . For both  $M$  and  $A$ , we generate 100 designs whose average criteria are presented in Fig. 1. While each one of the 100 designs  $M$  is independently randomized applying Owen's scrambling [8], designs  $A$  are constructed by randomly selecting matrix  $L$  (uniformly among all  $2^{r(r-1)/2}$  choices) and vectors  $\mathbf{e}_\ell$  used in equation (5). In addition, we also show in Fig. 1 the results obtained with an optimized Latin Hypercube design (LH design) according to each criterion for an equal number of points as in design  $A$ . The  $x$ -axis corresponds to the number of design points  $N$  and the  $y$ -axis to the value of the criterion. Although LH designs are the standard designs used in the

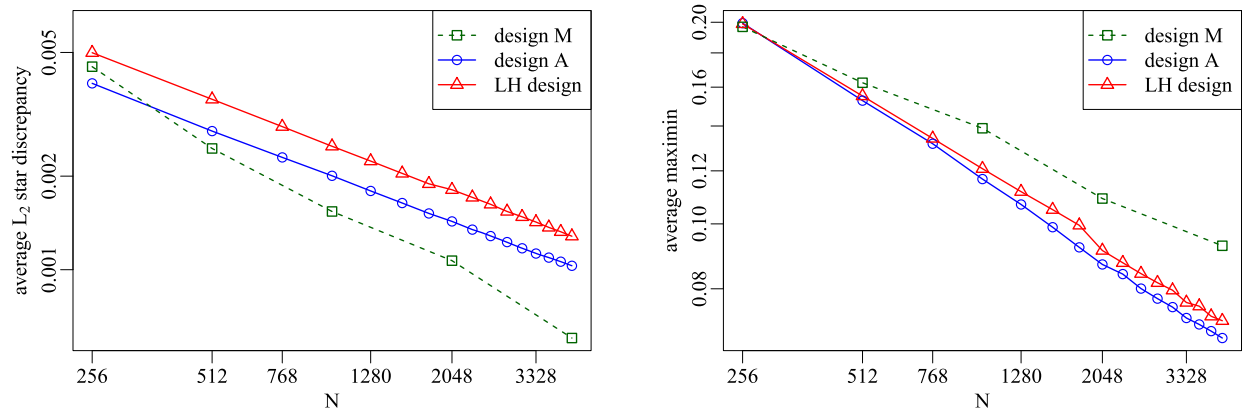


Fig. 1. Log-log graph of averaged  $L_2$  star discrepancy (left) and maximin (right) for designs  $M$  and  $A$  over 100 repetitions.

replication procedure to estimate first-order indices, the replicated design of an optimized LH design is not guaranteed to be optimal.

As expected, design  $M$  performs the best and the estimated slope of the discrepancy curve ( $-0.72$ ) falls within the expected range for Sobol' sequences [5]. Although design  $A$  does not perform as well as design  $M$ , it outperforms an optimized LH design for the discrepancy criterion. However, for the maximin criterion, design  $A$  shows slightly worse results. Concerning the number of steps, design  $A$  allows 15 refinement steps from  $2^8$  to  $2^{12}$  points, instead of only 4 steps for design  $M$ .

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