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Construction of nested space-filling designs using difference matrices

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ABSTRACT

Experiments that study complex real world systems in business, engineering and sciences can be conducted at different levels of accuracy or sophistication. Nested space-filling designs are suitable for such multi-fidelity experiments. In this paper, we propose a systematic method to construct nested space-filling designs for experiments with two levels of accuracy. The method that makes use of nested difference matrices can be easily performed, many nested space-filling designs for experiments with two levels of accuracy can thus be constructed, and the resulting designs achieve stratification in low dimensions. In addition, the proposed method can also be used to obtain sliced space-filling designs for conducting computer experiments with both qualitative and quantitative factors.

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1. Introduction and preliminaries

The experiments with various levels of accuracy or fidelity have become popular in practice because of its great value. They have been widely used in business, engineering and sciences to study the complex real world systems and attracted a recent surge of interests. Study of multi-fidelity experiments has been made to tackle the experimental planning. Nested space-filling designs are proposed for multi-fidelity experiments (Qian et al., 2009b). Qian et al. (2009a,b) and Qian and Ai (2010) constructed some nested space-filling designs for experiments with two levels of accuracy, i.e. the low-accuracy experiment (LE) and the high-accuracy experiment (HE), where HE is more accurate but more expensive than LE. The problem of modeling data from HE and LE has been discussed in Goldstein and Rougier (2004), Higdon et al. (2004), Kennedy and O'Hagan (2000, 2001), Reese et al. (2004), Qian et al. (2006), and Qian and Wu (2008). These methods of building surrogate models are mainly based on flexible Gaussian process models (Sacks et al., 1989; Welch et al., 1992; Santner et al., 2003; Fang et al., 2005).

Let S(n,m) be a space-filling design with n runs and m factors, each having n equidistant levels, we call S achieving stratification on $\underline{d \times \dots \times d}$ grids in $k \le m$ dimensions for some integer d, if for any k dimensional projection of S, $S[i_1, \dots, i_k]$,

its points locate evenly in $\underline{d \times \cdots \times d}$ grids, i.e., there are n/d^k points in each grid. If $n = d^k$, we call S achieving the

maximum stratification on $d \times \cdots \times d$ grids in k dimensions. The purpose of this paper is to construct two-fidelity

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experiments that are called the LE (D_l) and the HE (D_h) based on the three principles that were proposed by Qian et al. (2009b):

- *Economy*: the number of points in D_h is smaller than the number of points in D_i ;
- *Nested relationship*: D_h is nested within D_l , i.e., $D_h \subset D_l$;
- Space-filling: both D_h and D_l achieve stratification in low dimensions.

Qian et al. (2009b) first explicitly proposed the notion of nested space-filling designs and constructed such designs by making use of Galois fields and orthogonal arrays. Qian et al. (2009a) further presented another method to construct nested space-filling designs with the help of nested difference matrices. But the cases of nested difference matrices they constructed are limited. Qian and Ai (2010) constructed a new sampling scheme, called nested lattice sampling, with the knowledge of Galois field and incomplete pairwise orthogonal Latin squares. Haaland and Qian (2010) proposed a construction method of nested space-filling designs for multi-fidelity computer experiments based on existing (*t*,*s*)-sequences. The designs constructed in these four papers can achieve stratification in two dimensions. While, Qian (2009) used special permutations to construct nested Latin hypercubes, which achieve stratification only in one dimension. In this paper, we will present an easy method to construct more nested difference matrices. Nested space-filling designs for experiments with two levels of accuracy can thus be constructed from these nested difference matrices directly.

Now we present some basic concepts, notation and lemmas that will be used in the following sections.

Galois field. The set of residues modulo a prime number p, $\{0, 1, ..., p-1\}$, forms a field of p elements under addition '+' and multiplication modulo p, which is called a Galois field, denoted as GF(p). Knowing that the order of a Galois field must be a power of a prime, we now show how to obtain a Galois field of order $s = p^u$ for any prime number p and any positive number u. Let $g(x) = b_0 + b_1 x + \cdots + b_u x^u$, where $b_j \in GF(p)$ and $b_u = 1$, be an irreducible polynomial of degree u. Then the set of all polynomials of degree u-1 or lower, $\{a_0 + a_1 x + \cdots + a_{u-1} x^{u-1} | a_j \in GF(p)\}$, is a Galois field $GF(p^u)$ of order p^u under addition and multiplication of polynomials modulo g(x). For any polynomial f(x) with coefficients from GF(p), there exist unique polynomials q(x) and r(x) such that f(x) = q(x)g(x) + r(x) where the degree of r(x) is smaller than u. This r(x) is the residue of f(x) modulo g(x), which is usually written as $f(x) = r(x) \pmod{g(x)}$.

Orthogonal array and difference matrix. An orthogonal array OA(n,m,s,t) is an array of size $n \times m$, where each column has entries from $\{0, \ldots, s-1\}$, such that in any $n \times t$ subarray every possible *t*-tuple occurs an equal number of times λ as a row, and *t* is called the strength, λ is called the index of the orthogonal array. A difference matrix D(r,c,s) is an $r \times c$ array with entries from a finite Abelian group (A, +) of *s* elements such that every element of A appears equally often in the vector difference between any two columns of the array (Bose and Bush, 1952).

An easy way to construct a difference matrix is as follows.

Lemma 1 (Hedayat et al., 1999). Let the s elements of GF(s) be $\alpha_0, \ldots, \alpha_{s-1}$, and D be the $s \times s$ multiplication table of this field. Then D is a difference matrix D(s,s,s).

Nested difference matrix and Kronecker sum. Let *D* be a difference matrix $D(r_2, c, s_2)$, suppose there is a subarray of *D*, denoted by D_1 with r_1 rows, and a projection δ that collapses the s_2 levels of *D* into s_1 levels such that $\delta(D_1)$ is a $D(r_1, c, s_1)(r_2 > r_1, s_2 > s_1)$. Then *D*, or more precisely (D, D_1, δ) , is called a nested difference matrix (Qian et al., 2009a). For two matrices $A = (a_{ij})$ of order $n \times r$ and *B* of order $m \times g$ whose entries are all from an Abelian group A, define their Kronecker sum to be $A \oplus B = (B^{a_{ij}})$, where $B^k = (B + kJ)$ and *J* is the $m \times g$ matrix of ones. The rule of Kronecker sum combined with the difference matrices can became a simple but powerful tool for the construction of orthogonal arrays of strength two. The following lemma is an example.

Lemma 2 (Bose and Bush, 1952). Let A be an OA(n,m,s,2) and D be a difference matrix D(r,c,s) whose elements are all from an Abelian group A, then $A \oplus D$ is an OA(rn,cm,s,2).

Latin hypercube and OA-based Latin hypercube. An $n \times m$ matrix $L = (l_{ij})$ is called a Latin hypercube with n runs and m factors if each column of L is a permutation of $0, \ldots, n-1$. Let A be an OA(n,m,s,t) with its s levels being denoted by $0, \ldots, s-1$, then in every column of A, each level occurs q = n/s times. For each column of A, if we replace the q zeros by a permutation of $0, \ldots, q-1$, replace the q ones by a permutation of $q, \ldots, 2q-1$, and so on, we obtain an OA-based Latin hypercube (Tang, 1993). In addition to achieving maximum stratification in one dimension, OA-based Latin hypercubes achieve stratification in $k \le t$ dimensions.

This paper is organized as follows. Section 2 presents a general method for constructing nested difference matrices. In Section 3, we provide a construction of nested space-filling designs. There are some comparisons and concluding remarks in Section 4.

2. Construction of nested difference matrices

In this section, we propose an approach based on special multiplication tables of Galois fields to construct nested difference matrices. The method is flexible to construct more nested difference matrices which are different from those

given by Qian et al. (2009a) and Qian and Ai (2010). For convenience in presentation, we use $f_g(x)$ to denote the residue of f(x) modulo g(x) as Qian et al. (2009b) did. The following lemma will be critical to the proofs of Theorems 1 and 2 below.

Lemma 3. Suppose $g_i(x)$ is an irreducible polynomial that defines $F_i = GF(s_i)$, $s_i = p^{u_i}$ for i = 1, 2 and $u_1 < u_2$. Let ρ be a projection from $F = \{f(x) = a_0 + a_1x + \dots + a_tx^t \mid t \ge 0, a_i \in GF(p)\}$ to F_1 as $\rho(f(x)) = (f_{g_2})_{g_1}(x)$. Then we have:

(1) for any $f_1(x), f_2(x) \in F$, $\rho(f_1(x) + f_2(x)) = \rho(f_1(x)) + \rho(f_2(x))$; (2) if *A* is an *OA*(*n*,*m*,*s*₂,*t*) defined on *F*₂, then $\rho(A) = (\rho(a_{ij}))$ is an *OA*(*n*,*m*,*s*₁,*t*) defined on *F*₁; (3) if *D* is a *D*(*r*,*c*,*s*₂) defined on *F*₂, then $\rho(D) = (\rho(a_{ij}))$ is a *D*(*r*,*c*,*s*₁).

Proof. (1) Suppose $f_1(x) = q_1(x)g_2(x) + r_1(x)$, $f_2(x) = q_2(x)g_2(x) + r_2(x)$, $r_1(x) = n_1(x)g_1(x) + m_1(x)$ and $r_2(x) = n_2(x)g_1(x) + m_2(x)$, where $\partial(r_i(x)) < \partial(g_2(x))$, $\partial(m_i(x)) < \partial(g_1(x))$ for i = 1, 2, and $\partial(f(x))$ denotes the degree of polynomial f(x). Then

$$\rho(f_1(x) + f_2(x)) = ((f_1 + f_2)_{g_2})_{g_1} = (r_1 + r_2)_{g_1} = m_1 + m_2$$

$$\rho(f_1(x)) + \rho(f_2(x)) = ((f_1)_{g_2})_{g_1} + ((f_2)_{g_2})_{g_1} = (r_1)_{g_1} + (r_2)_{g_1} = m_1 + m_2$$

thus $\rho(f_1(x) + f_2(x)) = \rho(f_1(x)) + \rho(f_2(x)).$

(2) For any *t* columns $\mathbf{a}_{j,j} = 1, ..., t$, of *A* and any *t*-tuple $(b_1, ..., b_t), b_i \in F_1$, if we can prove that $(b_1, ..., b_t)$ occurs n/s_1^t times in the submatrix $[\rho(\mathbf{a}_1), ..., \rho(\mathbf{a}_t)]$, then the conclusion will be true. Let

 $B_i = \{f(x) | f(x) \in F_2, \rho(f(x)) = b_i\}$ and

$$B = \{(f_1(x), \ldots, f_t(x)) | f_i(x) \in B_i, i = 1, \ldots, t\}.$$

Obviously, $|B| = s_2^t/s_1^t$, where |B| denotes the cardinality of *B*. Since *A* is an *OA*(*n*,*m*,*s*₂,*t*), any *t*-tuple ($f_1(x), \ldots, f_t(x)$) occurs n/s_2^t times as the rows of submatrix (a_1, \ldots, a_t), therefore, (b_1, \ldots, b_t) occurs $(n/s_2^t)|B|$ times, i.e., n/s_1^t times as the rows of submatrix [$\rho(a_1), \ldots, \rho(a_t)$].

(3) Suppose $\mathbf{d}_j = (\mathbf{d}_{1j}, \dots, \mathbf{d}_{ij})'$ for j = 1, 2 are any two columns of D, then the vector difference between these two columns contains each element of F_2 equally often. Thus the vector $\rho(\mathbf{d}_1) - \rho(\mathbf{d}_2) = \rho(\mathbf{d}_1 - \mathbf{d}_2) = (\mathbf{d}_1 - \mathbf{d}_2)_{g_1(x)}$ contains each element of F_1 equally often, i.e., $\rho(D) = (\rho(\mathbf{d}_{ij}))$ is a $D(r, c, s_1)$. \Box

For a scalar α and a matrix or a set *A*, let α +*A* denote the element-wise sum of α and *A*. Suppose *F*₂ is as defined in Lemma 3, and let

$$E_1 = \{f(x) \in F_2 \mid \partial(f(x)) \le u_1 - 1\}$$

It is obvious that E_1 is a subgroup of F_2 under operation '+', then F_2 can be decomposed as

$$\Gamma = \{\gamma | \gamma = a_{u_2-1} x^{u_2-1} + \dots + a_{u_1} x^{u_1}, a_i \in GF(p), i = u_1, \dots, u_2-1\}$$

= $\{\gamma_0 = 0, \gamma_1, \dots, \gamma_{s_2/s_1-1}\}.$

 $F_2 = E_1 \cup (\gamma_1 + E_1) \cup \cdots \cup (\gamma_{s_2/s_1 - 1} + E_1)$ where $\gamma \in \Gamma$ and

Note that F_1 and E_1 have the same entries, but are defined on different Galois fields, i.e. $GF(s_1)$ and $GF(s_2)$, respectively. Define

 $C = \{ f(x) \in E_1 \, \big| \, \partial(f(x)) \le u_2 - u_1 \},\$

then it is easy to see that

$$|C| = \begin{cases} |E_1| = p^{u_1} = s_1 & \text{if } 2u_1 \le u_2 + 1, \\ p^{u_2 - u_1 + 1} & \text{otherwise.} \end{cases}$$

Now, let us construct an $s_2 \times |C|$ array *D* as follows.

Algorithm 1. Step 1. Label the columns of *D* with the elements of *C*, and label the first s_1 rows of *D* with the elements of E_1 , the next s_1 rows with the elements of $\gamma_1 + E_1$, and so on.

Step 2. Define the entry of *D* in the row labeled with $\delta \in F_2$ and the column labeled with $\beta \in C$ to be the product of δ and β , i.e., $\delta\beta$.

Step 3. Then D has the row partition configuration $(D'_{11}, \ldots, D'_{1,s_2/s_1})'$, where D_{1i} is an $s_1 \times |C|$ matrix.

From Lemmas 1 and 3, we can obtain the following result.

Theorem 1. Let $D = (D'_{11}, \ldots, D'_{1,s_2/s_1})'$ be the array constructed above and $D_1 = (D'_{11}, \ldots, D'_{1k})'$ with $k < s_2/s_1$, then D is a $D(s_2, |C|, s_2)$ defined on F_2 , $\rho(D_1)$ is a $D(s_1, |C|, s_1)$ defined on F_1 for $i = 1, \ldots, s_2/s_1$, $\rho(D_1)$ is a $D(ks_1, |C|, s_1)$ defined on F_1 , and (D, D_1, ρ) is a nested difference matrix, where |C| is given in (1).

Example 1. Let $p = 2, u_1 = 1, u_2 = 2, s_1 = p^{u_1} = 2, s_2 = p^{u_2} = 4$. We use $g_2(x) = x^2 + x + 1$ to define $F_2 = GF(s_2) = \{0, 1, x, x + 1\}$, $g_1(x) = x$ to define $F_1 = GF(s_1) = \{0, 1\}$. Then $E_1 = \{0, 1\}$, $C = \{0, 1\}$, $\Gamma = \{0, x\}$, and we can obtain a difference matrix

(1)

D(4, 2, 4) as

	0	1	
0	0	0	
1	0	1	D_1 .
x	0	x	
x + 1	0	x + 1	D_2

Here $\rho(0) = 0, \rho(1) = 1, \rho(x) = 0, \rho(x+1) = 1$, then

$$\rho(D) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 1 \end{pmatrix}$$

is a D(4, 2, 2) defined on GF(2). Thus (D, D_1, ρ) is a nested difference matrix.

3. Construction of nested space-filling designs

In this section, we use Lemma 2 to construct nested space-filling designs.

Algorithm 2. Step 1. Let $(D = (D'_1, D'_2)', D_1, \rho)$ be the nested difference matrix constructed in Theorem 1, A_1 be an $OA(n, m, s_2, 2)$ with levels taken from F_2 and $A = ((D_1 \oplus A_1)', (D_2 \oplus A_1)')'$. Then from Lemma 2, A is an $OA(ns_2, m |C|, s_2, 2)$.

Step 2. Relabel the levels of *A* as follows. Partition the $s_2 = p^{u_2}$ levels of *A* into $s_1 = p^{u_1}$ groups according to the scheme that two levels $f_1(x)$ and $f_2(x)$ belong to the same group if $f_1(x) = f_2(x) \pmod{g_1(x)}$. Arbitrarily label the s_1 groups as groups 1, ..., s_1 , and the s_2/s_1 levels within the *i*th group as $(i-1)s_2/s_1, \ldots, is_2/s_1-1$ for $i = 1, \ldots, s_1$.

Step 3. Use *A* to obtain an OA-based Latin hypercube *S*, then *S* has the configuration $S = (V'_1, V'_2)'$ corresponding to *A*. Algorithm 2 gives the construction method of space-filling designs. And the s_2 levels of *A* are labeled in the same way as in Qian et al. (2009b).

Theorem 2. Suppose *S* is constructed in Algorithm2, then $D_l = S$ and $D_h = V_1$ satisfy the three principles given in Section 1. In addition, D_h and D_l not only achieve stratification in any one dimension, but also achieve stratification on $s_1 \times s_1$ grids and $s_2 \times s_2$ grids in two dimensions, respectively.

Proof. Note that, for any two levels $f_1(x)$ and $f_2(x)$ of A, the necessary and sufficient condition for $f_1(x)$ and $f_2(x)$ being partitioned into a common group is $\rho(f_1(x)) = \rho(f_2(x))$. Thus, if we can prove that $\rho(D_1 \oplus A_1)$ is an $OA(nks_1, m|C|, s_1, 2)$, then the conclusion will be true. Since from Theorem 1, $\rho(D_1)$ is a $D(ks_1, |C|, s_1)$ defined on F_1 , then based on Lemmas 2 and 3, $\rho(D_1 \oplus A_1) = \rho(D_1) \oplus \rho(A_1)$ is an $OA(nks_1, m|C|, s_1, 2)$. \Box

Example 2 (*Example 1 continued*). *Step* 1. Let A_1 be an OA(16, 5, 4, 2) defined on GF(4) as shown in Table 1, then $A = ((D_1 \oplus A_1)', (D_2 \oplus A_1)')'$ is an OA(64, 10, 4, 2). It can be easily seen that $\rho(D_i \oplus A_1)$ is an OA(32, 10, 2, 2), i = 1, 2.

Step 2. We relabel the levels {0, 1, x, x+1} of *A* according to the scheme in Algorithm 2. The generated Latin hypercube $S = (V'_1, V'_2)'$ is listed in Table 2.

Step 3. Take $D_l = S_l D_h = V_1$, and plot the bivariate projections of *S*. For saving space, we only present four plots in Fig. 1 which shows that the points of bivariate projections of D_h and D_l achieve stratification on 2×2 grids and 4×4 grids, respectively.

Remark 1. In Example 2, A₁ is an OA(16, 5, 4, 2) and A has configuration

 $\begin{pmatrix} A_1 & A_1 \\ A_1 & 1+A_1 \\ A_1 & x+A_1 \\ A_1 & x+1+A_1 \end{pmatrix},$

then the bivariate projection on the *i*th and *j*th columns of V_1 or V_2 achieves stratification on

 $\begin{cases} 4 \times 4 \text{ grids in two dimensions} & \text{if } 1 \le ij \le 5 \text{ or } 6 \le ij \le 10 \\ \text{or } 1 \le i \le 5, 6 \le j \le 10 \text{ and } j \ne i+5, \end{cases}$ $2 \times 2 \text{ grids in two dimensions} & \text{if } 1 \le i \le 5, j = i+5. \end{cases}$

Refer to Fig. 1 for the illustrations of these cases.

Table 1

1	2	3	4	5
0	0	0	0	0
0	1	1	x	x+1
0	x	x	x+1	1
0	x+1	x+1	1	x
1	0	1	1	1
1	1	0	x+1	x
1	x	x+1	x	0
1	x+1	x	0	x+1
x	0	x	x	x
x	1	x+1	0	1
x	x	0	1	x+1
x	x+1	1	x+1	0
x+1	0	x+1	x+1	x+1
x+1	1	x	1	0
x+1	x	1	0	x
x+1	x+1	0	x	1

Table 2 $S = (V'_1, V'_2)'$ in Example 2.

V_1											V_2										
Run	1	2	3	4	5	6	7	8	9	10	Run	1	2	3	4	5	6	7	8	9	10
1	26	59	2	43	46	52	48	11	18	1	33	25	61	0	46	37	6	34	18	2	29
2	18	26	52	4	59	53	12	58	10	36	34	27	23	61	1	52	4	24	34	31	55
3	30	45	42	54	22	62	36	30	57	58	35	31	41	36	61	29	11	62	0	35	45
4	21	5	28	30	13	58	30	32	47	28	36	23	3	21	28	7	12	2	48	58	2
5	61	51	54	19	18	31	56	57	42	57	37	56	49	50	29	30	44	37	41	62	33
6	59	30	14	62	0	30	1	13	60	16	38	51	20	8	50	9	46	16	26	36	4
7	52	43	29	3	42	16	44	42	5	11	39	54	32	23	2	32	35	52	55	20	27
8	63	14	34	35	61	28	29	17	21	39	40	62	0	45	38	60	42	4	10	3	61
9	40	58	40	15	3	2	57	24	9	20	41	32	56	46	5	11	60	47	8	29	7
10	46	25	18	45	20	8	6	40	27	50	42	34	22	20	47	31	55	31	51	14	38
11	37	39	3	25	51	7	45	3	44	37	43	41	47	6	27	55	51	51	25	49	48
12	35	11	49	58	43	15	23	49	52	14	44	42	6	57	51	45	48	14	46	34	23
13	11	57	17	59	58	40	55	45	61	47	45	3	48	22	56	56	18	32	56	40	53
14	2	24	44	22	40	33	9	29	39	8	46	14	28	35	17	33	19	18	14	56	22
15	1	34	60	33	10	34	46	52	17	21	47	0	44	53	42	12	22	61	35	12	3
16	12	10	5	12	23	32	21	9	15	63	48	4	2	15	11	16	21	0	23	24	35
17	20	60	7	37	34	25	10	59	46	60	49	28	63	12	44	35	41	17	43	48	34
18	19	17	48	9	63	29	60	1	55	19	50	22	31	62	14	57	43	33	31	37	0
19	17	36	32	53	26	17	28	47	7	10	51	24	42	37	52	19	36	5	60	22	25
20	16	1	27	21	2	26	35	16	26	40	52	29	4	19	16	6	39	50	7	0	56
21	60	54	56	18	21	54	11	6	28	15	53	48	53	59	26	25	0	27	20	1	31
22	50	27	4	57	5	50	58	62	6	44	54	49	21	13	48	15	14	39	33	25	54
23	55	46	25	0	36	59	22	28	54	59	55	53	38	30	6	44	3	8	2	33	46
24	58	12	38	40	50	56	42	37	32	17	56	57	9	33	39	49	5	53	61	51	9
25	44	52	43	8	1	38	7	38	50	43	57	45	50	47	10	14	27	20	54	45	52
26	43	19	31	34	17	45	63	27	41	6	58	33	29	24	32	24	23	40	5	63	18
27	39	33	10	24	62	37	19	50	16	30	59	47	37	11	23	54	20	3	36	13	5
28	36	15	58	49	47	47	41	15	4	51	60	38	13	63	55	39	24	59	22	23	32
29	8	62	26	60	48	13	15	21	11	26	61	9	55	16	63	53	61	26	12	30	13
30	6	18	41	20	41	9	49	39	19	49	62	10	16	39	31	38	63	38	63	8	42
31	13	40	55	36	8	10	25	4	43	41	63	7	35	51	41	4	49	13	19	53	62
32	15	8	1	7	28	1	43	53	59	12	64	5	7	9	13	27	57	54	44	38	24

4. Discussion and concluding remarks

We have presented a general approach to constructing nested space-filling designs for experiments with two levels of accuracy or fidelity using nested difference matrices. These designs are easy to construct and achieve stratification in two dimensions, which are popular in physical vs. computer experiments or detailed vs. approximate computer experiments.



Fig. 1. Some bivariate projections among columns x_1, \ldots, x_{10} of *S* in Example 2 (V_i : block $V_i, i = 1, 2$).

Metho	ds	D	D_1^{a}	Constraints				
QAW	I II IV V	$\begin{array}{c} D(p^{m+1},p^2,p^{m+1})\\ D(p^{m+2},p^2,p^{m+2})\\ D(p^{m+2},p^3,p^{m+2})\\ D(p^{m+3},p^3,p^{m+3})\\ D(p^{m+3},p^4,p^{m+3}) \end{array}$	$\begin{array}{c} D(p^m,p^2,p^m) \\ D(p^m,p^2,p^m) \\ D(p^{m+1},p^3,p^m) \\ D(p^{m+1},p^3,p^m) \\ D(p^{m+2},p^4,p^m) \end{array}$	$m \ge 2$ p = 2, 3				
QA		$D(p^{u_2},p^{u_1},p^{u_2})$	$D(p^{u_1},p^{u_1},p^{u_1})$	$u_1 < u_2, u_1 u_2$				
PM		$D(p^{u_2}, C , p^{u_2})$	$D(kp^{u_1}, C , p^{u_1})$	$u_1 < u_2, k < p^{u_2 - u_1}$ $ C = \begin{cases} p^{u_1} & \text{for } 2u_1 \le u_2 + 1\\ p^{u_2 - u_1 + 1} & \text{for } 2u_1 > u_2 + 1 \end{cases}$ <i>p</i> is any prime number				

Comparisons between the nested difference matrices constructed by QAW and PM.

^a D_1 is nested in D.

Table 3

Note that Qian et al. (2009a) and Qian and Ai (2010) also used nested difference matrices to construct nested spacefilling designs. Now we give some comparisons among the nested difference matrices constructed by Qian et al. (2009a) (QAW), Qian and Ai (2010) (QA) and the proposed method (PM), the results are listed in Table 3. From this table, we can see that all the nested difference matrices obtained by QA can be generated by the proposed method. In addition, it can be easily verified that, by taking p=2,3 and some specific values for u_1,u_2 and k, the proposed method can generated almost all the nested difference matrices obtained by QAW, except for their case III with m=2, case IV with m=2, and case V with m=2,3. For instance, by taking $u_1 = m,u_2 = m+2,k=1$ and p=2,3, we can construct nested difference matrices $D = D(p^{m+2},p^2,p^{m+2}), D_1 = D(p^m,p^2,p^m)$ for m=2, and $D = D(p^{m+2},p^3,p^{m+2}), D_1 = D(p^m,p^3,p^m)$ for m > 2, which include all the matrices constructed in case II of QAW. Obviously, the proposed method has a more flexible choice of the parameters p, u_1, u_2 and k, and thus can generated much more new nested difference matrices.

Given an $OA(n,m,p^{u_2},t)$, the proposed method can generated nested space-filling designs D_h and D_l with m|C| factors, nkp^{u_1} and np^{u_2} runs, respectively, where p is a prime power, $u_1 < u_2$, $k < p^{u_2-u_1}$ and |C| is defined in (1). Usually, a larger value of t or (and) k may result in a more accurate surrogate model. In practice, the values of k and t can be chosen according to the experimental and economic considerations.

Basically, the study of multi-fidelity experiments involves two aspects, the experimental planning and surrogate model building. The design of a computer experiment often involves exploring a broad design space or region of design variable values. We want a design method to give a trade-off between the accuracy of a surrogate model and the resources needed to build it. The nested space-filling designs constructed in this paper can solve this trade-off problem. The design D_l can be used to conduct approximate simulations and the design D_h can be used to conduct detailed simulations. Since $D_h \subset D_l$, we can refine the surrogate model obtained based on D_l by incorporating the data from D_h to obtain a more accurate prediction model. To integrate the results from the detailed and approximate simulations, Qian et al. (2006) proposed a two-step approach based on the Gaussian process modeling, which can be illustrated using the design $S = (V'_1, V'_2)'$ constructed in Table 2 as follows: (1) fit a Gaussian process model based on the data obtained by conducting the approximate simulations using S (i.e., D_l); (2) adjust the fitted model with the data obtained by conducting the detailed simulations using V_1 (i.e., D_h). Details can refer to Qian et al. (2006).

One of the referees brought the designs based on Sobol sequences to our attention. Such designs were recently proposed by Challenor (2011) for computer experiments that involve switches. They may also be used for conducting multi-fidelity experiments, but usually the designs cannot achieve stratification in two or more dimensions, though the stratification in one dimension can be achieved. As for the comparison with the proposed designs in terms of reducing uncertainty of surrogate models, further study need to be carried out in the future research.

Recently, Qian and Wu (2009) suggested to use a sliced space-filling design to conduct a computer experiment with qualitative and quantitative factors. Since the difference matrices have the row partition configuration $D = (D'_{11}, \ldots, D'_{1,s_2/s_1})'$ (cf. Theorem 1), and by noting that $\rho(D_{1i} \oplus A_1)$ is an $OA(ns_1,m|C|,s_1,2)$ for $i = 1, \ldots, s_2/s_1$, then it is easy to obtain a sliced space-filling design from $((D_{11} \oplus A)', \ldots, (D_{1,s_2/s_1} \oplus A)')'$. Thus, the resulting designs obtained by the proposed method can also be used to conduct computer experiments with qualitative and quantitative factors. For the analysis of computer experiments with both quantitative and qualitative input variables, refer to Han et al. (2009) and the references therein.

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