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Flexible sliced designs for computer experiments

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Abstract Sliced Latin hypercube designs are popularly adopted for computer experiments with qualitative factors. Previous constructions require the sizes of different slices to be identical. Here we construct sliced designs with flexible sizes of slices. Besides achieving desirable one-dimensional uniformity, flexible sliced designs (FSDs) constructed in this paper accommodate arbitrary sizes for different slices and cover ordinary sliced Latin hypercube designs as special cases. The sampling properties of FSDs are derived and a central limit theorem is established. It shows that any linear combination of the sample means from different models on slices follows an asymptotic normal distribution. Some simulations compare FSDs with other sliced designs in collective evaluations of multiple computer models.

Keywords Central limit theorem · Latin hypercube design · Sampling property · Sliced design

1 Introduction

A central issue in computer experiments is to estimate the mean of the response of a computer model. McKay et al. (1979) proposed Latin hypercube designs (LHDs) which achieve maximum stratification in univariate margins simultaneously. Stein (1987) showed that a Latin hypercube sample provides a smaller variance for the sample mean compared with the independently identical distribution sample.

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When the experiment contains several batches or multiple computer models based on similar mathematics (Williams et al. 2009), sliced designs are considered as appropriate choices since their different slices can be arranged to different batches or models, respectively. Qian (2012) introduced sliced LHDs (SLHDs) with multislices and univariate stratification, whereas both sliced LHDs and general sliced LHDs require the sizes of different slices to be identical. Same restrictions on the sample size can be found in variants of sliced LHDs discussed in Ai et al. (2014), Yin et al. (2014), Ai et al. (2016), Ba et al. (2015), and Hwang et al. (2016).

Consider the following cases: (i) There exists several different codes with different accuracies and complexities which can be used as alternative models for the same problem; (ii) several experiment centers have different limitation of time or budget in studying the same project. In these two cases, different computational complexities and different experimental resources lead to different available sample sizes for slices. The data should be able to be analyzed both separately and together, and the design should be robust to the failure of some slices.

In this paper, we construct flexible sliced designs which can suit for different slices of arbitrary sample sizes. The proposed design is robust to the failure of its sub-designs. We refer to these new designs as FSDs for convenience. When all slices share the same sample size, FSDs reduce to SLHDs. Detailed sampling properties of FSDs are derived, which cover the results for SLHDs in Qian (2012). Qian (2012) proved that, compared with independent LHDs, SLHDs enjoy smaller variance of linear combinations of the sample mean from different models in each slice. With the same assumption, we will show that FSDs lead to a further variance reduction. Simulations show that FSDs provide variance reduction compared with SLHDs in estimating linear combinations of the means of functions from different slices.

The aforementioned linear combination of the sample mean from different models in each slice is considered as an important estimator in sliced designs. In this paper, a central limit theorem is established for FSDs. It shows that any linear combination of the sample mean with different models on each slice follows an asymptotic normal distribution. No similar result has been given for sliced designs with multiple models yet. It covers the related result for sliced LHDs given by He and Qian (2015).

The paper is organized as follows. In Sect. 2, a general method for constructing FSDs is proposed. Section 3 derives sampling properties for FSDs and compares FSDs with other two alternative design schemes. A central limit theorem is established in Sect. 4. In Sect. 5, some simulations are given to support our theoretical results. Section 6 concludes this paper with some discussions. All proofs are given in "Appendix."

2 Constructing flexible FSDs

Before constructing FSDs, we introduce some commonly used definitions and notation. Let Z_n denote the set $\{1, \ldots, n\}$ for any positive integer n and $U(0, 1)$ be the uniform distribution on (0, 1). Let $Z_n \oplus p$ denote the set $\{1 + p, \ldots, n + p\}$. The least common multiple of k integers a_i, $i = 1, \ldots, k$, is denoted by $lcm(a_1, \ldots, a_k)$. In other words,

$$lcm(a_1, \ldots, a_k) = \min\{\, l \mid l > 0 \text{ and is a multiple of } a_i \text{ for any } 1 \le i \le k\}.$$

Let $|D|$ denote the sample size of a design D. A randomized Latin hypercube with n runs and m factors is an $n \times m$ matrix in which each column is an independent permutation on Z_n. An LHD of N runs constructed in McKay et al. (1979) is denoted by LHD(N). SLHDs with n N-run slices, denoted by SLHD(N, n), is a design scheme whose each slice is statistically equivalent to an ordinary LHD(N) and combined design is an LHD($N \times n$). For details of the SLHD(N, n), we refer to Qian (2012).

Consider an experiment containing $\sum_{i=1}^{k} n_i$ batches among which n_i batches have an sample size of N_i. Without loss of generality, $N_{i_1} \neq N_{i_2}$ for any $i_1 \neq i_2$. There are totally $\sum_{i=1}^{k} n_i$ batches and $\sum_{i=1}^{k} N_i n_i$ runs. To make it clear, consider an experiment with three batches for which the first two design $|D_{1,1}| = |D_{1,2}| = 6$ and the third slice $|D_{2,1}| = 4$. SLHDs are unavailable since the sizes of three slices are not same. To deal this situation, we provide three alternative schemes:

(i) ILs which contain $\sum_{i=1}^{k} n_i$ independent LHD of given sample sizes,
(ii) ISs which contain independent SLHD(N_i, n_i) for $i = 1, \ldots, k$,
(iii) FSDs generated in this paper.

Now we introduce the construction of FSDs. Given integers $k, n_1, \ldots, n_k$, and $N_1, \ldots, N_k$, let $l = lcm(N_1 n_1, \ldots, N_k n_k)$ and $n = \sum_{i=1}^{k} n_i$. The design matrix of an m-dimensional FSD containing n_i slices of N_i runs, for $i = 1, \ldots, k$, is constructed through following steps.

Step 1 Let $M = (m_{i,h})_{k \times l}$ be a $k \times l$ matrix whose hth column is a random permutation of $Z_k \oplus (h-1)k$.

Step 2 For $i = 1, \ldots, k$ and $q = 1, \ldots, N_i n_i$, draw $a_q^{(i)}$ from the discrete uniform distribution on $\{m_{i,(q-1)\lambda_i+1}, m_{i,(q-1)\lambda_i+2}, \ldots, m_{i,q\lambda_i}\}$ where $\lambda_i = \frac{l}{N_i n_i}$. Let $M^{(i)} = (m_{j,u}^{(i)})_{n_i \times N_i}$ be an $n_i \times N_i$ matrix whose uth column is a random permutation of $\{a_{(u-1)n_i+1}^{(i)}, \ldots, a_{un_i}^{(i)}\}$. Randomly permute the N_i elements of each row of $M^{(i)}$, the resulting matrix is still denoted by $M^{(i)}$.

Step 3 For $i = 1, \ldots, k$, $j = 1, \ldots, n_i$ and $u = 1, \ldots, N_i$, let

$$d_{i,j,u,1} = (kl)^{-1} \left(m_{j,u}^{(i)} - \varepsilon_{i,j,u} \right), \tag{1}$$

where $\varepsilon_{i,j,u}$'s are independent random variables following $U(0, 1)$.

Step 4 Repeat last three steps to generate $d_{i,j,u,2}, \ldots, d_{i,j,u,m}$. For $i = 1, \ldots, k$, $j = 1, \ldots, n_i$, let $D_{i,j} = (d_{i,j,u,v})_{N_i \times m}$ denote an $N_i \times m$ matrix where $u = 1, \ldots, N_i$ and $v = 1, \ldots, m$. Sequentially define $D_i = (D_{i,1}^T, \ldots, D_{i,n_i}^T)^T$ and $D = (D_1^T, \ldots, D_k^T)^T$.

When $k = n_1 = 1$, this algorithm gives the construction ordinary N_1-run LHDs. When $k = 1$, this construction is equivalent to that of SLHD(N_1, n_1). For details of the construction of LHDs and SLHDs, we refer to McKay et al. (1979) and Qian (2012), respectively. The whole design D contains $D_{i,j}$'s as n slices with arbitrary sample sizes. The FSD constructed above is denoted by FSD($N_1 \times n_1 + \cdots + N_k \times n_k$). To distinguish D_i's from $D_{i,j}$'s, we call them sub-designs and slices, respectively.

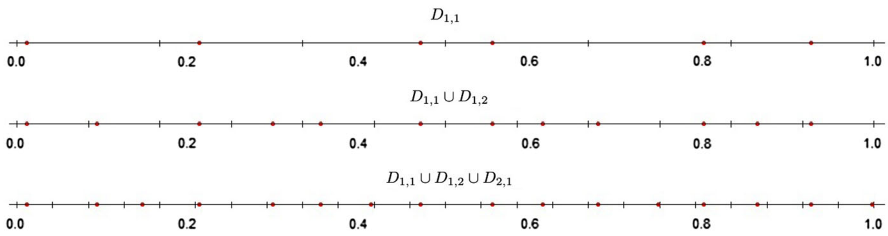

Fig. 1 Three plots of the distribution of design points in $D_{1,1}$, $D_{1,1} \cup D_{1,2}$, and $D_{1,1} \cup D_{1,2} \cup D_{2,1}$, respectively, in Example 1

Now we provide an example to illustrate the construction. Note that each dimension of the design is generated independently through the same processes, we only construct one-dimensional FSDs for illustration.

Example 1 Consider generating a one-dimensional FSD$(6 \times 2 + 4 \times 1)$. In this case, N_1=6, $n_1 = 2$, $N_2 = 4$, n_2=1, $k = 2$, $l = 12$, $\lambda_1 = 1$ and $\lambda_2 = 3$. Generate a 2×12 matrix M as

$$\begin{pmatrix} 1 & 3 & 6 & 8 & 9 & 12 & 14 & 15 & 17 & 20 & 21 & 23 \\ 2 & 4 & 5 & 7 & 10 & 11 & 13 & 16 & 18 & 19 & 22 & 24 \end{pmatrix}.$$

Then we have $(a_1^{(1)}, \ldots, a_{12}^{(1)}) = (1, 3, 6, 8, 9, 12, 14, 15, 17, 20, 21, 23)$ and generate $M^{(1)}$ as

$$\begin{pmatrix} 23 & 14 & 6 & 20 & 1 & 12 \\ 8 & 17 & 3 & 15 & 21 & 9 \end{pmatrix}.$$

Randomly generate $(a_1^{(2)}, \ldots, a_4^{(2)}) = (4, 10, 18, 24)$ and $M^{(2)} = (18, 24, 10, 4)$. By substituting $M^{(1)}$ and $M^{(2)}$ into construction (1), we generate $D_{1,1} = (0.926, 0.555, 0.213, 0.801, 0.012, 0.471)^T$, $D_{1,2} = (0.299, 0.678, 0.093, 0.613, 0.864, 0.354)^T$, and $D_{2,1} = (0.748, 0.998, 0.413, 0.146)^T$.

The design points generated in Example 1 are depicted in Fig. 1 to provide a visual approach to the design.

3 Sampling properties of FSDs

This section establishes a theoretical framework of the sampling properties for FSDs and compares FSDs with other two alternative design schemes. To provide some intuition of the space-filling properties of FSDs, we revisit Example 1 and Fig. 1. It can be easily seen that $D_{1,1}$ is an LHD(6), $D_{1,1}$ and $D_{1,2}$ are two slices of an SLHD(6,2), and the totally combined design $D_{1,1} \cup D_{1,2} \cup D_{2,1}$ has no two points falling in the same small interval of length 1/24. Now we discuss these space-filling properties theoretically.

Actually, an SLHD(N_1, n_1) is statistically equivalent to an FSD$(N_1 \times n_1)$. Thus, SLHDs constructed in Qian (2012) are special cases of FSDs and the general theories of FSDs cover He and Qian's (2015) related results.

Proposition 1 *For the FSD$(N_1 \times n_1 + \cdots + N_k \times n_k)$ constructed by our proposed algorithm, we have*

(i) *slice $D_{i,j}$ is statistically equivalent to an ordinary LHD(N_i),*
(ii) *sub-design $D_i = \cup_{j=1}^{n_i} D_{i,j}$ is statistically equivalent to an SLHD(N_i, n_i).*

Proposition 1 reveals that a sub-design D_i of $N_i n_i$ runs has the same statistical properties with an SLHD(N_i, n_i) proposed by Qian (2012). Next proposition gives the joint distribution of two design points from two different sub-designs D_{i_1} and D_{i_2} where $i_1 \neq i_2$. For $0 \leq r_1, r_2 \leq 1$ and a positive integer p, define $\delta_p(r_1, r_2) = 1$ if $\lceil pr_1 \rceil = \lceil pr_2 \rceil$ and $\delta_p(r_1, r_2) = 0$ if $\lceil pr_1 \rceil \neq \lceil pr_2 \rceil$.

Proposition 2 *For the FSD$(N_1 \times n_1 + \cdots + N_k \times n_k)$ constructed by our proposed algorithm, each point in D follows the uniform distribution on $[0, 1]^m$. Let $X_{i_1} = (x_{i_1,1}, \ldots, x_{i_1,m}) \in D_{i_1}$ and $X_{i_2} = (x_{i_2,1}, \ldots, x_{i_2,m}) \in D_{i_2}$ denote two design points, we have the joint density function of X_{i_1} and X_{i_2} as*

$$\left(\frac{k}{k-1}\right)^m \prod_{b=1}^{m} \left[\frac{k-1}{k} + \frac{1}{k}\delta_l(x_{i_1,b}, x_{i_2,b}) - \delta_{kl}(x_{i_1,b}, x_{i_2,b})\right], \tag{2}$$

where $i_1 \neq i_2$, $X_{i_1} = (x_{i_1,1}, \ldots, x_{i_1,m})$ and $X_{i_2} = (x_{i_2,1}, \ldots, x_{i_2,m})$.

Proposition 2 gives only the joint distribution of two points from different sub-designs. For the joint distribution of two point from the same sub-design, we refer to Lemma 1 in Qian (2012) for details since the sub-design D_i is statistically equivalent to an SLHD(N_i, n_i) generated in Qian (2012).

Lehmann (1966) introduced the concept of negatively quadrant dependent variables. Two random variables τ_1 and τ_2 are negatively quadrant dependent if $P(\tau_1 \leq v_1, \tau_2 \leq v_2) \leq P(\tau_1 \leq v_1)P(\tau_2 \leq v_2)$ for any v_1 and v_2. Proposition 3 shows that any two points from different sub-designs of an FSD are negatively quadrant dependent.

Proposition 3 *For the FSD$(N_1 \times n_1 + \cdots + N_k \times n_k)$ constructed by our proposed algorithm, given that $X_{i_1} = (X_{i_1,1}, \ldots, X_{i_1,m}) \in D_{i_1}$ and $X_{i_2} = (X_{i_2,1}, \ldots, X_{i_2,m}) \in D_{i_2}$ where $i_1 \neq i_2$, we have that $X_{i_1,b}$ and $X_{i_2,b}$ are negatively quadrant dependent for any $b \in Z_m$.*

With assumption on the monotonicity of $f^{(i,j)}$'s, it is known that negatively quadrant-dependent variables have a negative covariance (Lehmann 1966). This property is often used in variance comparison among different designs as in Theorem 1 from Qian (2012). We are now ready to compare FSDs with other two design schemes introduced in Sect. 2.

Consider an ensemble experiment using n similar computer models $\{f^{(1,1)}, \ldots, f^{(1,n_1)}, f^{(2,1)}, \ldots, f^{(2,n_2)}, \ldots, f^{(k,1)}, \ldots, f^{(k,n_k)}\}$, where $n = \sum_{i=1}^{k} n_i$. Slice $D_{i,j}$ is arranged to $f^{(i,j)}$. The inputs of these models follow the uniform measure on $[0, 1]^m$. For $1 \leq i \leq k$ and $1 \leq j \leq n_i$, define

$$\mu_{i,j} = E\{f^{(i,j)}(X)\} \quad \text{and} \quad \eta = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \lambda_{i,j}\mu_{i,j},$$

where $\lambda_{i,j}$'s are nonnegative real numbers and X is uniformly distributed on $[0, 1]^m$. We now move on to the estimation of $\mu_{i,j}$'s and η through FSDs. Throughout, $x = (x_1, x_2, \ldots, x_m)$ and $f^{(i,j)}(x)$'s are continuous on $[0, 1]^m$. Let $\mathrm{d}x_{-u} = \prod_{b \in Z_m \setminus u} \mathrm{d}x_b$ for any $u \subseteq Z_m$. Decompose $f^{(i,j)}$'s as

$$f^{(i,j)}(x) = \sum_{\emptyset \subseteq u \subseteq Z_m} f_u^{(i,j)}(x),$$

where $f_\emptyset^{(i,j)}(x) = \mu_{i,j}$ and $f_u^{(i,j)}(x)$ is the u-factor interaction of $f^{(i,j)}$ defined recursively by

$$f_u^{(i,j)}(x) = \int_{[0,1]^{m-|u|}} \left[f^{(i,j)}(x) - \sum_{v \subset u} f_v^{(i,j)}(x) \right] \mathrm{d}x_{-u}.$$

If only main effects are considered, $f^{(i,j)}$ can be decomposed as

$$f^{(i,j)}(x) = \mu_{i,j} + \sum_{b=1}^{m} f_b^{(i,j)}(x_b) + r_{i,j}(x), \tag{3}$$

where $r_{i,j}(x)$ is the residual containing all multivariate interactions of $f^{(i,j)}$. The unbiased estimators of $\mu_{i,j}$ and η are

$$\hat{\mu}_{i,j} = \frac{1}{N_i} \sum_{x \in D_{i,j}} f^{(i,j)}(x) \quad \text{and} \quad \hat{\eta} = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \lambda_{i,j} \hat{\mu}_{i,j},$$

respectively. It should be mentioned that these estimators are also unbiased in for IL and IS. This can be verified immediately from the sampling properties of IL and IS given in McKay et al. (1979) and Qian (2012). Theorem 1 compares the variance of these estimators from the three alternative schemes mentioned in Sect. 2.

Theorem 1 *For $1 \le i \le k$ and $1 \le j \le n_i$, the three alternative schemes share the same variance of $\hat{\mu}_{i,j}$'s, i.e.,*

$$\mathrm{Var}_{\mathrm{FSD}}(\hat{\mu}_{i,j}) = \mathrm{Var}_{\mathrm{IS}}(\hat{\mu}_{i,j}) = \mathrm{Var}_{\mathrm{IL}}(\hat{\mu}_{i,j}).$$

Suppose that $f^{(i,j)}$'s are all increasing (or all decreasing) in each argument x_b of x. For the variance of $\hat{\eta}$, we have

$$\mathrm{Var}_{\mathrm{FSD}}(\hat{\eta}) \le \mathrm{Var}_{\mathrm{IS}}(\hat{\eta}) \le \mathrm{Var}_{\mathrm{IL}}(\hat{\eta}).$$

Note that $\lambda_{i,j}$'s are nonnegative real numbers, Theorem 1 also compares the variance of $\hat{\mu}_i = \sum_j \lambda_{i,j} \hat{\mu}_{i,j}$ $(i = 1, \ldots, k)$ for the three design schemes by setting $\lambda_{r,j}$ $(r \neq i)$ to 0 as a special case of $\hat{\eta}$.

4 Central limit Theorem for FSDs

Before giving the central limit theorem for FSDs, we introduce the definition of Lipschitz continuous. A function f is called Lipschitz continuous if there exists a constant c such that for any two points x_1 and x_2 in $[0, 1]^m$, it always holds that $|f(x_1) - f(x_2)| \leq c \parallel x_1 - x_2 \parallel$, where $\parallel x_1 - x_2 \parallel$ represents the Euclidean distance between x_1 and x_2. In this section, we establish a central limit theorem for FSDs. The asymptotic distribution of $\hat{\eta}$ helps in providing confidence intervals.

Owen (1992) introduced the central limit theorem of LHDs. Compared with independent LHDs, different slices in FSDs have complex joint distributions. Thus, it is hard to establish a central limit theorem for elaborate space-filling designs. The following theorem gives the asymptotic distribution of $\hat{\eta}$ for FSDs which covers Theorem 8 in He and Qian (2015).

Theorem 2 *Assume that* (i) $f^{(i,j)}$*'s are Lipschitz continuous, and* (ii) k, $n_1, \ldots, n_k$ *are fixed and* N_{i_1}/N_{i_2} *is bounded as* $(N_1, \ldots, N_k) \to \infty$ *for any* $i_1 \neq i_2$. *For the FSD*$(N_1 \times n_1 + \cdots + N_k \times n_k)$ *constructed by our proposed algorithm, we have*

$$(\hat{\eta} - \eta) \Big/ \left(\int_{[0,1]^m} \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{\lambda_{i,j}^2}{N_i} r_{i,j}^2(x) \mathrm{d}x \right)^{1/2} \to N(0, 1)$$

as $(N_1, \ldots, N_k) \to \infty$.

Note that the SLHD(N_1, n_1) constructed in Qian (2012) is statistically equivalent to FSD$(N_1 \times n_1)$. Theorem 2 covers the central limit theorem for SLHDs in Theorem 8 in He and Qian (2015).

5 Simulations

In this section, we present three examples to illustrate the advantages of FSDs by comparing FSDs with two alternative schemes ILs and ISs. For convenience, ILs and ISs containing n_i slices of N_i runs for $i = 1, \ldots, k$ are denoted by IL$(N_1 \times n_1 + \cdots + N_k \times n_k)$ and IS$(N_1 \times n_1 + \cdots + N_k \times n_k)$, respectively. We will not compare these three alternative space-filling designs with IID sampling since even ILs outperform IID sampling.

Example 2 Consider the five-dimensional function in Drew and Homem-de Mello (2005):

$$f(x) = \log(x_1 x_2 x_3 x_4 x_5)$$

to act as a computer code whose input x follows a uniform distribution on $[0, 1]^5$. Two 6-run slices and one 4-run slice are available. Suppose $f^{(1,1)} = f^{(1,2)} = f^{(2,1)} = f$, $\lambda_{1,1} = \lambda_{1,2} = 0.3$ and $\lambda_{2,1} = 0.4$. Figure 1 presents the MSE (mean squared error) and distribution of $\hat{\eta}$ over the 10^5 replicates for ILs, ISs and FSDs, respectively. The distribution of $\hat{\eta}$ is compared with a normal distribution of the same mean and variance.

Figure 2 shows that FSDs provide variance reduction compared with ISs and fit the asymptotic normal distribution well. Figure 2 also reveals another interesting advantage of FSDs in this problem. However, the log function tends to $-\infty$ as $x \to 0$. Consider one-dimensional projection of these schemes. FSDs drop only one point in $[0, 24^{-1}]$, while other two schemes may contain more than one point in this interval. Thus, ISs and ILs are likely to give a heavy left tail distribution for the estimator compared with FSDs.

When a sophisticated integration problem is studied by multiple machines or places as batches, some of these batches may fail or encounter delay. In this case, FSDs generated in this paper provides a robust way to allocate computing resources. In the following example, we randomly drop one slice from the whole design to show the robustness of FSDs.

Example 3 Consider the experiment in Example 2. In each simulation, we randomly drop one slice and the sample mean estimator $\hat{\mu}$ is based on the rest two slices. Figure 3 presents the MSE and distribution of the sample mean estimator over the 10^5 replicates for ILs, ISs and FSDs, respectively.

Example 3 reveals that FSDs outperform ISs and ILs when some slices fail and so are robust. Next example consider a group of different functions used in Qian (2012). It illustrates the performance of FSDs when their different slices are arranged to different models based on similar mathematics.

Example 4 Consider two-dimensional functions in Qian (2012):

$$
\begin{aligned}
f^{(1,1)}(x) &= \log\left(\frac{1}{\sqrt{x_1}} + \frac{1}{\sqrt{x_2}}\right)\\
f^{(1,2)}(x) &= \log\left(\frac{0.98}{\sqrt{x_1}} + \frac{0.95}{\sqrt{x_2}}\right)\\
f^{(2,1)}(x) &= \log\left(\frac{1.02}{\sqrt{x_1}} + \frac{1.02}{\sqrt{x_2}}\right)
\end{aligned}
$$

where $x = (x_1, x_2)$ follows a uniform distribution on $[0, 1]^2$. Similar to that in Example 2, the experiment contains two 6-run slices and one 4-run slice. For $\lambda_{1,1} = \lambda_{1,2} = 0.3$ and $\lambda_{2,1} = 0.4$, Fig. 4 shows the MSE and distribution of $\hat{\eta}$ over the 10^5 replicates for ILs, ISs and FSDs, respectively. As depicted in 4, FSDs enjoy 18.42% variance reduction compared with ISs, which is greater than the 13.15% variance reduction from substituting ISs for ILs.

6 Discussion

In this paper, we propose flexible sliced designs (FSDs) for multi-slice computer experiments. Compared with existing sliced space-filling designs such as SLHDs in Qian (2012), FSDs permit different sample sizes for different slices. We derive a theoretical framework of the sampling properties of FSDs. Compared with two alternative

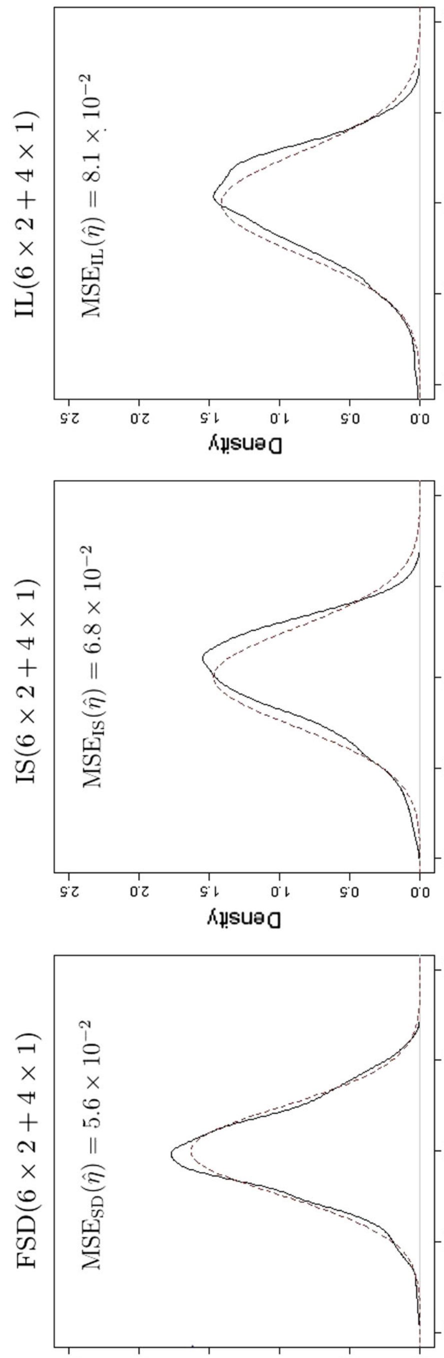

Fig. 2 Three plots of the distribution of $\hat{\eta}$ over the 10^5 replicates for FSD$(6 \times 2 + 4 \times 1)$, IS$(6 \times 2 + 4 \times 1)$ and IL$(6 \times 2 + 4 \times 1)$, respectively, in Example 2

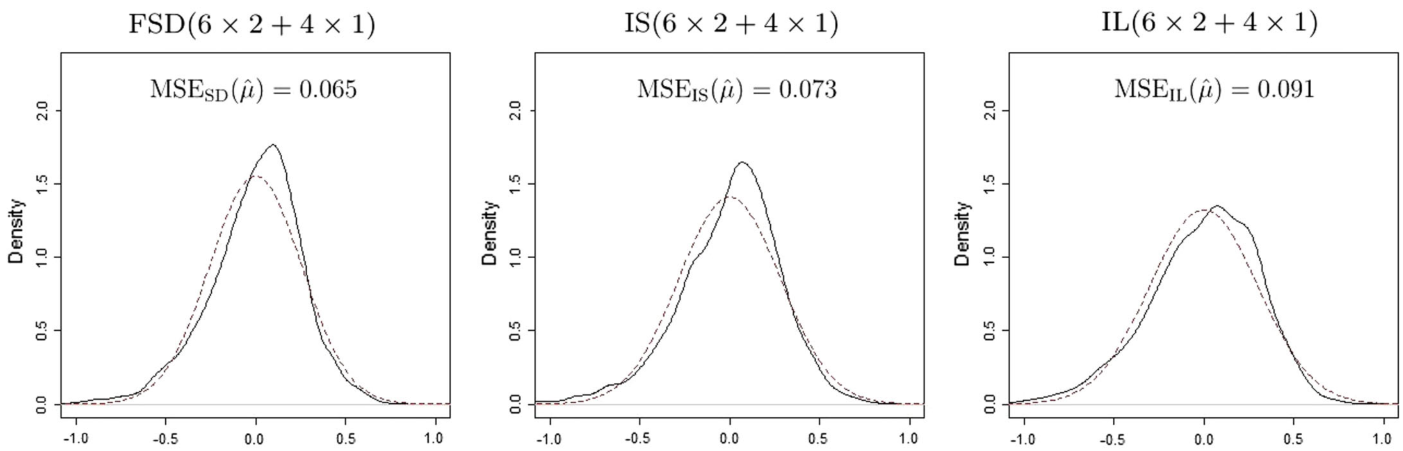

Fig. 3 Three plots of the distribution of $\hat{\mu} - \mu$ over the 10^5 replicates for FSD$(6 \times 2 + 4 \times 1)$, IS$(6 \times 2 + 4 \times 1)$ and IL$(6 \times 2 + 4 \times 1)$, respectively, in Example 3

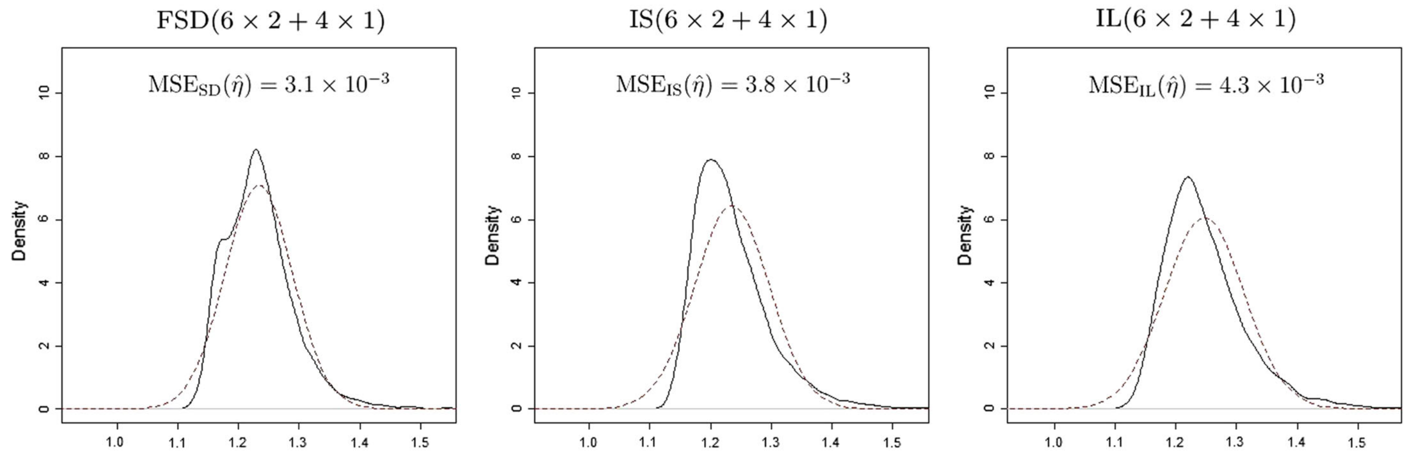

Fig. 4 Three plots of the distribution of $\hat{\eta}$ over the 10^5 replicates for FSD($6 \times 2 + 4 \times 1$), IS($6 \times 2 + 4 \times 1$) and IL($6 \times 2 + 4 \times 1$), respectively, in Example 4

schemes, FSDs permit a smaller variance of $\hat{\eta}$. The parameter η can be any linear combination of sample mean from different slices. A central limit theorem is established showing that $\hat{\eta}$ follows an asymptotic normal distribution.

FSDs can be further refined according to different criterion such as correlation control (Owen 1994) and maximin inter-site distance. Using the ranked Gram–Schmidt (RGS) algorithm (Owen 1994) for each slice, we can control the correlations of columns for FSDs (Morris and Mitchell 1995).

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Appendix: proofs of Propositions and Theorems

Proof of Proposition 1 First, we prove that $D_{i,j}$ is statistically equivalent to an ordinary LHD(N_i). Let $H = (h_{i,j})_{N\times m}$ be the design matrix of an experiment. Let $h_{(1),j}, \ldots, h_{(N),j}$ denote the ordered statistics of $h_{1,j}, \ldots, h_{N,j}$. Review the construction of LHD(N_i). Simple analysis shows that if (i) $h_{1,j}, \ldots, h_{N,j}$ is a random permutation of $h_{(1),j}, \ldots, h_{(N),j}$, (ii) $h_{i,j}$ follows the uniform distribution on $(\frac{i-1}{N}, \frac{i}{N}]$, and (iii) each column is generated independently, and then design H is statistically equivalent to an ordinary LHD(N). For the design matrix $D_{i,j}$ given in our algorithm, the columns are generated independently. Let $d_{i,j,(1),v}, \ldots, d_{i,j,(N_i),v}$ denote the ordered statistics of $d_{i,j,1,v}, \ldots, d_{i,j,N_i,v}$. The random permutation of each row of $M^{(i)}$ reveals that the second condition is satisfied. It is now sufficient to show that $d_{i,j,(u),v}$ follows the uniform distribution on $(\frac{u-1}{N_i}, \frac{u}{N_i}]$ for $u = 1, \ldots, N_i$. Simple analysis shows that, before the row-element permutation, we have (i) $m^{(i)}_{j,u}$ follows the discrete uniform distribution on $\{a^{(i)}_{(u-1)n_i+b_1} : b_1 = 1, \ldots, n_i\}$, (ii) $a^{(i)}_{(u-1)n_i+b_1}$ follows the discrete uniform distribution on $\{m_{i,[(u-1)n_i+b_1-1]\lambda_i+b_2} : b_2 = 1, \ldots, \lambda_i\}$ and (iii) $m_{i,[(u-1)n_i+b_1-1]\lambda_i+b_2}$ follows the discrete uniform distribution on $Z_k \oplus \{[(u-1)n_i + b_1 - 1]\lambda_i + b_2 - 1\}k$. Thus, $m^{(i)}_{j,u}$ follows the uniform distribution on $\{\frac{kl}{N_i n_i}(u-1)+1, \frac{kl}{N_i n_i}(u-1)+2, \ldots, \frac{kl}{N_i n_i}u\}$. From Eq. (1), we know that $d_{i,j,(1),v}$ follows the uniform distribution on $(\frac{u-1}{N_i}, \frac{u}{N_i}]$ for $u = 1, \ldots, N_i$, which completes the proof. □

Then we prove that D_i is statistically equivalent to an SLHD(N_i, n_i). Review the construction of SLHD(N_i, n_i). An SLHD(N_i, n_i) is statistically equivalent to a n_i-slice design which (i) each slice is statistically equivalent to an ordinary LHD(N_i), and (ii) the combined design is an LHD($N_i n_i$). $D_{i,j}$ is statistically equivalent to LHD(N_i) and the combined design of all $D_{i,j}$'s is also an LHD since matrix $\lceil D_i \cdot N_i n_i \rceil$ is an $N_i n_i$-row Latin hypercube. And Proposition 1 right follows.

Proof of Proposition 2 The uniform distribution of each design point is trivial and so omitted here. We move on to the joint distribution of X_{i_1} and X_{i_2}. Note that the m

dimensions are generated independently. Consider only the one-dimensional projection of the design.

In Step 1 of construction (1), we actually divide [0, 1] to kl intervals. Given $X_{i_1} = (x_{i_1,1}, \ldots, x_{i_1,m})$, we know that there exists $j_1 \in Z_{n_{i_1}}$ and $u_1 \in Z_{N_{i_1}}$ such that $d_{i_1,j_1,u_1,1} = x_{i_1,1}$. Similarly, there exists $j_2 \in Z_{n_{i_2}}$ and $u_2 \in Z_{N_{i_2}}$ such that $x_{i_2,1} = d_{i_2,j_2,u_2,1}$. Let $a_{i_1} = \lceil d_{i_1,j_1,u_1,1} \cdot kl \rceil$. First, we figure out the distribution of $d_{i_2,j_2,u_2,1}$ conditional on $x_{i_1,1}$. Let R_{i_2} denote the i_2th row of the matrix M and be *random* conditional on a_{i_1}. For an arbitrary integer $b \in Z_{kl}$, simple analysis reveals that
Case 1 $P(b \in R_{i_2}) = 0$ if $b = a_{i_1}$;
Case 2 $P(b \in R_{i_2}) = \frac{1}{k-1}$ if $b \neq a_{i_1}$ and $\lceil \frac{b}{k} \rceil = \lceil \frac{a_{i_1}}{k} \rceil$;
Case 3 $P(b \in R_{i_2}) = \frac{1}{k}$ if $\lceil \frac{b}{k} \rceil \neq \lceil \frac{a_{i_1}}{k} \rceil$.

Review the construction process given in Steps 2 and 3. Similar analysis as that in the proof of Proposition 1 reveals that, if $b \in R_{i_2}$, then the $P(m^{(i_2)}_{j_2,u_2} = b) = l^{-1}$. From Eq. (1), we know $d_{i_2,j_2,u_2,1}$ follows the uniform distribution on $(\frac{m^{(i_2)}_{j_2,u_2}-1}{kl}, \frac{m^{(i_2)}_{j_2,u_2}}{kl}]$ In Step 2, a is chosen with a uniform probability of $\frac{N_i n_i}{l}$. Thus, for any $b \in Z_{kl}$, the conditional density function of $d_{i_2,j_2,u_2,1}$ on $(\frac{b-1}{kl}, \frac{b}{kl}]$ is

$$P(b \in R_{i_2}) \cdot P(m^{(i_2)}_{j_2,u_2} = b) \cdot kl = k \cdot P(b \in R_{i_2}).$$

Note that the single-point distribution of $X_{i_1,1}$ is the uniform distribution on (0, 1]. This immediately gives the one-dimensional joint distribution of $X_{i_1,1}$ and $X_{i_2,1}$ as

$$\frac{k}{k-1}\left[\frac{k-1}{k} + \frac{1}{k}\delta_l(x_{i_1,1}, x_{i_2,1}) - \delta_{kl}(x_{i_1,1}, x_{i_2,1})\right].$$

The conditional density function of X_{i_2} given X_{i_1} right follows. □

Proof of Proposition 3 Let $\lfloor r \rfloor$ denote the largest integer not greater than a real number r. Without loss of generality, assume $v_1 \le v_2$. From Eq. 4, $P(X_{i_1,1} \le v_1, X_{i_2,1} \le v_2)$ can be calculated as

$$\begin{aligned}
&\int_0^{v_1}\int_0^{v_2} \frac{k}{k-1}\left[\frac{k-1}{k} + \frac{1}{k}\delta_l(x_{i_1,1}, x_{i_2,1}) - \delta_{kl}(x_{i_1,1}, x_{i_2,1})\right] \mathrm{d}x_{i_1,1}\mathrm{d}x_{i_2,1} \\
&\quad = v_1 v_2 + \frac{k}{k-1}\int_0^{v_1}\int_0^{v_2}\left[\frac{1}{k}\delta_l(x_{i_1,1}, x_{i_2,1}) - \delta_{kl}(x_{i_1,1}, x_{i_2,1})\right] \mathrm{d}x_{i_1,1}\mathrm{d}x_{i_2,1}. \qquad (4)
\end{aligned}$$

Note that $X_{i_1,1}$ and $X_{i_2,1}$ Then $P(X_{i_1,1} \le v_1, X_{i_2,1} \le v_2) - P(X_{i_1,1} \le v_1)P(X_{i_2,1} \le v_2)$ can be calculated as Let $\lambda = \lfloor l v_1 \rfloor$, where $\lfloor r \rfloor$ is the largest integer not greater than r. Let $\widetilde{v}_1 = v_1 - l^{-1}\lambda$ and $\widetilde{v}_2 = v_2 - l^{-1}\lambda$. Note that for any positive integer b and $x_{i_2,1}$, we have

$$\int_{((b-1)l^{-1}, bl^{-1}]}\left[\frac{1}{k}\delta_l(x_{i_1,1}, x_{i_2,1}) - \delta_{kl}(x_{i_1,1}, x_{i_2,1})\right] \mathrm{d}x_{i_1,1} = 0.$$

So integral (4) can be rewritten as

$$\frac{k}{k-1}\int_0^{\widetilde{v}_1}\int_0^{\widetilde{v}_2}\left[\frac{1}{k}\delta_l(x_{i_1,1},x_{i_2,1})-\delta_{kl}(x_{i_1,1},x_{i_2,1})\right]\mathrm{d}x_{i_1,1}\mathrm{d}x_{i_2,1}. \tag{5}$$

Case 1 $\widetilde{v}_2 \geq \frac{1}{l}$. The integral equals 0.
Case 2 $0 \leq \widetilde{v}_2 \leq \frac{1}{l}$ and $\lceil x_{i_1,1}\cdot kl\rceil \neq \lceil x_{i_2,1}\cdot kl\rceil$. The integral equals $k^{-1}\widetilde{v}_1(\widetilde{v}_2-l^{-1}) \leq 0$.
Case 3 $0 \leq \widetilde{v}_2 \leq \frac{1}{l}$ and $\lceil x_{i_1,1}\cdot kl\rceil = \lceil x_{i_2,1}\cdot kl\rceil$. Let $p=\lfloor\widetilde{v}_2\cdot kl\rfloor=\lfloor\widetilde{v}_1\cdot kl\rfloor$, $r_1=\widetilde{v}_1\cdot kl-p$ and $r_2=\widetilde{v}_2\cdot kl-p$. The integral equals to $\frac{(r_1+p)(r_2+p)l}{(kl)^3}-\frac{p+r_1r_2}{(kl)^2}$. Note that $k\geq p+1$. The integral is no greater than $-\frac{p(1-r_1)(1-r_2)}{(p+1)(kl)^2}\leq 0$.

Thus, integral (5) is no greater than 0, which completes the proof. □

Proof of Theorem 1 For $i_1 \neq i_2$, let $X_{(i_1,j_1)}$ and $X_{(i_2,j_2)}$ denote design points from two different slices D_{i_1,j_1} and D_{i_2,j_2}, respectively. By Theorem 1 of Lehmann (1966), Proposition 3 and the assumption on $f^{(i,j)}$'s yield that

$$\mathrm{Cov}_{\mathrm{FSD}}\left[f^{(i_1,j_1)}\left(X_{(i_1,j_1)}\right), f^{(i_2,j_2)}\left(X_{(i_2,j_2)}\right)\right]\leq 0. \tag{6}$$

Consider $\hat{\eta}=\sum_{i=1}^{k}\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}$. By combining Proposition 1 with Theorem 1 in Qian (2012), we have $\mathrm{Var}_{\mathrm{FSD}}(\hat{\mu}_{i,j})=\mathrm{Var}_{\mathrm{IL}}(\hat{\mu}_{i,j})=\mathrm{Var}_{\mathrm{IS}}(\hat{\mu}_{i,j})$ since each slice of these designs is statistically equivalent to an ordinary LHD(N_i), and

$$\mathrm{Var}_{\mathrm{FSD}}\left(\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}\right)=\mathrm{Var}_{\mathrm{IS}}\left(\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}\right)\leq \mathrm{Var}_{\mathrm{IL}}\left(\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}\right). \tag{7}$$

Note that $\hat{\eta}$ is an unbiased estimator of η for these three schemes. By combining (6) and (7), we have

$$\begin{aligned}\mathrm{Var}_{\mathrm{FSD}}(\hat{\eta})&=\sum_{i=1}^{k}\mathrm{Var}_{\mathrm{FSD}}\left(\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}\right)\\&\quad+\sum_{i_1\neq i_2}\sum_{j_1=1}^{n_{i_1}}\sum_{j_2=1}^{n_{i_2}}\sum_{X\in D_{i_1,j_1}}\sum_{Y\in D_{i_2,j_2}}\mathrm{Cov}_{\mathrm{FSD}}\left[f^{(i_1,j_1)}(X), f^{(i_2,j_2)}(Y)\right]\\&\leq\sum_{i=1}^{k}\mathrm{Var}_{\mathrm{IS}}\left(\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}\right)=\mathrm{Var}_{\mathrm{IS}}(\hat{\eta})\\&\leq\sum_{i=1}^{k}\mathrm{Var}_{\mathrm{IL}}\left(\sum_{j=1}^{n_i}\lambda_{i,j}\hat{\mu}_{i,j}\right)=\mathrm{Var}_{\mathrm{IL}}(\hat{\eta}),\end{aligned}$$

which completes the proof. □

Proof of Theorem 2 For the FSD($N_1 \times n_1 + \cdots + N_k \times n_k$) and $i = 1, \ldots, k$, define a group of functions $\phi_i : (0, 1) \to (0, 1)$ as

$$\phi_i(y) = \{ykl - \lfloor ykl \rfloor + \lfloor yN_i \rfloor\}/N_i.$$

For $x = (x_1, \ldots, x_m)$, let $\Phi_i(x) = (\phi_i(x_1), \ldots, \phi_i(x_m))$. For the FSD($N_1 \times n_1 + \cdots + N_k \times n_k$), let

$$D^*_{i,j} = \{\Phi_i(x), x \in D_{i,j}\}.$$

Simple analysis shows that $D^*_{i,j}$'s are statistically equivalent to $\sum_{i=1}^k n_i$ independent LHDs with the same sample size.

For $1 \le i \le k$ and $1 \le j \le n_i$, let

$$\hat{\mu}^*_{i,j} = \sum_{x \in D^*_{i,j}} f^{(i,j)}(x) \quad \text{and} \quad \hat{\eta}^* = \sum_{i=1}^{k} \sum_{j=1}^{n_i} \lambda_{i,j} \hat{\mu}^*_{i,j}.$$

Note that $0 < a < \frac{N_{i_1}}{N_{i_2}} < b$ as $N_i \to \infty$ and $D^*_{i,j}$'s are independent designs. From Theorem 1 in Owen (1992), we have

$$(\hat{\eta}^* - \eta) / \left(\int_{[0,1]^m} \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{\lambda^2_{i,j}}{N_i} r^2_{i,j}(x) \mathrm{d}x \right)^{1/2} \to N(0, 1) \tag{8}$$

as $N_i \to \infty$. For any $X_i \in D_i$, we have $||X_i - \Phi_i(X_i)|| = O(N_i^{-1})$. Note that $f^{(i,j)}$'s are Lipschitz continuous. We have

$$\frac{1}{N_i} \sum_{X \in D_{i,j}} \left[f^{(i,j)}(X) - f^{(i,j)}(\Phi_i(X)) \right] = O\left(N_i^{-1}\right). \tag{9}$$

From Eq. (9), a simple calculation reveals that

$$(\hat{\eta} - \hat{\eta}^*) / \left(\int_{[0,1]^m} \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{\lambda^2_{i,j}}{N_i} r^2_{i,j}(x) \mathrm{d}x \right)^{1/2} = o(1). \tag{10}$$

Let $\{X_n\}$ and $\{Y_n\}$ be sequences of random variables. The Slutsky's theorem says that if X_n converges in distribution to a random element X, and Y_n converges in probability to a constant c, then $X_n + Y_n$ converges in distribution to $X + c$. By combining (8), (10) and the Slutsky's theorem, we have

$$(\hat{\eta} - \eta) \Big/ \left(\int_{[0,1]^m} \sum_{i=1}^{k} \sum_{j=1}^{n_i} \frac{\lambda_{i,j}^2}{N_i} r_{i,j}^2(x) \mathrm{d}x \right)^{1/2} \to N(0, 1),$$

which completes the proof. □

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