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A GENERAL THEORY FOR ORTHOGONAL ARRAY BASED LATIN HYPERCUBE SAMPLING

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Abstract: Orthogonal array based Latin hypercube sampling (LHS) is popularly adopted for computer experiments. Because of its stratification on multivariate margins in addition to univariate uniformity, the associated samples may provide better estimators for the gross mean of a complex function on a domain. In this paper, for some LHS methods based on an orthogonal array of strength t, a unified expression of the variance of the sample mean is developed by introducing a new discrete function. An approximate estimator for the variance of the sample mean is also established that is helpful in obtaining the confidence interval of the gross mean. We extend these statistical properties to three types of LHS: strong orthogonal array-based LHS, nested orthogonal array-based LHS, and correlation-controlled orthogonal array-based LHS. Some simulations are given to verify our results.

Key words and phrases: Functional decomposition, Latin hypercube sampling, orthogonal array, statistical property.

1. Introduction

Let $f(x)$ be a real function defined on the unit cube $[0,1)^m$. Consider its gross mean $\mu = \int_{[0,1)^m} f(x)dx$. After sampling n design points $\{X_1, \ldots, X_n\}$ in $[0,1)^m$, we can use $\hat{\mu} = n^{-1}\sum_{i=1}^n f(X_i)$ to estimate μ. For the independent and identically distributed (iid) sample with each point following a uniform distribution on $[0,1)^m$, the variance of $\hat{\mu}$ can be calculated by

$$\mathrm{var}(\hat{\mu}) = n^{-1}\mathrm{var}(f(X_1)) = n^{-1}\int_{[0,1)^m}[f(x)-\mu]^2 dx. \tag{1.1}$$

In order to obtain a better estimator of μ, McKay, Beckman, and Conover (1979) proposed Latin hypercube sampling (LHS) which can achieve maximum stratification in univariate margins. Stein (1987) provided an elaborate expression of $\mathrm{var}(\hat{\mu})$ if LHS is adopted, and further showed that the LHS can filter out the variance components of main effects of the function $f(x)$ and offer a more precise estimator of μ compared with the iid sampling.

Later, Tang (1993) independently introduced LHS based on an orthogonal array (OA), called U-designs hereafter. These U-designs not only preserve univariate uniformity, but also achieve stratifications in multivariate margins. Moreover, Tang (1993) showed that a U-design can filter out one- and two-dimensional variance components from $\mathrm{var}(\hat{\mu})$ if an OA of strength two is applied. Almost simultaneously, Owen (1994) derived a similar formula for $\mathrm{var}(\hat{\mu})$ for randomized orthogonal arrays (ROAs). It reveals that the variance components of all g-factor interactions of $f(x)$, $g \leq t$, are removed when an OA of strength t is employed. Tang's (1993) derivation of $\mathrm{var}(\hat{\mu})$ is based on a conditional density function, whose complexity grows quickly as the strength of the OA increases. Moreover, the structure of OA-based LHS is more sophisticated than that of the ROAs in Owen (1994). Thus, both methods cannot be adopted for U-designs based on OAs of higher strength or other types of OA-based LHS.

In this paper, we extend Tang's (1993) theoretical result to any U-design based on an OA of any strength. As in Owen (1994), a unified decomposition of $\mathrm{var}(\hat{\mu})$ is developed. The derivation is based on a new discrete function and is not a trivial extension of Tang's (1993) and Owen's (1994) analysis. Furthermore, we provide an approximate estimator of $\mathrm{var}(\hat{\mu})$ through introducing some consistent estimators of the lower-order interactions. Thus, an approximate confidence interval for μ can be established if a U-design is applied.

The remainder of this paper is as follows. Section 2 presents some definitions and preliminaries. In Section 3, by using the technique of functional decomposition, a unified expression of $\mathrm{var}(\hat{\mu})$ is derived for U-designs based on an OA of any strength; This covers Tang's (1993) result as a special case. Some consistent estimators for these lower-order interactions are provided in order to establish an approximate confidence interval of the gross mean. Section 4 extends these statistical properties to other types of sampling methods: strong orthogonal array (SOA) based LHS (He and Tang (2013)), nested orthogonal array (NOA) based LHS (He and Qian (2011)), and correlation-controlled OA-based LHS (Chen and Qian (2014)). Some simulations are given to support our results in Section 5. Section 6 concludes this paper with some discussions. All proofs are given in the Appendix.

2. Definitions and Preliminaries

An orthogonal array (OA) with n runs, m factors, and strength t ($1 \leq t \leq m$), denoted by $OA(n, s^m, t)$, is an $n \times m$ matrix in which each column contains s levels from $\{1, \ldots, s\}$ and all possible level combinations occur equally often as rows in every $n \times t$ submatrix. For convenience, we define $\lambda = n/s^t$. According to Owen (1994), an $OA(n, s^m, t)$ is called free of coincidence defect if no two rows agree in its any $t+1$ columns.

Let Z_m denote the set $\{1,\ldots,m\}$ for any positive integer m and $U(0,1]$ be the uniform distribution on $(0,1]$. For an $OA(n,s^m,t)$ A, a U-design $D=\{X_1,\ldots,X_n\}$ based on A can be constructed in the following steps, as described in Tang (1993).

Step 1. For each column of A, relabel the s levels with a random permutation of Z_s.

Step 2. For $j=1,\ldots,m$ and $e=1,\ldots,s$, replace the ns^{-1} positions of e in the jth column of A with a random permutation of $Z_{ns^{-1}}$. Denote by $B=(b_{ij})_{n\times m}$ the resulting array from A after such replacements.

Step 3. For $i=1,\ldots,n$ and $j=1,\ldots,m$, let

$$X_{ij}=s^{-1}(a_{ij}-1)+n^{-1}(b_{ij}-\varepsilon_{ij}), \tag{2.1}$$

where a_{ij} is the (i,j)-th entry of A and ε_{ij}'s are independent random variables following $U(0,1]$.

Thus, a U-design D is constructed by collecting the design points $X_i=(X_{i1},\ldots,X_{im})^T$ for $i=1,\ldots,n$. By noting that $ns^{-1}(a_{ij}-1)+b_{ij}$ is a discrete random variable that is uniform distribution on Z_n, it is known that X_{ij} is uniformly distributed on $[0,1)$ and $X_i=(X_{i1},\ldots,X_{im})$ is uniformly on $[0,1)^m$. The sample mean $\hat{\mu}$ is unbiased for μ. If we remove Step 2 and replace formula (2.1) with $X_{ij}=s^{-1}(a_{ij}-\varepsilon_{ij})$ in Step 3, then the above construction procedure reduces to the procedure for constructing an ROA.

Without loss of clearness, let $|u|$ be the cardinality of u if u is a set. Throughout, $x=(x_1,x_2,\ldots,x_m)$. Let $dx_{-u}=\prod_{i\in Z_m\setminus u}dx_i$ for any $u\subseteq Z_m$. Owen (1994) decomposed the function $f(x)$ as

$$f(x)=\sum_{\emptyset\subseteq u\subseteq Z_m} f_u(x), \tag{2.2}$$

where $f_\emptyset(x)=\mu$ and $f_u(x)$ is the u-factor interaction defined recursively by

$$f_u(x)=\int_{[0,1)^{m-|u|}}[f(x)-\sum_{v\subset u} f_v(x)]dx_{-u}. \tag{2.3}$$

It can be verified that $\int_{[0,1)^m} f_u(x)dx=0$ for any nonempty set $u\subseteq Z_m$ and $\int_{[0,1)^m} f_u(x)f_v(x)dx=0$ for any $u,v\subseteq Z_m$ with $u\neq v$.

For convenience, take

$$\sigma_u^2=\int_{[0,1)^m} f_u^2(x)dx \tag{2.4}$$

for any nonempty $u \subseteq Z_m$. By (1.1) and (2.2), it follows that $\mathrm{var}(\hat{\mu}) = n^{-1} \sum_{|u|>0} \sigma_u^2$ for an iid n-point sample. For a U-design based on an $OA(n, s^m, 2)$ with $n = s^2$, Tang (1993) proved that

$$\mathrm{var}(\hat{\mu}) = n^{-1} \sum_{|u|>2} \sigma_u^2 + o(n^{-1}).$$

For an ROA based on an $OA(n, s^m, t)$ free of coincidence defect, Owen (1994) showed that

$$\mathrm{var}(\hat{\mu}) = n^{-1} \sum_{|u|>t} \sigma_u^2 + o(n^{-1}).$$

Throughout we assume that the function $f(x)$ is continuous.

3. A General Theory for U-designs

3.1. Statistical properties for U-designs

Let $\Omega = [0,1)^m$ and $\mathcal{F}$ be the collection of all Borel sets in $[0,1)^m$. Let $\mathcal{Q} = \{[0, s^{-1}), [s^{-1}, 2s^{-1}), \ldots, [1 - s^{-1}, 1)\}$. For any $u \subseteq Z_m$, let $\prod_{j \in u} Q_j$ be the subset $\{x \in [0,1)^m : x_j \in Q_j, j \in u\}$ of $[0,1)^m$, where $Q_j \in \mathcal{Q}$ for all $j \in u$. Let $\sigma(\mathcal{Q}^u)$ denote the smallest σ-field containing all elements in $\{\prod_{j \in u} Q_j : Q_j \in \mathcal{Q}\}$. It is easily shown that $E[f(x)|\sigma(\mathcal{Q}^u)]$ is a discrete function on $[0,1)^m$ which takes on the value $s^{|u|} \int_{\prod_{j \in u} Q_j} f(z)dz$ if $x \in \prod_{j \in u} Q_j$.

Let $\bar{f}(x) = E[f(x)|\sigma(\mathcal{Q}^{Z_m})]$ for simplification. Since $\bar{f}(x)$ is a constant on each cell of $\prod_{j \in Z_m} Q_j$, Owen's (1994) result about ROAs can be used to analyze the variance of the sample mean of $\bar{f}(x)$.

Similar to (2.3), let $\bar{f}_u(x)$ be the u-factor interaction in $\bar{f}(x)$. We can obtain a connection between $f_u(x)$ and $\bar{f}_u(x)$.

Lemma 1. *We have (i) $\bar{f}_u(x) = E[f_u(x)|\sigma(\mathcal{Q}^u)]$; (ii) $f_u(x) \to \bar{f}_u(x)$ as $s \to \infty$.*

For any $u \subseteq Z_m$ and a given $OA(n, s^m, t)$ $A = (a_{ij})$, let $\omega_{ik}(u) = \{j \in u : a_{ij} = a_{kj}\}$ and $M(u, r) = \sum_{i,k=1}^{n} \mathbf{1}_{\{|\omega_{ik}(u)|=r\}}$, where $\mathbf{1}_{\{\cdot\}}$ is the indicator function. Based on Lemma 1, we can obtain the result of Owen (1994) for ROAs.

Theorem 1. *For a U-design based on $OA(n, s^m, t)$ A with $n = \lambda s^t$, as $s \to \infty$ with λ fixed, we have*

$$\mathrm{var}(\hat{\mu}) = n^{-2} \sum_{|u|>t} \sum_{r=0}^{|u|} M(u,r)(1-s)^{r-|u|} \sigma_u^2 + o(n^{-1}).$$

Furthermore, if A is free of coincidence defect, the above formula can be simplified as

$$\mathrm{var}(\hat{\mu}) = n^{-1} \sum_{|u|>t} \sigma_u^2 + o(n^{-1}). \tag{3.1}$$

3.2. Estimation of $f_u(x)$

In this subsection, we estimate the functions $f_u(x)$'s for all $u \subseteq Z_m$ with $|u| < t$ and analyze the related asymptotic property when a U-design is adopted. Since $f(x) = \sum_{\emptyset \subseteq u \subseteq Z_m} f_u(x)$, it is obvious that a better estimation of $f_u(x)$'s for all $u \subseteq Z_m$ with $|u| < t$ will help us to get closer to $f(x)$.

For an $OA(n, s^m, t)$ A free of coincidence defect, let $D = \{X_1, \ldots, X_n\}$ be the U-design based on A via the three steps in (2.1). For any $u \subseteq Z_m$, let

$$g_u(x) = \int_{[0,1)^{m-|u|}} \bar{f}(x) dx_{-u}. \tag{3.2}$$

By Lemma 1, $g_u(x)$ is a discrete function closely approximating the component $\int_{[0,1)^{m-|u|}} f(x) dx_{-u}$ of the function $f_u(x)$ in (2.3).

Let $\lceil a \rceil$ as the smallest integer not smaller than a. For any $x = (x_1, \ldots, x_m)$ in $[0, 1)^m$ and any $u \subseteq Z_m$ with $|u| < t$, take $\gamma(x, u) = \{i : \lceil sX_{ij} \rceil = \lceil sx_j \rceil$ for all $j \in u\}$. By (3.2), a naive estimator of $g_u(x)$ is

$$\hat{g}_u(x) = \frac{1}{ns^{-|u|}} \sum_{i \in \gamma(x,u)} \bar{f}(X_i). \tag{3.3}$$

According to (2.3), (3.2), and (3.3), the estimators of $f_u(x)$'s ($|u| < t$) can be given inductively as follows. First, the gross mean $f_\emptyset(x)$ is estimated by

$$\hat{f}_\emptyset(x) = \frac{1}{n} \sum_{i=1}^{n} f(X_i).$$

Then the higher-order interactions $f_u(x)$'s ($0 < |u| < t$) are estimated recursively by

$$\hat{f}_u(x) = \frac{1}{ns^{-|u|}} \sum_{i \in \gamma(x,u)} f(X_i) - \sum_{v \subset u} \hat{f}_v(x).$$

We turn to the asymptotic property of the estimator $\hat{f}_u(x)$.

Lemma 2. *For a U-design based on an $OA(n, s^m, t)$ free of coincidence defect with $n = \lambda s^t$, as $s \to \infty$ with λ fixed, we have*

$$n^{1/2} s^{-|u|/2} (\hat{g}_u(x) - g_u(x)) \to N(0, c(f)) \tag{3.4}$$

for any $u \subseteq Z_m$ with $|u| < t$, where $c(f)$ is a constant depending only on the function $f(\cdot)$.

Theorem 2. *For a U-design based on an $OA(n, s^m, t)$ free of coincidence defect with $n = \lambda s^t$, as $s \to \infty$ with λ fixed, we have*

$$n^{1/2} s^{-|u|/2} (\hat{f}_u(x) - \bar{f}_u(x)) \to N(0, c(f)) \tag{3.5}$$

for any $u \subseteq Z_m$ *with* $|u| < t$*, where* $c(f)$ *is a constant depending only on the function* $f(\cdot)$*.*

3.3. Estimation of var($\hat{\mu}$)

In this subsection, we provide an estimator of $\mathrm{var}(\hat{\mu})$ when a U-design is adopted and then use it to establish an approximate confidence interval of the gross mean μ.

Using the estimator $\hat{f}_u(x)$ of $f_u(x)$ provided in Section 3.2, we propose to estimate σ_u^2 by

$$\hat{\sigma}_u^2 = s^{-|u|} \sum_{i_1,\ldots,i_{|u|}=1}^{s} [\hat{f}_u((i_1 - 0.5)s^{-1}, \ldots, (i_{|u|} - 0.5)s^{-1})]^2$$

for any $u \subseteq Z_m$ with $0 < |u| < t$. By Theorem 2, the following result is immediate.

Theorem 3. *For a* U*-design based on an* $OA(n, s^m, t)$ *free of coincidence defect with* $n = \lambda s^t$*, as* $s \to \infty$ *with* λ *fixed, we have*

$$\hat{\sigma}_u^2 = \int_{[0,1)^m} \bar{f}_u^{\,2}(x)dx + O_p(n^{-1/2}s^{|u|/2}) = \sigma_u^2 + o_p(1)$$

for any $u \subseteq Z_m$ *with* $0 < |u| < t$*.*

Let $\sigma^2 = \int_{[0,1)^m}[f(x) - \mu]^2 dx$. By (2.2), we have $\sigma^2 = \sum_{\emptyset \subset u \subseteq Z_m} \sigma_u^2$. It is well known that the sample variance $\hat{\sigma}^2 = (n-1)^{-1} \sum_{i=1}^{n} [f(X_i) - \hat{\mu}]^2$ is an unbiased estimator of σ^2 for an iid n-point sample. For a U-design based on an $OA(n, s^m, t)$ free of coincidence defect, it follows directly from Lemma 4.2 of He and Qian (2014) that $\hat{\sigma}^2 = \sigma^2 + O_p(n^{-1/2})$. The ratio $S_u = \hat{\sigma}_u^2/\hat{\sigma}^2$ can be used in variable selection because it can be interpreted as a measure of the importance of the u-factor interaction. By choosing a small constant c, 1% for example, one can ignore all the u-factor interactions with $S_u \le c$. Under this circumstance, the response surface $f(x)$ is approximated by the estimator $\sum_{S_u > c} \hat{f}_u(x)$. By (3.1), we propose to use

$$\widehat{\mathrm{var}}(\hat{\mu}) = n^{-1}\Big(\hat{\sigma}^2 - \sum_{|u|<t} \hat{\sigma}_u^2\Big) \tag{3.6}$$

as an approximate estimator of $\mathrm{var}(\hat{\mu})$.

From Theorem 4.4 in He and Qian (2014), the interval

$$\Big(\hat{\mu} - z_{\alpha/2} n^{-1/2} \widehat{\mathrm{var}}(\hat{\mu})^{1/2}, \hat{\mu} + z_{\alpha/2} n^{-1/2} \widehat{\mathrm{var}}(\hat{\mu})^{1/2}\Big) \tag{3.7}$$

is an approximate $1-\alpha$ confidence interval for the gross mean μ, where $z_{\alpha/2}$ is the $\alpha/2$ percentile of $N(0,1)$.

Compared with iid samples of the same size, a U-design not only provides a better estimator of the gross mean, but also yields a dramatically shorter confidence interval. Example 1 in Section 5 will illustrate this advantage.

It should be mentioned that Owen's (1992) estimator of σ_u^2 does not perform well if the proportion of inner cells is small. For example, on two-dimensional margins, there are s^2 cells of $\prod_{j\in Z_2} Q_j$ in total and $(s-2)^2$ of them are inner cells. It can be seen that as dimension increases, the proportion of inner cells decreases. Meanwhile, Owen's method may give a negative estimator for $\mathrm{var}(\hat{\mu})$, especially when $\sum_{|u|>t}\sigma_u^2$ is small. Thus, Owen's estimation is deficient when high-dimensional interactions are involved.

4. Extensions

Apart from U-designs, other types of OA-based Latin hypercubes have been proposed for computer experiments, such as strong orthogonal array (SOA) based LHS, nested orthogonal array (NOA) based LHS and correlation controlled OA-based LHS. In constructing these designs, more sophisticated randomization procedures are needed. However, the statistical properties for such designs can be obtained by similar analyse. For this we assume that $f(x)$ is Lipschitz continuous.

4.1. Extension to SOA-based LHS

The formal definition of an SOA was given by He and Tang (2013). An SOA with n runs, m factors, s^t levels and strength t $(1\le t\le m)$, denoted by $SOA(n,m,s^t,t)$, is an $n\times m$ matrix in which each column contains s^t levels from $\{1,\cdots,s^t\}$ such that every $n\times g$ submatrix can be collapsed into an $OA(n, s^{u_1}\times s^{u_2}\times\ldots\times s^{u_g}, g)$ for any positive integers $u_1,\ldots,u_g$ with $u_1+\ldots+u_g=t$ and $1\le g\le t$, where the collapsing into s^{u_j} levels is done by $\lceil a/s^{t-u_j}\rceil$ for $a=1,\ldots,s^t$.

He and Tang (2014) constructed $SOA(s^3, s+1, s^3, 3)$ for any prime power s. We construct LHS based on such SOAs. Let A be an $SOA(n,m,s^3,3)$ with $n=s^3$. For a random permutation of Z_s, say π, let $\pi(i)$ be the image of i.

Step 1. For each column of A, replace the entry $(i-1)s^2+(j-1)s+k$ with $(\pi_1(i)-1)s^2+(\pi_2(j)-1)s+\pi_3(k)$, where $i,j,k\in Z_s$, and π_1,π_2,π_3 are independent random permutations of Z_s. Denote by B the resulting array from A after such replacements.

Step 2. For $i=1,\ldots,n$ and $j=1,\ldots,m$, let

$$X_{ij}=n^{-1}(b_{ij}-\varepsilon_{ij}), \tag{4.1}$$

where b_{ij} is the (i,j)-th entry of B and ε_{ij}'s are independent random variables from $U(0,1]$.

It can be verified that the level replacements in Step 1 do not destroy the structure of an SOA and thus the array B is an SOA randomized from A. An SOA-based LHS is constructed by collecting the design points $X_i = (X_{i1},\ldots,X_{im})^T$, $i=1,\ldots,n$. By construction, it is known that each X_i is uniform on $[0,1)^m$ and thus the sample mean $\hat{\mu}$ is unbiased for μ.

Theorem 4. *For the constructed LHS based on $SOA(n,m,s^3,3)$ with $n=s^3$, as $s\to\infty$, we have*

$$var(\hat{\mu}) = n^{-1}\sum_{|u|>3}\sigma_u^2 + o(n^{-1}).$$

4.2. Extension to NOA-based LHS

A nested orthogonal array $NOA((n_1,n),s^m,(t_1,t))$ is an $OA(n,s^m,t)$ in which the first n_1 rows form an $OA(n_1,s^m,t_1)$. He and Qian (2011) constructed NOA-based LHS and analyzed their statistical properties when NOAs with $t=2$ and $t_1=t-1$ are employed. Here we generalize their results to any $t\geq 2$.

Let A_0 be an $OA(n,s^{m+1},t)$ free of coincidence defect, with the last column arranged in ascending order. Drop the last column of A_0 to obtain an $OA(n,s^m,t)$ A. Randomly shuffle the levels of A column by column. Then A is an $NOA((n_1,n),s^m,(t-1,t))$ with $n_1=ns^{-1}$. Write $A=(A_1^T,A_2^T)^T$, where A_1 consists of the first n_1 rows of A. The construction of LHS based on A is described as follows.

Step 1. For each column of A_1 and any $q\in Z_s$, replace the ns^{-2} positions of entry q with a random permutation of $\{(q-1)ns^{-2}+1,\ldots,qns^{-2}\}\oplus(q-1)ns^{-2}$. Denote by $B_1=(b_{ij}^{(1)})$ the resulting array after such replacements. For $i=1,\ldots,n_1$ and $j=1,\ldots,m$, let

$$X_{ij} = n^{-1}(b_{ij}^{(1)} - \varepsilon_{ij}), \tag{4.2}$$

where ε_{ij}'s are independent $U(0,1]$ random variables.

Step 2. For each column of A_2 and any $q\in Z_s$, replace the $ns^{-2}(s-1)$ positions of entry q with a random permutation of $\{(q-1)n_1+1,\ldots,qn_1\}\setminus\{\lceil nX_{1j}\rceil,\lceil nX_{2j}\rceil,\ldots,\lceil nX_{n_1,j}\rceil\}$. Denote by $B_2=(b_{ij}^{(2)})$ the resulting array after such replacements. For $i=n_1+1,\ldots,n$ and $j=1,\ldots,m$, let

$$X_{ij} = n^{-1}(b_{i-n_1,j}^{(2)} - \varepsilon_{ij}), \tag{4.3}$$

where ε_{ij}'s are independent $U(0,1]$ random variables.

The NOA-based LHS is constructed by collecting the design points $X_i = (X_{i1}, \ldots, X_{im})^T$, $i = 1, \ldots, n$. It can be used for computer experiments containing two codes of different accuracies. The first n_1 points are used for high-accuracy code, and n points are used for low-accuracy code.

Denote by $h(x)$ and $l(x)$ the high-accuracy and low-accuracy codes, respectively. Similar to (2.3), define $h_u(x)$ and $l_u(x)$ as their associated u-factor interactions for any $u \subseteq Z_m$. Let $\sigma^2_{u(h)} = \int_{[0,1)^m} h^2_u(x)dx$ and $\sigma^2_{u(l)} = \int_{[0,1)^m} l^2_u(x)dx$. By adopting the NOA-based LHS, we estimate the gross means $\mu_h = \int_{[0,1)^m} h(x)dx$ and $\mu_l = \int_{[0,1)^m} l(x)dx$ by $\hat{\mu}_h = n_1^{-1}\sum_{i=1}^{n_1} h(X_i)$ and $\hat{\mu}_l = n^{-1}\sum_{i=1}^{n} l(X_i)$, respectively. By construction, $\hat{\mu}_h$ and $\hat{\mu}_l$ are unbiased for μ_h and μ_l, respectively.

Theorem 5. *For the constructed LHS based on $NOA((n_1, n), s^m, (t-1, t))$ with $n_1 = ns^{-1}$, as $s \to \infty$ for fixed $\lambda = ns^{-t}$, we have*

(i) $\mathrm{var}(\hat{\mu}_h) = n_1^{-1}\sum_{|u|>t-1} \sigma^2_{u(h)} + o(n_1^{-1})$;

(ii) $\mathrm{var}(\hat{\mu}_l) = n^{-1}\sum_{|u|>t} \sigma^2_{u(l)} + o(n^{-1})$.

Theorem 4 covers the result of Theorem 1 of He and Qian (2011) as the special case $t = 2$.

4.3. Extension to correlation-controlled OA-based LHS

Chen and Qian (2014) constructed correlation-controlled LHS with n points and m factors based on an $OA(n, s^{m+1}, t)$. Sampling based on such designs can achieve multi-dimensional stratification and lower the correlation between any two factors. They investigated the statistical properties of these designs when $\lambda = ns^{-2} = 1$ and $t = 2$. Here we consider a correlation-controlled LHS when an $OA(n, s^{m+1}, 2)$ free of coincidence defect is employed. The sample mean $\hat{\mu}$ of such LHS is also unbiased for μ by the construction method in Chen and Qian (2014).

Theorem 6. *For a correlation-controlled LHS based on an $OA(n, s^{m+1}, 2)$ free of coincidence defect, as $s \to \infty$ for fixed $\lambda = ns^{-2}$, we have*

$$var(\hat{\mu}) = n^{-1}\sum_{|u|>2} \sigma^2_u + o(n^{-1}).$$

Theorem 6 covers the result in Theorem 1 of Chen and Qian (2014) as a special case when $\lambda = 1$.

5. Simulations

We provide several examples to support our results.

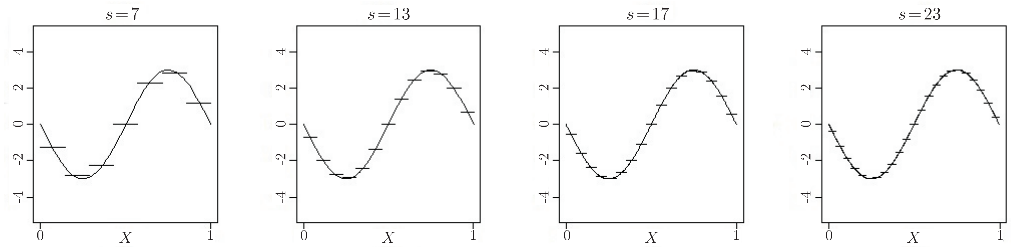

Figure 1. Estimation of $f_{\{1\}}(x)$ in Example 1 for four values s's. The real function $f_{\{1\}}(x)$ and its estimator $\hat{f}_{\{1\}}(x)$ are presented by the curve and the piecewise function, respectively.

Example 1. Consider the function

$$\begin{aligned} f(x) = & \, 3\sin(2\pi x_1 - \pi) + 2(x_2 - 0.5) - 5(x_3 - 0.5) + 2(x_4 - 0.5) \\ & +2(x_2 - 0.5)\sin(2\pi x_1 - \pi) - 2(x_1 - 0.5)(x_3 - 0.5) \\ & +2(x_1 - 0.5)(x_2 - 0.5)(x_4 - 0.5) + 10. \end{aligned}$$

We constructed U-designs based on $OA(s^2, s^3, 2)$, $s = 7, 13, 17, 23$. The estimate of $f_{\{1\}}(x)$ is shown in Figure 1 with respect to different s. It reveals that on every $[i/s, (i+1)/s)$, the estimator is close to the average of $f_{\{1\}}(x)$ on this interval. Furthermore, as $s \to \infty$, our estimator tends to $f_{\{1\}}(x)$.

We also estimated σ_u^2 for $|u| = 1$ with $s = 7$, repeating the process 1,000 times independently. The average and standard deviation over these 1,000 estimated $\hat{\sigma}_u^2$'s are shown in Table 1 by $ave(\hat{\sigma}_u^2)$ and $std(\hat{\sigma}_u^2)$, respectively. We also used (3.6) to estimate $\mathrm{var}(\hat{\mu})$. For comparison, we list the corresponding results via Owen's (1992) method, denoted by $ave_o(\hat{\sigma}_u^2)$, $std_o(\hat{\sigma}_u^2)$. Our method estimates σ_u^2 more accurately than Owen's. In these 1,000 repetitions, there were 372 Owen negative estimators for $\mathrm{var}(\mu)$, while our method always gives positive estimators.

We compared the estimated confidence interval given by (3.7) with that given by iid sampling. Here we took the sample size as $s^2 = 7^2$, repeating the process 10^5 times independently. Table 2 presents the rate at which the estimated confidence intervals accurately cover the true μ and the average length of the estimated confidence intervals for U-designs and iid samples, respectively.

Example 2. Consider the high-accuracy function and low-accuracy functions

$$\begin{cases} h(x) = 0.48\sin(x_1 - 0.5)\pi + 0.9(x_2 - 0.5)(x_3 - 0.5) + 0.8\displaystyle\prod_{i=1}^{3}(x_i - 0.5), \\ l(x) = (x_1 - 0.5) + (x_2 - 0.5)(x_3 - 0.5) + \prod_{i=1}^{3}(x_i - 0.5), \end{cases}$$

Table 1. Comparison of $ave(\hat{\sigma}_u^2)$ and $std(\hat{\sigma}_u^2)$ for $\hat{\sigma}_u^2$'s in Example 1.

u	$\{1\}$	$\{2\}$	$\{3\}$	$\{4\}$
σ_u^2	4.500	0.333	2.083	0.333
$ave(\hat{\sigma}_u^2)$	4.320	0.332	2.048	0.333
$std(\hat{\sigma}_u^2)$	0.055	0.037	0.086	0.038
$ave_o(\hat{\sigma}_u^2)$	4.307	0.030	1.788	0.110
$std_o(\hat{\sigma}_u^2)$	0.472	0.043	0.681	0.061

Table 2. Comparison of the estimated confidence intervals for μ in Example 1.

sample	coverage rate	average length
U-design	0.999	0.151
iid sample	0.997	1.69

Table 3. MSEs for NOA-based LHS in Example 2.

s		3	7	13	23	37
MSE($\hat{\mu}_h$) $\times s^2$	$t=3$	3.2×10^{-3}	9.7×10^{-4}	5.6×10^{-4}	4.4×10^{-4}	3.3×10^{-4}
	$t=2$	2.1×10^{-2}	4.8×10^{-2}	7.1×10^{-2}	0.17	0.26
MSE($\hat{\mu}_l$) $\times s^3$	$t=3$	2.8×10^{-3}	3.1×10^{-4}	1.1×10^{-4}	3.1×10^{-5}	1.2×10^{-5}
	$t=2$	4.8×10^{-3}	5.0×10^{-3}	8.5×10^{-3}	1.4×10^{-2}	2.6×10^{-2}

Table 4. MSEs for correlation-controlled OA-based LHS in Example 3.

s	5	11	17	23	29
MSE($\hat{\mu}$) $\times 2s^4$	0.582	0.178	0.133	0.101	0.102

respectively. For $s = 3, 7, 13, 23, 37$ and $t = 2, 3$, we constructed an $NOA((s^2, s^3), s^3, (t-1, t))$ by the method in Section 4.2. For each case, we generated 100 NOA-based LHS independently and then used them to estimate μ_h and μ_l. The mean square errors (MSEs) of $\hat{\mu}_h$ and $\hat{\mu}_l$ are given in Table 3. There the MSE decreases as s becomes larger for fixed t, and the MSE for $t = 3$ is smaller than that for $t = 2$ in each case.

Example 3. Consider the function $f(x) = 12(x_2-0.5)\sin(x_1-0.5)+3(x_2-0.5)+3\sin(x_1-0.5)$. For $s = 5, 11, 17, 23, 29$, we randomly generated an $OA(2s^2, s^2, 2)$ and constructed 100 correlation-controlled LHS based on it by the method in Chen and Qian (2014). The MSE of $\hat{\mu}$ for each case is given in Table 4. It shows that the order of MSE($\hat{\mu}$) is $O(n^{-1}s^{-2})$.

A final example compares five types of LHS including ordinary LHS (OLHS), U-designs based on OAs of strength two (Us), U-designs based on OAs of strength

Table 5. MSEs for the five types of LHS in Example 4.

	OLHS	Us	HUs	MMs	CLHS
$s = 8$	0.19433	0.00843	0.00474	0.05082	0.18235

three (HUs), maximin LHS (MMs in abrreation, proposed by Johnson, Moore, and Ylvisaker (1990)), and correlation-controlled LHS (CLHS) based on an OA of strength two.

Example 4. The borehole function used by Morris, Mitchell, and Ylvisaker (1993) is

$$\frac{20\pi T_u(H_u - H_l)}{\log(r/r_u)[1 + 2LT_u/\{\log(r/r_\omega)r_\omega^2 K_\omega\} + T_u/T_l]},$$

in which the eight input variables, after appropriate scaling, lie in $[0,1]^8$. Consider the five types of LHS with 8^3 points and eight factors: OLHS, Us, HUs, MMs and CLHS. Each type of sampling method was repeated 100 times. The MSEs of $\hat{\mu}$ for them are presented in Table 5. There HUs are the best, because they have better space-filling properties in high-dimensional margins.

6. Discussions

This paper provides a general analysis of the statistical properties for U-designs. A unified expression of the variance of the sample mean and its approximate estimator is established. Consequently, we obtain an effective confidence interval of the gross mean. By similar analysis, we also give the statistical properties for SOA-based LHS, NOA-based LHS, and correlation-controlled OA-based LHS.

For computer experiments with both qualitative and quantitative factors, sliced space-filling designs based on OAs of sliced structure have been proposed (Qian and Wu (2009) and Ai, Jiang, and Li (2014)). For a sliced space-filling designs, the whole design and any slice constitute NOA-based LHS. Therefore, by the similar analysis of NOA-based LHS, it can be shown that the variance components of lower-order interactions are filtered out for each slice and the whole design.

The formula of $\mathrm{var}(\hat{\mu})$ for U-designs based on an OA of strength t implies that the stability of the sample mean depends only on $\{M(u,r) : |u| > t\}$. So it is natural to use $M(u,r)$'s to compare different OAs. Since the lower-order interactions are considered to be more significant, we can define the sequence

$$\Bigg(\sum_{|u|=t+1} M(u,t+1), \sum_{|u|=t+2} M(u,t+2), \sum_{|u|=t+3} M(u,t+3), \ldots\Bigg)$$

as a criterion to distinguish OAs of the same strength t. A promising direction is to find the best OAs which minimize this sequence; we can investigate the lower bounds for this sequence theoretically.

Appendix

Proof of Lemma 1. Let $\mathcal{P} = \{[0, n^{-1}), [n^{-1}, 2n^{-1}), \ldots, [1-n^{-1}, 1)\}$ and $\mathcal{S} = \{\prod_{j=1}^m P_j : P_j \in \mathcal{P}, j = 1, \ldots, m\}$. Recall that $\mathcal{Q} = \{[0, s^{-1}), [s^{-1}, 2s^{-1}), \ldots, [1-s^{-1}, 1)\}$. Let $\mathcal{L} = \{\prod_{j=1}^m Q_j : Q_j \in \mathcal{Q}, j = 1, \ldots, m\}$. Hereafter, we refer to members of $\mathcal{S}$ and $\mathcal{L}$ as small cells and large cells, respectively. Similarly, for any $u \subseteq Z_m$, take $\prod_{j\in u} P_j$ as the subset of $[0,1)^m$ that consists of all points $(x_1, \ldots, x_m)$'s with $x_j \in P_j$ for $j \in u$ and $x_j \in [0,1)$ for $j \notin u$, provided $P_j \in \mathcal{P}$ for all $j \in u$. For convenience, write $\prod_{j\in u} Q_j$ and $\prod_{j\in u} P_j$ as Q^u and P^u, respectively.

The proof of part (i) is given inductively. It is trivial for $u = \emptyset$. Assume that part (i) holds for any $u \subseteq Z_m$ with $|u| < k$. Consider the case of $|u| = k$. For any set $v \subset u$, we have

$$\int_{Q^v} \bar{f}_v(x)dx = \int_{Q^v} E[f_v(x)|\sigma(\mathcal{Q}^v)]dx = \int_{Q^v} f_v(x)dx \tag{A.1}$$

for any Q^v. By the definition of $\bar{f}(x)$, we have

$$\int_{Q^u} \bar{f}(x)dx = \int_{Q^u} f(x)dx \tag{A.2}$$

for any Q^u. By the (A.1) and (A.2), it can be verified that

$$\begin{aligned}\int_{Q^u} \bar{f}_u(x)dx &= \int_{Q^u} \int_{[0,1)^{m-|u|}} [\bar{f}(x) - \sum_{v\subset u} \bar{f}_v(x)]dx_{-u}dx \\ &= \int_{Q^u} \int_{[0,1)^{m-|u|}} [f(x) - \sum_{v\subset u} f_v(x)]dx_{-u}dx \\ &= \int_{Q^u} f_u(x)dx. \end{aligned} \tag{A.3}$$

Thus, $\bar{f}_u(x) = E[f_u(x)|\sigma(\mathcal{Q}^u)]$ and part (i) is obtained. Since $|f(x_1) - f(x_2)| \to 0$ for any $x_1, x_2 \in Q^{Z_m}$, as $s \to \infty$, part (ii) follows directly.

Proof of Theorem 1. Consider a U-design $D = \{X_1, \ldots, X_n\}$ based on an $OA(n, s^m, t)$ constructed in (2.1). By Lemma 1, we know $E[f(X_i) - \bar{f}(X_i)]^2 = o(1)$. Decompose $\mathrm{var}(\hat{\mu})$ as

$$\begin{aligned}\mathrm{var}(\hat{\mu}) = \mathrm{var}\big(n^{-1} \sum_{X_i\in D} \bar{f}(X_i)\big) &+ n^{-2} \sum_{i,j=1}^n E[(f(X_i) - \bar{f}(X_i))(\bar{f}(X_j) - \mu)] \\ &+ n^{-2} \sum_{i\neq j} E[(f(X_i) - \bar{f}(X_i))(f(X_j) - \bar{f}(X_j))] + o(n^{-1}). \end{aligned} \tag{A.4}$$

By Theorem 1 in Owen (1994), we have

$$\mathrm{var}\big(n^{-1}\sum_{X_i\in D}\bar f(X_i)\big)=n^{-2}\sum_{|u|>t}\sum_{r=0}^{|u|}M(u,r)(1-s)^{r-|u|}\sigma_u^2+o(n^{-1}). \tag{A.5}$$

Next, we are ready to prove

$$n^{-2}\sum_{i,j=1}^{n}E[(f(X_i)-\bar f(X_i))\bar f(X_j)]=o(n^{-1}), \tag{A.6}$$

$$n^{-2}\sum_{i\neq j}E[(f(X_i)-\bar f(X_i))(f(X_j)-\bar f(X_j))]=o(n^{-1}). \tag{A.7}$$

For $i=1,\ldots,n$, let $Q_i^{Z_m}$ and $P_i^{Z_m}$ be the large and small cell in which X_i lies, respectively. Since $E[(f(X_i)-\bar f(X_i))\bar f(X_j)]=E\{E[(f(X_i)-\bar f(X_i))\bar f(X_j)|X_i\in Q_i^{Z_m},X_j\in Q_j^{Z_m}]\}=0$, (A.6) follows.

For $i\neq j$, write $P_i^{Z_m}=\prod_{k=1}^m P_k$ and $Q_j^{Z_m}=\prod_{k=1}^m Q_k$. Let $\Delta_a\subset Q_j^{Z_m}$ be the area that X_j cannot lie in and $\Delta_b=Q_j^{Z_m}\setminus\Delta_a$. Take V_a and V_b as the volumes of Δ_a and Δ_b, respectively.

Case 1. $V_a=0$. We have $E[f(X_j)-\bar f(X_j)|X_j\in\Delta_b,V_a=0]=0$. Thus $E[(f(X_i)-\bar f(X_i))(f(X_j)-\bar f(X_j))]=E\{(f(X_i)-\bar f(X_i))E[f(X_j)-\bar f(X_j)|X_j\in\Delta_b,V_a=0]\}=0$.

Case 2. $V_a\neq 0$. Here $X_{jk}\notin P_k$ for $k\in Z_m$. We have $V_a=O(n^{-1}s^{1-m})$ and $V_b=O(s^{-m})$. Since $E[f(x)-\bar f(x)|x\in Q_j^{Z_m}]=0$, we obtain

$$V_aE[f(x)-\bar f(x)|x\in\Delta_a]+V_bE[f(x)-\bar f(x)|x\in\Delta_b]=0. \tag{A.8}$$

By (A.8), it can be shown that $E[f(X_j)-\bar f(X_j)|X_j\in\Delta_b,V_a\neq 0]=o(s/n)$. Thus $E[(f(X_i)-\bar f(X_i))(f(X_j)-\bar f(X_j))]=E\{(f(X_i)-\bar f(X_i))E[f(X_j)-\bar f(X_j)|X_j\in\Delta_b,V_a=0]\}=o(s/n)$.

One has $V_a\neq 0$ if and only if $P_k\subset Q_k$ for some k, which means the ith row and jth row of the $OA(n,s^m,t)$ agree in some positions. Thus the number of (i,j)'s such that $V_a\neq 0$ is $O(n^2s^{-1})$. A direct calculation shows that the (A.7) holds. In view of (A.4), (A.5), (A.6), and (A.7), the first expression of $\mathrm{var}(\hat\mu)$ follows. If the OA is free of coincidence defect, then $\sum_{r=0}^{|u|}M(u,r)(1-s)^{r-|u|}=n+o(n)$ for any $|u|>t$. The proof of Theorem 1 concludes.

Proof of Lemma 2. For the U-design $D=\{X_1,\ldots,X_n\}$ based on an $OA(n,s^m,t)$ free of coincidence defect constructed in (2.1), we further define $D_{(-u)}=\{X_{1(-u)},\ldots,X_{n(-u)}\}$ for $u\subset Z_m$, where $X_{i(-u)}$ is obtained by dropping all the components of X_i in u for $i=1,\ldots,n$. For a given $x\in[0,1)^m$, let $D_{(-u)}(x)=$

$\{X_{i(-u)} : i \in r(x,u)\}$, the subdesign of $D_{(-u)}$ consisting of all points labeled in $r(x,u)$. It is known that $D_{(-u)}(x)$ is a design based on an $OA(ns^{-|u|}, s^{m-|u|}, t-|u|)$ free of coincidence defect. Note that $g_u(x)$ is an discrete function. Thus, the consistency for the estimator $\hat{g}_u(x)$ with $|u| < t$ can be easily obtained by Theorem 4.4 of He and Qian (2014).

Proof of Theorem 2. In view of formulas (3.3), (3.4), and (3.5), it's sufficient to verify that

$$n^{-1/2}s^{|u|/2}\sum_{i\in\gamma(x,u)}[\bar{f}(X_i)-f(X_i)] = o_p(1). \tag{A.9}$$

By using arguments as in (A.8), it can be shown that

$$E[(f(X_i)-\bar{f}(X_i))(f(X_j)-\bar{f}(X_j))] = o(s/n) \tag{A.10}$$

for any $i, j \in r(x,u)$ with $i \neq j$. By (A.10), we have

$$n^{-1}s^{|u|}\mathrm{var}\big(\sum_{i\in\gamma(x,u)}[f(X_i)-\bar{f}(X_i)]\big) = o(1),$$

which indicates (A.9) by Chebyshev's inequality.

Proof of Theorem 4. Consider the design $D = \{X_1, \ldots, X_n\}$ based on an $SOA(n, s^m, t)$ constructed in (4.1). Similar to the proof of Theorem 1, we only need to verify the equation (A.7). Denote the $SOA(s^3, m, s, 3)$ as $A = (a_{ik})$. For any $i, j \in Z_n$ with $i \neq j$, consider two cases.

Case 1. For all $k \in Z_m$, $\lceil a_{ik}s^{-2}\rceil \neq \lceil a_{jk}s^{-2}\rceil$. Then $E[f(X_j)-\bar{f}(X_j)|X_i] = 0$. So $E[(f(X_i)-\bar{f}(X_i))(f(X_j)-\bar{f}(X_j))] = 0$.

Case 2. There exists $k_0 \in Z_m$ such that $\lceil a_{ik_0}s^{-2}\rceil = \lceil a_{jk_0}s^{-2}\rceil$ and $\lceil a_{ik}s^{-1}\rceil \neq \lceil a_{jk}s^{-1}\rceil$ for any $k \in Z_m$. We use the arguments and notation as in the proof of Theorem 1. Then $V_a = O(s^{-m-1})$ and $V_b = O(s^{-m})$. By (A.8), we have $E[f(X_j)-\bar{f}(X_j)|X_i] = O(s^{-2})$. So $E[(f(X_i)-\bar{f}(X_i))(f(X_j)-\bar{f}(X_j))] = O(s^{-3})$.

By the structure of A, the number of (i,j)'s that satisfy Case 1 is $O(n^2)$, which for Case 2 is $O(n^2s^{-1})$. For (i,j)'s beyond these two cases, the number is $O(n^2s^{-2})$ and $E[(f(X_i)-\bar{f}(X_i))(f(X_j)-\bar{f}(X_j))] = O(s^{-2})$ since $f(x)$ is Lipschitz continuous. By straightforward calculations, (A.7) follows.

Proof of Theorem 5. Consider the design $D = \{X_1, \ldots, X_n\}$ based on the $NOA((n_1, n), s^m, (t-1, t))$ A with $n_1 = ns^{-1}$ constructed in (4.2) and (4.3). As in the proof of Theorem 1, part (i) is straightforward. For part (ii), we only need to verify (A.7) where $f(\cdot)$ is replaced with $l(\cdot)$. For any $i, j \in Z_n$ with $i \neq j$, consider two cases.

Case 1. $i, j \le n_1$. By the structure of A, we know that $V_a = O(n^{-1}s^{2-m})$ and $V_b = O(s^{-m})$ when $\Delta_a \neq \emptyset$. Using (A.8), we have

$$E[l(X_j) - \bar{l}(X_j)|X_i, Q_j^{Z_m}] = O(n^{-1}s).$$

Thus $E[(l(X_i) - \bar{l}(X_i))(l(X_j) - \bar{l}(X_j))] = O(n^{-1}s^{-1})$. When $\Delta_a = \emptyset$, it is obvious that $E[l(X_j) - \bar{l}(X_j)|X_i, Q_j^{Z_m}] = 0$.

Case 2. $i > n_1$ or $j > n_1$. When $\Delta_a \neq \emptyset$, we have $V_a = O(n^{-1}s^{1-m})$. Similarly, $E[l(X_j) - \bar{l}(X_j)|X_i, Q_j^{Z_m}] = O(n^{-1})$, which leads to $E[(l(X_i) - \bar{l}(X_i))(l(X_j) - \bar{l}(X_j))] = O(n^{-1}s^{-2})$. When $\Delta_a = \emptyset$, we have $E[l(X_j) - \bar{l}(X_j)|X_i,\, Q_j^{Z_m}] = 0$.

For $\Delta_a \neq \emptyset$, the number of (i, j)'s satisfying Case 1 is $O(n_1^2 s^{-1})$ and that for Case 2 is $O(n^2 s^{-1})$. Then (A.7) follows by direct calculations.

Proof of Theorem 6. Consider the correlation-controlled LHS $D = \{X_1, \ldots, X_n\}$ based on an $OA(n,\, s^{m+1}, 2)$ $A = (a_{ik})$ free of coincidence defect. As in the proof of Theorem 1, we only need to verify (A.7).

For any $i, j \in Z_m$ with $i \neq j$, if $a_{i,m+1} \neq a_{j,m+1}$, then $V_a = O(s^{-m-1})$. By (A.8), we have $E[(f(X_i) - \bar{f}(X_i))(f(X_j) - \bar{f}(X_j))] = O(s^{-3})$. If $a_{i,m+1} = a_{j,m+1}$, we obtain $E[(f(X_i) - \bar{f}(X_i))(f(X_j) - \bar{f}(X_j))] = O(s^{-2})$ since $f(x)$ is Lipschitz continuous. The number of (i, j)'s for $a_{i,m+1} \neq a_{j,m+1}$ is $O(n^2)$ and that for $a_{i,m+1} = a_{j,m+1}$ is $O(ns)$. Then (A.7) follows by direct calculation.

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