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A CENTRAL LIMIT THEOREM FOR GENERAL ORTHOGONAL ARRAY BASED SPACE-FILLING DESIGNS

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Orthogonal array based space-filling designs (Owen [*Statist. Sinica* **2** (1992a) 439–452]; Tang [*J. Amer. Statist. Assoc.* **88** (1993) 1392–1397]) have become popular in computer experiments, numerical integration, stochastic optimization and uncertainty quantification. As improvements of ordinary Latin hypercube designs, these designs achieve stratification in multi-dimensions. If the underlying orthogonal array has strength t, such designs achieve uniformity up to t dimensions. Existing central limit theorems are limited to these designs with only two-dimensional stratification based on strength two orthogonal arrays. We develop a new central limit theorem for these designs that possess stratification in arbitrary multi-dimensions associated with orthogonal arrays of general strength. This result is useful for building confidence statements for such designs in various statistical applications.

1. Introduction. Latin hypercube designs achieve maximum uniformity in univariate margins [McKay, Beckman and Conover (1979)]. Orthogonal arrays based Latin hypercube designs [Tang (1993)], called *U designs*, improve upon them by achieving uniformity in multivariate dimensions. Another type of orthogonal array based design is the randomized orthogonal array [Owen (1992a), Patterson (1954)]. The two classes of designs are widely used in computer experiments, numerical integration, stochastic optimization and uncertainty quantification.

Consider a K-dimensional numerical integration problem

$$\mu = E\{f(x)\} = \int_{[0,1)^K} f(x)\,dx.$$

After evaluating f at N runs, $X_1, \ldots, X_N$, μ is estimated by

$$\hat{\mu} = N^{-1} \sum_{i=1}^{N} f(X_i^1, \ldots, X_i^K), \tag{1}$$

where X_i^k is the kth dimension of X_i. Tang (1993) gives a variance formula of $\hat{\mu}$ for a U design, and Owen (1994) derives variance formulas for a randomized

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orthogonal array free of coincidence defect. Methods to numerically estimate this variance are discussed in Owen (1992a, 1994).

When an orthogonal array based space-filling design is used in numerical integration, stochastic optimization [Birge and Louveaux (2011), Shapiro, Dentcheva and Ruszczyński (2009), Tang and Qian (2010)], uncertainty quantification [Xiu (2010)] and other applications, one is often interested in a central limit theorem for deriving a confidence statement. Derivation of a central limit theorem for such designs is a very challenging problem because of their complicated combinatorial structure and sophisticated dependence across the rows after randomization. Loh (1996, 2008) was first to address this problem and derived central limit theorems for these designs associated with orthogonal arrays of index one and strength two, which achieve uniformity up to two-dimensional projections. In Loh (2008), the integrand is assumed to be Lipschitz continuous mixed partial of order K.

Different from the work of Loh (1996, 2008), we propose a new approach to construct a new central limit theorem for orthogonal array based space-filling designs. This approach works for these designs that achieve uniformity in arbitrary multi-dimensions associated with orthogonal arrays of general strength. As in Owen (1994), we assume the underlying orthogonal array is free of coincidence defect. Let λ and n denote the index and the number of levels for the orthogonal array, respectively. As N tends to infinity, we assume λ is fixed or λ/n tends to zero. Our method is inspired by the method of moments used in Owen (1992b) for ordinary Latin hypercube designs but with new combinational techniques to deal with the complexity of orthogonal arrays. Section 2 presents useful definitions and notation. Sections 3 and 4 provide central limit theorems for orthogonal array based space-filling designs. Section 5 gives numerical illustration of the derived theoretical results. Section 6 concludes with some brief discussion.

2. Definitions and notation. An N by K matrix is said to be a Latin hypercube if each of its columns consists of $\{0, 1, \dots, N-1\}$. A uniform permutation on a set of a numbers is randomly generated with all $a!$ permutations equally probable. An ordinary Latin hypercube design [McKay, Beckman and Conover (1979)] is constructed by

$$X_i^k = \pi_k(i)/N + \eta_i^k/N,$$

where the π_k are uniform permutations on $\{0, 1, \dots, N-1\}$, the η_i^k are generated from uniform distributions on $[0, 1)$ and the π_k and the η_i^k are generated independently.

An N by K matrix is said to be an orthogonal array $OA(N, K, n, h)$ if its entries are from $0, 1, \dots, n-1$ and for any $p \le h$ columns of the matrix, the n^p combinations of values appear exactly the same number of times in rows [Hedayat, Sloane and Stufken (1999)]. For an $OA(N, K, n, h)$, if additionally no two rows from any

TABLE 1
An orthogonal array with 18 *runs*

0	0	0	0	0	0
1	1	1	1	1	1
2	2	2	2	2	2
0	0	1	2	1	2
1	1	2	0	2	0
2	2	0	1	0	1
0	1	0	2	2	1
1	2	1	0	0	2
2	0	2	1	1	0
0	2	2	0	1	1
1	0	0	1	2	2
2	1	1	2	0	0
0	1	2	1	0	2
1	2	0	2	1	0
2	0	1	0	2	1
0	2	1	1	2	0
1	0	2	2	0	1
2	1	0	0	1	2

$N \times (h+1)$ submatrices are the same, the orthogonal array is said to be free of coincidence defect [Owen (1994)]. For illustration, Table 1 gives an $OA(18, 6, 3, 2)$ of index two and free of coincidence defect.

Let H denote an $OA(N, K, n, h)$ with the (i, k)th element H_i^k. A randomized orthogonal array [Owen (1992a)] based on H is constructed by

$$X_i^k = \pi_k\big(H^k_{\gamma^{-1}(i)}\big)/n + \eta_i^k/n, \tag{2}$$

where the γ is a uniform permutation on $\{1, \dots, N\}$, the π_k are uniform permutations on $\{0, 1, \dots, n-1\}$, the η_i^k are generated from the uniform distribution on $[0, 1)$ and the γ, the π_k and the η_i^k are generated independently.

Compared with (2), a U design [Tang (1993)] based on H is constructed with one additional step,

$$X_i^k = \pi_k\big(H^k_{\gamma^{-1}(i)}\big)/n + \alpha^k_{\gamma^{-1}(i)}/N + \eta_i^k/N, \tag{3}$$

where the γ is a uniform permutation on $\{1, \dots, N\}$, the π_k are uniform permutations on $\{0, 1, \dots, n-1\}$, all the α_i^k's related to entries in the kth column with level x in H consist of a permutation of $\{0, 1, \dots, N/n-1\}$, the η_i^k are generated from uniform distributions on $[0, 1)$ and the γ, the π_k, the $\alpha^i_{k,x}$ and the η_i^k are generated independently.

For illustration, let H be the orthogonal array in Table 1. We generate a randomized orthogonal array and a U design based on H. The bivariate projections to the first two dimensions of the two designs are depicted in Figure 1. For both designs,

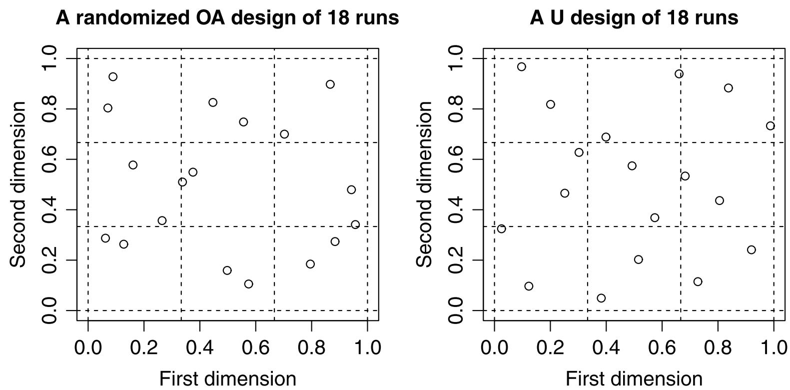

FIG. 1. *Bivariate projections to the first two dimensions of a randomized orthogonal array design and a U design generated from the orthogonal array in Table 1. For both designs, each of the nine squares by dashed lines contains exactly two points. Furthermore, for the U design, each of the* 18 *equally spaced intervals of* $[0, 1)$ *contains exactly one point.*

each of the nine squares by dashed lines contains exactly two points. Furthermore, for the U design, each of the 18 equally spaced intervals of [0, 1) contains exactly one point.

Next, we introduce the functional analysis of variance decomposition [Owen (1994)]. Let F be the uniform measure on $[0, 1)^K$ with $dF = \prod_{k=1}^{K} dF_{\{k\}}$, where $F_{\{k\}}$ is the uniform measure on $[0, 1)$. Under the assumption f is a continuous function in $[0, 1]^K$, f is bounded and has finite variance $\int f(x)^2\, dF$. Express f as

$$f(x) = \mu + \sum_{\phi \subset u \subseteq \{1,\dots,K\}} f_u(x),$$

where $\mu = \int f(x)\, dF$ and f_u is defined recursively via

$$f_u(x) = \int \left\{ f(x) - \sum_{v \subset u} f_v(x) \right\} dF_{\{1,\dots,K\}\setminus u}.$$

If $u \cap v \neq \phi$,

$$\int_v f_u\, dx = 0. \tag{4}$$

Following Owen (1994), for the two classes of designs of strength h without coincidence defect, the f_u part with $|u| \le h$ is balanced out from the design. The remaining part r of f is defined via

$$f(x) = \mu + \sum_{0<|u|\le h} f_u(x) + r. \tag{5}$$

The variance of $\hat{\mu}$ from (1) is

$$\operatorname{var}(\hat{\mu}) = N^{-1} \int r(X)^2 \, dF(X) + o(N^{-1}).$$

Let $I(\cdot)$ be the indicator function. For a real number x, let $\lfloor x \rfloor$ be the largest integer no greater than x, and the subdivision of x with length $1/z$ is

$$\delta_z(x) = [\lfloor zx \rfloor / z, (\lfloor zx \rfloor + 1)/z). \tag{6}$$

Let $|D|$ be the volume of region D. Let E_{IID}, E_{ROA} and E_{UD} be the expectation of a function from samples generated identically and independently, from a randomized orthogonal array and from a U design, respectively.

3. A central limit theorem for randomized orthogonal arrays. We now derive a central limit theorem for randomized orthogonal arrays. Assume f is a continuous function from $[0, 1]^K$ to $\mathscr{R}$. Let H be an $OA(N, K, n, h)$ free of coincidence defect and $\lambda = N/n^h$. Take $X_1, \dots, X_N$ in (1) to be the design points from a randomized orthogonal array constructed in (2). For fixed K and h, we suppose there is a sequence of H such that N and n tend to infinity with λ/n tending to zero. Lemma 3.1 on the method of moments [Durrett (2010)] is used throughout.

LEMMA 3.1. *Suppose that $A_1, A_2, \dots$ are random variables, and their distribution functions $F_1, F_2, \dots$ have finite moments. Namely, for any $p = 1, 2, \dots$ and $n = 1, 2, \dots,$*

$$m_n^{(p)} = \int_{-\infty}^{+\infty} x^p \, dF_n$$

is finite. Suppose that F is a distribution function with finite moments. Namely,

$$m^{(p)} = \int_{-\infty}^{+\infty} x^p \, dF$$

is finite. Also assume

$$\limsup_{p \to \infty} \{ (m^{(2p)})^{1/2p} / (2p) \} < \infty.$$

Finally, suppose for any $p = 1, 2, \dots,$

$$\lim_{n \to \infty} m_n^{(p)} = m^{(p)}.$$

Then A_n converges in distribution to F.

Because the density function of multiple points among $X_1, \dots, X_N$ is complicated, we consider the conditional density $g = g(d_1, \dots, d_K)$ of X_s given other points $X_1, \dots, X_{s-1}$, $s = 1, \dots, N$. Unfortunately, the conditional density is not uniquely determined by the definition of orthogonal arrays and N, K, n, h and depends on the specific construction algorithm of H. A key to overcome this difficulty is to express g in big O terms. Let M_{s-1} denote an $(s-1) \times K$ matrix with the (i,k)th element being z if $z < i$, and z is the smallest number such that X_i^k matches X_z^k, that is, $\lfloor nX_{i,k} \rfloor = \lfloor nX_{z,k} \rfloor$. If X_i^k does not match to any other point X_z^k with $z < i$, the (i,k)th element of M_{s-1} is defined to be zero and the first row of M_{s-1} is zero. According to this definition, M_{s-1} contains full information on pairwise coincidence among $X_1, \dots, X_{s-1}$.

LEMMA 3.2. *For a randomized orthogonal array in* (2), *the conditional density of* X_s *given* $X_1, \dots, X_{s-1}$ *is*

$$\begin{aligned} &g_s(d_1, \dots, d_K) \\ &\quad = \sum_{i_1,\dots,i_K=0}^{s-1} b_s(i_1, \dots, i_K, M_{s-1}) I\big(d_1 \in D_{i_1}^1, \dots, d_K \in D_{i_K}^K\big), \end{aligned} \tag{7}$$

where $D_i^k = \delta_n(X_i^k)$ *for* $i = 1, \dots, s-1$ *and* $k = 1, \dots, K$, $D_0^k = [0,1) \setminus \{\bigcup_{i=1}^{s-1} \delta_n(X_i^k)\}$ *for* $k = 1, \dots, K$ *and* $b_s(\cdot)$ *is a deterministic function on* $d_1, \dots, d_K, M_{s-1}$ *with*

$$b_s(i_1, \dots, i_k, M_{s-1}) = \begin{cases} 1 + O(n^{-1}), & |w| < h, \\ O(1), & |w| = h, \\ 0, & |w| > h, \max(|w_1|, \dots, |w_{s-1}|) > h, \\ O(n^{|w|}/N), & \textit{otherwise}, \end{cases}$$

where $w(i_1, \dots, i_K)$ *is the dimensions of nonzero elements in* $(i_1, \dots, i_K)$, $w = \{k : i_k \neq 0\}$, $w_z(i_1, \dots, i_K) = \{k : i_k = z\}$ *and* $w = \bigcup w_z$.

Lemma 3.2 shows that the conditional density is a constant except in the subdivisions of $X_1, \dots, X_{s-1}$ and $|w|$ indicates the number of dimensions that X_s is inside the subdivisions of any length. For illustration, Figure 2 displays subdivisions of $\delta_n(X_i^k)$ for $n = 5$, $h = 2$, $K = 2$ and $s = 3$. In this example, $X_1 = (0 \cdot 332, 0 \cdot 542)$ and $X_2 = (0 \cdot 722, 0 \cdot 734)$. The subdivisions of X_1 and X_2 are $\delta_5(X_1^1) = [0 \cdot 2, 0 \cdot 4)$, $\delta_5(X_1^2) = [0 \cdot 4, 0 \cdot 6)$, $\delta_5(X_2^1) = [0 \cdot 6, 0 \cdot 8)$ and $\delta_5(X_2^2) = [0 \cdot 6, 0 \cdot 8)$. The regions with $|w| = 0$, $|w| = 1$ and $|w| = 2$ are in white, light gray and gray colors, respectively. The proof of Lemma 3.2 is given in the Appendix.

Next, we state two lemmas for the conditional expectation of $f(X_s)$ given points $X_1, \dots, X_{s-1}$ from a randomized orthogonal array. These lemmas parallel the results for ordinary Latin hypercube designs in Owen (1992b) but use more complicated arguments.

LEMMA 3.3. *For any bounded function* f *and* $s > 1$, *as* $N \to \infty$,

$$E_{\mathrm{ROA}}\{f(X_s) | X_1, \dots, X_{s-1}\} = E_{\mathrm{IID}}\{f(X_s)\} + O(n^{-1}).$$

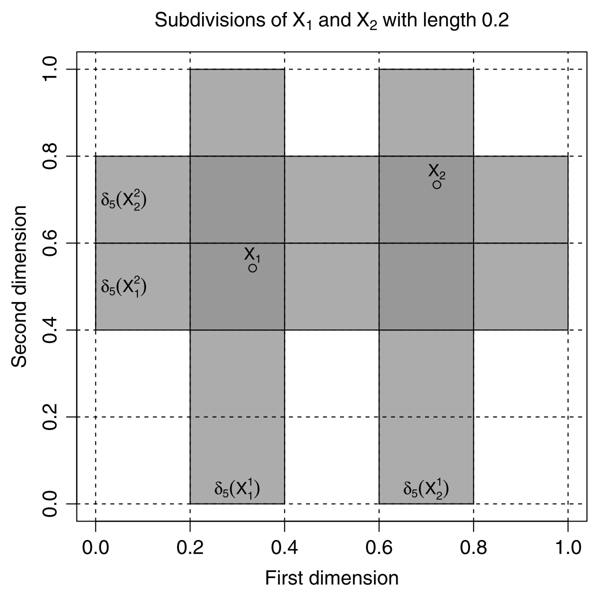

FIG. 2. *The subdivisions of* X_1 *and* X_2 *with length* $1/5$ *for an example with* $n = 5$, $h = 2$, $K = 2$ *and* $s = 3$. *The white, light gray and gray regions represent the cases with* $|w| = 0$, $|w| = 1$ *and* $|w| = 2$, *respectively.*

LEMMA 3.4. *Let*

$$\bar{R} = N^{-1} \sum_{i=1}^{N} r(X_i).$$

Then for any positive integer p,

$$E_{\mathrm{ROA}}\{(N^{1/2}\bar{R})^p\} = E_{\mathrm{IID}}\{(N^{1/2}\bar{R})^p\} + o(1).$$

Lemma 3.3 is a direct consequence of Lemma 3.2. The proof of Lemma 3.4 is given in the Appendix.

We are now ready for our main theorem for randomized orthogonal arrays.

THEOREM 3.5. *Suppose that* f *is a continuous function from* $[0, 1]^K$ *to* $\mathscr{R}$, $\hat{\mu}$ *in* (1) *is based on a randomized orthogonal array in* (2) *without coincidence defect*, λ *is fixed or* $\lambda = o(n)$. *Then, as* $N \to \infty$,

$$N^{1/2}(\hat{\mu} - \mu) \to N\left(0, \int r(x)^2\, dx\right).$$

PROOF. The mean of $N^{1/2}(\hat{\mu} - \mu)$ is 0 and the variance of $N^{1/2}(\hat{\mu} - \mu)$ tends to $\int r(x)^2\, dx$. From Lemma 3.4, for $p = 1, 2, \ldots,$

$$E_{\mathrm{ROA}}\{(N^{1/2}\bar{R})^p\} = E_{\mathrm{IID}}\{(N^{1/2}\bar{R})^p\} + o(1).$$

When the points are generated identically and independently, $N^{1/2}\bar{R}$ follows a normal distribution with mean zero and variance $\sigma^2 = \int r(x)^2\,dx$. From Owen (1980),

$$E_{\mathrm{IID}}\{(N^{1/2}\bar{R})^p\} = \begin{cases} 0, & p = 1, 3, 5, \ldots, \\ \sigma^p(p-1)!!, & p = 2, 4, 6, \ldots. \end{cases}$$

Note that

$$\limsup_{p\to\infty} \bigl(\sigma^p(p-1)!!\bigr)^{1/p}/p = 0.$$

From Lemma 3.1, $N^{1/2}\bar{R}$ from randomized orthogonal array has the same limiting distribution as $N^{1/2}\bar{R}$ where the points are generated identically and independently, which yields a normal distribution. $\square$

We can easily extend Theorem 3.5 to a multivariate function $f = (f_1, \ldots, f_P)$. Parallel to (5), define r_i via

$$f_i(x) = \mu_i + \sum_{0<|u|\le h} f_{i,u}(x) + r_i.$$

The following theorem gives a central limit theorem for a multivariate f.

COROLLARY 3.6. *Suppose that f is a continuous function from $[0,1]^K$ to $\mathscr{R}^P$, $\hat{\mu}$ in* (1) *is based on a randomized orthogonal array in* (2) *without coincidence defect, λ is fixed or $\lambda = o(n)$. Then, as $N \to \infty$,*

$$N^{1/2}(\hat{\mu} - \mu) \to N(0, \Sigma),$$

where Σ is a $P \times P$ matrix with the (i, j)th element $\Sigma_{i,j} = \int r_i(x) r_j(x)\,dx$.

The normality of multivariate f follows from the fact that any linear combinations of $(f_1, \ldots, f_P)$ has a limiting normal distribution.

4. A central limit theorem for *U* designs. Next, we derive a central limit theorem for U designs. As before, we assume f is a continuous function from $[0,1]^K$ to $\mathscr{R}$. Let H be an $OA(N, K, n, h)$ free of coincidence defect and $\lambda = N/n^h$. Take $X_1, \ldots, X_N$ in (1) to be the design points from a U design constructed in (3). For fixed K and h, we suppose there is a sequence of H such that N and n tend to infinity with λ/n tending to zero. Analogous to Lemma 3.2, we first derive the conditional density function of X_s given $X_1, \ldots, X_{s-1}$.

LEMMA 4.1. *For a U design in* (3) *from H, the conditional density of X_s given $X_1, \ldots, X_{s-1}$ is*

$$g_s(d_1, \ldots, d_K) = \sum_{i_1, \ldots, i_K = 0}^{s-1} b_s(i_1, \ldots, i_K, M_{s-1}) I\bigl(d_1 \in D^1_{i_1}, \ldots, d_K \in D^K_{i_K}\bigr),$$

where $D_i^k = \delta_n(X_i^k) \setminus \{\bigcup_{j=1}^{s-1} \delta_N(X_j^k)\}$ *for* $i = 1, \ldots, s-1$ *and* $k = 1, \ldots, K$, $D_i^k = \delta_N(X_{i-(s-1)}^k)$ *for* $i = s, \ldots, 2s-2$ *and* $k = 1, \ldots, K$, $D_0^k = [0, 1) \setminus \{\bigcup_{j=1}^{s-1} \delta_n(X_j^k)\}$ *for* $k = 1, \ldots, K$ *and* $b_s(\cdot)$ *is a deterministic function on* $d_1, \ldots, d_K, M_{s-1}$ *with*

$$b_s(i_1, \ldots, i_k, M_{s-1}) = \begin{cases} 0, & \textit{there is a } k \textit{ such that } i_k > s-1, \\ 1 + O(n^{-1}), & i_1, \ldots, i_K \le s-1, |w| < h, \\ O(1), & i_1, \ldots, i_K \le s-1, |w| = h, \\ 0, & |w| > h, \max(|w_1|, \ldots, |w_{s-1}|) > h, \\ O(n^{|w|}/N), & \textit{otherwise}, \end{cases}$$

where $w(i_1, \ldots, i_K)$ *is the dimensions of nonzero elements in* $(i_1, \ldots, i_K)$, $w = \{k : i_k \neq 0\}$, $w_z(i_1, \ldots, i_K) = \{k : i_k = z\}$ *and* $w = \bigcup w_z$.

The proof of Lemma 4.1 is given in the Appendix. Analogous to Lemmas 3.3 and 3.4, we state two lemmas for the conditional expectation of $f(X_s)$ given points $X_1, \ldots, X_{s-1}$ from a U design.

LEMMA 4.2. *For any bounded function* f *and* $s > 1$, *as* $N \to \infty$,

$$E_{\mathrm{UD}}\{f(X_s)|X_1, \ldots, X_{s-1}\} = E_{\mathrm{IID}}\{f(X_s)\} + O(n^{-1}).$$

LEMMA 4.3. *Let*

$$\bar{R} = N^{-1} \sum_{i=1}^{N} r(X_i).$$

Then for any positive integer p,

$$E_{\mathrm{UD}}\{(N^{1/2}\bar{R})^p\} = E_{\mathrm{IID}}\{(N^{1/2}\bar{R})^p\} + o(1).$$

Lemma 4.2 is a direct consequence of Lemma 4.1. A sketch to prove Lemma 4.3 is given in the Appendix. A central limit theorem for U designs is given below.

THEOREM 4.4. *Suppose that* f *is a continuous function from* $[0, 1]^K$ *to* $\mathscr{R}$, $\hat{\mu}$ *in* (1) *is based on a* U *design in* (3) *without coincidence defect*, λ *is fixed or* $\lambda = o(n)$. *Then, as* $N \to \infty$,

$$N^{1/2}(\hat{\mu} - \mu) \to N\left(0, \int r(x)^2\, dx\right).$$

PROOF. $E\{N^{1/2}(\hat{\mu} - \mu)\} = 0$ and $\mathrm{var}\{N^{1/2}(\hat{\mu} - \mu)\}$ tends to $\int r(x)^2\, dx$. From Lemma 4.3 and Owen (1980), for $p = 1, 2, \ldots,$

$$\begin{aligned} E_{\mathrm{UD}}\{(N^{1/2}\bar{R})^p\} &= E_{\mathrm{IID}}\{(N^{1/2}\bar{R})^p\} + o(1) \\ &= \begin{cases} 0 + o(1), & p = 1, 3, 5, \ldots, \\ \sigma^p (p-1)!! + o(1), & p = 2, 4, 6, \ldots, \end{cases} \end{aligned}$$

where $\sigma^2 = \int r(x)^2\,dx$ with

$$\limsup_{p\to\infty} \bigl(\sigma^p (p-1)!!\bigr)^{1/p}/p = 0.$$

From Lemma 3.1, $N^{1/2}\bar{R}$ from U design has the same limiting distribution as $N^{1/2}\bar{R}$ where the points are generated identically and independently, which yields a normal distribution. $\square$

Similarly, the result can be extended to a multivariate f.

COROLLARY 4.5. *Suppose that f is a continuous function from $[0, 1]^K$ to $\mathscr{R}^P$, $\hat{\mu}$ in (1) is based on a U design in (3) without coincidence defect, λ is fixed or $\lambda = o(n)$. Then, as $N \to \infty$,*

$$N^{1/2}(\hat{\mu} - \mu) \to N(0, \Sigma),$$

where Σ is a $P \times P$ matrix with the (i, j)th element $\Sigma_{i,j} = \int r_i(x) r_j(x)\,dx$.

5. Numerical illustration. We provide two numerical examples to validate the central limit theorems in Sections 3 and 4. In the first experiment, the orthogonal array with 18 runs, three levels and strength two in Table 1 of Section 2 is used to generate a randomized orthogonal array and a U design. Consider estimating the mean output of a function [Cox, Park and Singer (2001)]

$$f = x_1/\Bigl[2\Bigl\{\sqrt{1 + (x_2 + x_3^2)x_4/x_1^2} - 1\Bigr\}\Bigr] + x_1 + 3x_4,$$

where $x_1, \ldots, x_4$ follow the uniform distribution on $[0, 1)$. The true value of μ is approximately $2 \cdot 160$, computed from a large ordinary Latin hypercube design. We compute $\hat{\mu} = \sum_{i=1}^{18} f(X_i)/18$ as in (1) for the two designs. This procedure is repeated for 100,000 times. The density plots of $\hat{\mu}$ for the two designs are shown in Figure 3, where both distributions are close to a normal distribution.

In the second experiment, an orthogonal array with 25 runs, five levels and strength two is used for generating a randomized orthogonal array and a U design. We estimate the mean output μ of the Branin function [Branin (1972)]

$$f = \left(x_2 - \frac{5.1}{4\pi^2}x_1^2 + \frac{5}{\pi}x_1 - 6\right) + 10\left(1 - \frac{1}{8\pi}\right)\cos(x_1) + 10$$

on the domain $[-5, 10] \times [0, 15]$. The true value of μ is approximately $54 \cdot 31$, computed from a large grid design. We compute $\hat{\mu} = \sum_{i=1}^{25} f(X_i)/25$ for the two designs. This procedure is repeated for 100,000 times. The density plots of $\hat{\mu}$ from

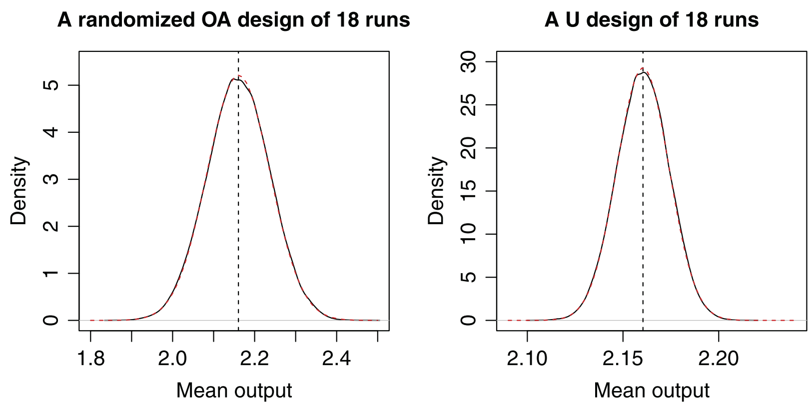

FIG. 3. *Density plots of $\hat{\mu}$ based on a randomized orthogonal array (left) and a U design (right) from the orthogonal array given in Table 1, both of which are close to a normal distribution.*

the two designs are shown in Figure 4, both of which are close to a normal distribution.

6. Conclusions. A new central limit theorem has been derived for orthogonal array based space-filling designs. One might be interested in extending our technique to derive a central limit theorem for scrambled nets [Owen (1997)]. Another possible direction for future research is to use this new result to study validation of sample average approximation solutions for a stochastic program [Shapiro, Dentcheva and Ruszczyński (2009)]. Finally, it is an important problem to estimate the variance $\int r(x)^2\,dx$ from a U design.

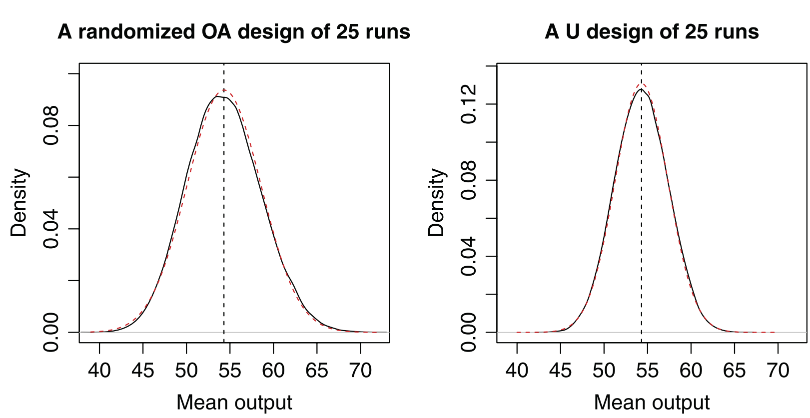

FIG. 4. *Density plots of $\hat{\mu}$ based on a randomized orthogonal array (left) and a U design (right) from an orthogonal array with 25 runs, both of which are close to a normal distribution.*

APPENDIX

A.1. Proof of Lemma 3.2. We first work on the $g_s(d_1, \dots, d_K)$ on the cells $D = (D^1, \dots, D^K)$, where $D^k \in \{[0, 1/n), [1/n, 2/n), \dots, [(n-1)/n, 1)\}$ for $k = 1, \dots, K$. Consider the matrix $\tilde{H}$ obtained by dropping rows $\gamma^{-1}(1), \dots, \gamma^{-1}(s-1)$ of H. $g_s(d_1, \dots, d_K)$ is nonzero if $(\lfloor nd_1 \rfloor, \dots, \lfloor nd_K \rfloor)$ can be obtained from a row of $\tilde{H}$ by some operators π_k, which means $\lfloor nd_1 \rfloor = \pi_1(H_r^1), \dots, \lfloor nd_K \rfloor = \pi_K(H_r^K)$ for a row $H_r = (H_r^1, \dots, H_r^K)$ in $\tilde{H}$. Let x be the number of rows in $\tilde{H}$ from which $(\lfloor nd_1 \rfloor, \dots, \lfloor nd_K \rfloor)$ can be obtained. The value of $g_s(d_1, \dots, d_K)$ is closely related to x because X_s has the same probability $1/(N - (s-1))$ being permuted from each row of $\tilde{H}$.

Because level permutations do not affect the result on whether two rows of H take same value in a particular column, x is closely related to M_s and w. Below we compute x by types of w.

For the type of $|w| = 0$, since there are at most $(s-1)(N/n - 1)$ rows taking value in $\bigcup_{i=1}^{s-1}\{H^k_{\gamma^{-1}(i)}\}$ in the kth column for $k = 1, \dots, K$, $N - (s-1) - K(s-1)(N/n - 1) \le x \le N - (s-1)$ and $x = N(1 - O(n^{-1}))$. Since the volume of cells for $w = \phi$ is $1 - O(n^{-1})$ and $g_s(d)$ is the same in such cells, $g_s(d_1, \dots, d_K) = 1 + O(n^{-1})$.

For the type of $|w| = 1$, without loss of generality, assume $w = \{1\}$ and $w_1 = \{1\}$. There are at least $N/n - (s-1)$ rows and at most $N/n - 1$ rows taking value $\{H^1_{\gamma^{-1}(1)}\}$ in the first column. Out of those rows, there are at most $(s-1)(N/n^2 - 1)$ rows taking value in $\bigcup_{i=1}^{s-1}\{H^k_{\gamma^{-1}(i)}\}$ in the kth column for $k = 2, \dots, K$. Therefore, $x = N/n(1 - O(n^{-1}))$. Since the volume of cells for $w = \{1\}$ is $n^{-1}(1 - O(n^{-1}))$ and $g_s(d)$ is the same in such cells, $g_s(d_1, \dots, d_K) = 1 + O(n^{-1})$. Similarly, we obtain $g_s(d_1, \dots, d_K) = 1 + O(n^{-1})$ for any w with $|w| < h$.

For the type of $|w| = h$, there are at most N/n^h rows in $\tilde{H}$ that match X_s in w. Since the volume of cells is $n^{-h}(1 + O(n^{-1}))$, $g_s(d_1, \dots, d_K) = O(1)$.

For the type of $|w| > h$, because H is free of coincidence defect, there is zero or one row in $\tilde{H}$ that matches X_s in w. Since the volume of cells is $n^{-|w|}(1 + O(n^{-1}))$, $g_s(d_1, \dots, d_K) = O(n^{|w|}/N)$. A special case is when $|w| > h$ and $|w_z| > h$ for a z with $1 \le z \le s-1$. In this case, no row in $\tilde{H}$ can match X_s and $g_s(d_1, \dots, d_K) = 0$.

Thus

$$g_s(d_1, \dots, d_K) = \begin{cases} 1 + O(n^{-1}), & |w| < h, \\ O(1), & |w| = h, \\ 0, & |w| > h, \max(|w_1|, \dots, |w_{s-1}|) > h, \\ O(n^{|w|}/N), & \text{otherwise}. \end{cases}$$

Furthermore, the value of $g_s(d_1,\dots,d_K)$ is the same in any regions defined by $D^1_{i_1}\times\cdots\times D^K_{i_K}$ in which $i_k=0,1,\dots,s-1$ for $k=1,\dots,K$. Thus, write

$$g_s(d_1,\dots,d_K)=\sum_{i_1,\dots,i_K=0}^{s-1} b_s(i_1,\dots,i_K,M_{s-1})I\bigl(d_1\in D^1_{i_1},\dots,d_K\in D^K_{i_K}\bigr),$$

where

$$b_s(i_1,\dots,i_K,M_{s-1})=\begin{cases}1+O(n^{-1}), & |w|<h,\\ O(1), & |w|=h,\\ 0, & |w|>h,\max\bigl(|w_1|,\dots,|w_{s-1}|\bigr)>h,\\ O\bigl(n^{|w|}/N\bigr), & \text{otherwise,}\end{cases}$$

and $b_s(\cdot)$ is a deterministic function on $d_1,\dots,d_K$ and M_{s-1}.

A.2. Proof of Lemma 3.4. The idea to prove Lemma 3.4 is as follows. Note that

$$(8)\qquad E_{\mathrm{ROA}}\bigl\{\bigl(N^{1/2}\bar{R}\bigr)^p\bigr\}=N^{-p/2}\sum_{a_1+\cdots+a_N=p,a_1,\dots,a_N\ge 0} E_{\mathrm{ROA}}\left(\prod_{i=1}^N r_i^{a_i}\right).$$

Let t be the number of a_i's being one and s be the number of nonzero a_i's; there are at most $O(N^s)$ terms in (8). Thus it suffices to show that for any $s\le p$,

$$E_{\mathrm{ROA}}\left(\prod_{i=1}^s r_i^{a_i}\right)-E_{\mathrm{IID}}\left(\prod_{i=1}^s r_i^{a_i}\right)=o\bigl(N^{p/2-s}\bigr).$$

If $t=0$, then $s\le p/2$. From Lemma 3.3,

$$E_{\mathrm{ROA}}\left(\prod_{i=1}^s r_i^{a_i}\right)-E_{\mathrm{IID}}\left(\prod_{i=1}^s r_i^{a_i}\right)=O\bigl(n^{-1}\bigr)=o\bigl(N^{p/2-s}\bigr).$$

If $t>0$, $E_{\mathrm{IID}}(\prod_{i=1}^s r_i^{a_i})=0$. Thus it suffices to show that for any $1\le t\le s\le p$, $t+a_{t+1}+\cdots+a_s=p, a_{t+1},\dots,a_s>1$,

$$E_{\mathrm{ROA}}\left(\prod_{i=1}^t r_i\prod_{i=t+1}^s r_i^{a_i}\right)=o\bigl(N^{p/2-s}\bigr).$$

Because $t+2(s-t)\le p$, $-t/2\le p/2-s$. Since $r_i=\sum_{|u|>h} f_u(x_i)$, and we can rearrange the order of $\prod_{i=1}^t r_i$ by sorting $|u_i|$, it suffices to show for any $1\le t\le s$, $|u_1|\ge|u_2|\ge\cdots\ge|u_t|>h$ and continuous functions $f,q_{t+1},\dots,q_s$,

$$E_{\mathrm{ROA}}\left\{\prod_{i=1}^t f_{u_i}(x_i)\prod_{i=t+1}^s q_i(x_i)\right\}=o\bigl(N^{-t/2}\bigr).$$

From Lemma 3.3, if $s > t$,

$$
\begin{aligned}
&E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i) \prod_{i=t+1}^{s} q_i(x_i)\right\} \\
&\quad = E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i) \prod_{i=t+1}^{s-1} q_i(x_i) E_{\mathrm{ROA}}\bigl(q_s(x_s)|x_1, \ldots, x_{s-1}\bigr)\right\} \\
&\quad = E_{\mathrm{ROA}}\left[\prod_{i=1}^{t} f_{u_i}(x_i) \prod_{i=t+1}^{s-1} q_i(x_i)\bigl\{E_{\mathrm{IID}}\bigl(q_s(x_s)\bigr) + O\bigl(n^{-1}\bigr)\bigr\}\right] \\
&\quad = E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i) \prod_{i=t+1}^{s-1} q_i(x_i)\right\} E_{\mathrm{IID}}\bigl(q_s(x_s)\bigr) + O\bigl(n^{-1}\bigr).
\end{aligned}
$$

Inducting on s, it is not hard to conclude that it is suffice to show

$$
E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i)\right\} = o\bigl(N^{-t/2}\bigr). \tag{9}
$$

To show (9), first express

$$
E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i)\right\} = E_{\mathrm{ROA}}\left[\prod_{i=1}^{t-1} f_{u_i}(x_i) E_{\mathrm{ROA}}\bigl\{f_{u_t}(X_t)|X_1, \ldots, X_{t-1}\bigr\}\right].
$$

From Lemma 3.2,

$$
\begin{aligned}
&E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i)\right\} \\
&\quad = \sum_{i_1,\ldots,i_K} E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t-1} f_{u_i}(X_i) b_t(i_1, \ldots, i_K, M_{t-1})\left(\int_{D_t} f_{u_t}(y)\,dy\right)\right\},
\end{aligned} \tag{10}
$$

where $D_t = D_{i_1}^1 \times \cdots \times D_{i_K}^K$ and $D_i^k = \delta_n(X_i^k)$. From (4),

$$
\int_{\tilde{D}^1 \times \cdots \times \tilde{D}^K} f_u(y)\,dy = 0
$$

if there is at least one k such that $\tilde{D}^k = [0, 1)$ and $k \in u$. Therefore,

$$
\int_{D_0^1 \times \tilde{D}^2 \times \cdots \times \tilde{D}^K} f_{u_t}(y)\,dy = -\sum_{j=1}^{t-1} \int_{\delta_n(X_j^1) \times \tilde{D}^2 \times \cdots \times \tilde{D}^K} f_{u_t}(y)\,dy.
$$

Consequently, $\int_{D_t} f_{u_t}(y)\,dy$ has order $O(n^{-|w \cup u_t|})$ where $w(d_1, \ldots, d_K) = \{k : d_k > 0\}$, and (10) has order $O(N^{-1})$.

We can further reduce the order of (10) if $t > 1$. For any term in the sum of (10),

$$
\begin{aligned}
&E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t-1} f_{u_i}(X_i) b_t(i_1,\ldots,i_K,M_{t-1})\left(\int_{D_t} f_{u_t}(y)\,dy\right)\right\}\\
&\quad=\sum_{j_1,\ldots,j_K} E_{\mathrm{ROA}}\Bigg[\prod_{i=1}^{t-2} f_{u_i}(X_i) b_{t-1}(j_1,\ldots,j_K,M_{t-2})\\
&\qquad\qquad\times\left\{\int_{D_{t-1}} b_t(i_1,\ldots,i_K,M_{t-1})\right.\\
&\qquad\qquad\qquad\left.\times\left(\int_{D_t} f_{u_t}(y_t)\,dy_t\right) f_{u_{t-1}}(y_{t-1})\,dy_{t-1}\right\}\Bigg],
\end{aligned}\tag{11}
$$

where $D_{t-1} = D_{j_1}^1 \times \cdots \times D_{j_K}^K$ and $D_j^k = \delta_n(X_i^k)$. In any region D_{t-1}, $b_t(\cdot)$ becomes a deterministic function on $i_1,\ldots,i_K, M_{t-2}$ with the same order as in Lemma 3.2. Let $b_t'(\cdot)$ denote this function. Then

$$
\begin{aligned}
&E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t-1} f_{u_i}(X_i) b_t(i_1,\ldots,i_K,M_{t-1})\left(\int_{D_t} f_{u_t}(y)\,dy\right)\right\}\\
&\quad=\sum_{j_1,\ldots,j_K} E_{\mathrm{ROA}}\Bigg[\prod_{i=1}^{t-2} f_{u_i}(X_i) b_{t-1}(j_1,\ldots,j_K,M_{t-2}) b_t'(i_1,\ldots,i_K,M_{t-2})\\
&\qquad\qquad\times\left\{\int_{D_{t-1}}\left(\int_{D_t} f_{u_t}(y_t)\,dy_t\right) f_{u_{t-1}}(y_{t-1})\,dy_{t-1}\right\}\Bigg].
\end{aligned}
$$

So far we have showed the first two steps to reduce the order of magnitudes for $E_{\mathrm{ROA}}\{\prod_{i=1}^t f_{u_i}(x_i)\}$. In (10), we took $f_{u_t}(X_t)$ out of the product and reached the $O(N^{-1})$ order. We keep taking out the $f_{u_i}(X_i)$ terms as in (11) and work on a more general formula as follows:

$$
\begin{aligned}
&\left(\prod_{l=1}^{L} |D_l|\right)^{-1} E_{\mathrm{ROA}}\Bigg[\prod_{i=1}^{t} f_{u_i}(X_i)\rho(M_t)\\
&\qquad\times\left\{\int_{\prod_{l=1}^L D_l}\left(\prod_{l=1}^{L} f_{v_l}(y_l)\right) dy_1\cdots dy_L\right\}\Bigg],
\end{aligned}\tag{12}
$$

where $\rho(M_t)$ is a deterministic function on M_t which has order $O(1)$ for any M_t. Suppose G is an arbitrary term by (12) with the following parameters: $0 \le t \le p$, $|u_1| \ge |u_2| \ge \cdots \ge |u_t| > h$, L is a nonnegative integer, $v_l \subseteq \{1,\ldots,K\}$, $|v_l| > h$, $D_l = D_l^1 \times \cdots \times D_l^K$ and D_l^k is either $[0,1)$ or $\delta_n(X_i^k)$ with $1 \le i \le t$, or $\delta_n(y_i^k)$ with $l < i \le L$. Suppose that C is an $t \times K$ zero–one matrix with the (i,k)th element being one if and only if $k \in u_i$ and for any $1 \le l \le L$, $D_l^k \ne \delta_n(X_i^k)$. Let c_i

be the number of ones in the ith row of C, and let $\theta = \sum_{i=1}^{t} c_i/|u_i|$. The following two lemmas give the orders of G by the number of ones in C.

LEMMA A.1. *The quantity G has order $O(N^{-\theta/2})$.*

PROOF. We show this by induction on t. If $t = 0$, then $\theta = 0$, and the result clearly holds. Next, assume the result holds for $t = 0, \dots, z-1$ with $z \geq 1$. It suffices to show the result holds for $t = z$. Express

$$\begin{aligned}
G &= \left(\prod_{l=1}^{L} |D_l|\right)^{-1} E_{\mathrm{ROA}}\left[\prod_{i=1}^{t} f_{u_i}(X_i)\rho(M_t)\left\{\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\,dy_1\cdots dy_L\right\}\right] \\
&= \left(\prod_{l=1}^{L} |D_l|\right)^{-1} \\
&\quad \times E_{\mathrm{ROA}}\left[\prod_{i=1}^{t-1} f_{u_i}(X_i)\right. \\
&\qquad \times E_{\mathrm{ROA}}\left\{\rho(M_t) f_{u_t}(X_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\,dy_1\cdots dy_L\right)\right| \\
&\qquad\qquad \left.\left.\{X_1, \dots, X_{t-1}\}\right\}\right].
\end{aligned}$$

From Lemma 3.2 and similar to (10) and (11),

$$\begin{aligned}
&E_{\mathrm{ROA}}\left\{\rho(M_t) f_{u_t}(X_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\,dy_1\cdots dy_L\right)\middle|\{X_1, \dots, X_{t-1}\}\right\} \\
&\quad = \int g(x_t)\rho(M_t) f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t \\
&\quad = \sum_{i_1,\dots,i_K} b_t(i_1, \dots, i_K, M_{t-1}) \\
&\qquad \times \int_{D_{L+1}} \rho(M_t) f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t,
\end{aligned}$$

where $g(x_t)$ is the conditional density of X_t, $D_{L+1} = D_{L+1}^1 \times \cdots \times D_{L+1}^K$, $D_{L+1}^k = \delta_n(X_{i_k}^k)$ if $i_k > 0$ and $D_{L+1}^k = [0, 1) \setminus \bigcup_{i=1}^{t-1} \delta_n(X_i^k)$ if $i_k = 0$.

In any D_{L+1}, $\rho(M_t)$ is a deterministic function on M_{t-1}. Let $\rho_{i_1,\dots,i_K}(M_{t-1})$ denote this function. Then for any M_{t-1}, $\rho_{i_1,\dots,i_K}(M_{t-1}) = O(1)$. Thus

$$\begin{aligned}G = \sum_{i_1,\dots,i_K} \left(\prod_{l=1}^{L} |D_l|\right)^{-1}& \\ \times E_{\mathrm{ROA}}\Bigg[\prod_{i=1}^{t-1} f_{u_i}(X_i) b_t(i_1,\dots,i_K, M_{t-1}) \rho_{i_1,\dots,i_K}(M_{t-1})& \\ \times \int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t\Bigg].&\end{aligned} \tag{13}$$

If $i_1 = 0$, $D_{L+1}^1 = [0,1) \setminus \bigcup_{i=1}^{t-1} \delta_n(X_i^1)$. If additionally $k \notin u_t$,

$$\begin{aligned}&\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t \\ &\quad = \rho_0(M_{t-1}) \\ &\qquad \times \int_{[0,1)\times D_{L+1}^2 \times \cdots \times D_{L+1}^K} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t,\end{aligned}$$

where $\rho_0(M_{t-1}) = O(1)$. If $k \in u_t$,

$$\begin{aligned}&\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t \\ &\quad = \int_{[0,1)\times D_{L+1}^2 \times \cdots \times D_{L+1}^K} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t \\ &\qquad - \sum_{j=1}^{t-1} \Bigg\{\rho_j(M_{t-1}) \\ &\qquad\qquad \times \int_{D_j^1 \times D_{L+1}^2 \times \cdots \times D_{L+1}^K} f_{u_t}(x_t) \\ &\qquad\qquad\qquad \times \left(\int_{\prod_{l=1}^{L} D_l} \prod_{l=1}^{L} f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t\Bigg\},\end{aligned}$$

where $\rho_j(M_{t-1}) = O(1)$ for $j = 1,\dots,t-1$. Let

$$\tilde{b}_t(i_1,\dots,i_k) = \begin{cases} 1, & |w| \le h, \\ n^{|w|}/N, & |w| > h. \end{cases}$$

Then $\tilde{b}_t$ is not related to M_{t-1} and $\tilde{b}_t(0, i_2, \dots, i_K) \le \tilde{b}_t(j, i_2, \dots, i_K)$ for any $j > 0$.

From the arguments above, it suffices to show

$$
\begin{aligned}
&J(i_1,\dots,i_K)\\
&\qquad =\tilde{b}_t(i_1,\dots,i_K)\left(\prod_{l=1}^{L}|D_l|\right)^{-1}\\
&\qquad\qquad \times E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t-1} f_{u_i}(X_i)\rho(M_{t-1})\right.\\
&\qquad\qquad\qquad \left.\times\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^{L} D_l}\prod_{l=1}^{L} f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t\right\}
\end{aligned}\tag{14}
$$

has order $O(N^{-\theta/2})$ for any $i_1,\dots,i_K=0,1,\dots,t-1$, $\rho(M_{t-1})=O(1)$, $D_{L+1}=D_{L+1}^1\times\cdots\times D_{L+1}^K$, $D_{L+1}^k=\delta_n(X_{i_k}^k)$ if $i_k>0$, $k=1,\dots,K$, $D_{L+1}^1=[0,1)$ if $i_1=0$ and $D_{L+1}^k=[0,1)\setminus\bigcup_{j=1}^{t-1}\delta_n(X_j^k)$ if $i_k=0$, $k=2,\dots,K$.

From similar arguments, it suffices to show (14) has order $O(N^{-\theta/2})$ for any $i_1,\dots,i_K=0,1,\dots,t-1$, $\rho(M_{t-1})=O(1)$, $D_{L+1}=D_{L+1}^1\times\cdots\times D_{L+1}^K$, $D_{L+1}^k=\delta_n(X_{i_k}^k)$ if $i_k>0$ and $D_{L+1}^k=[0,1)$ if $i_k=0$, $k=1,\dots,K$.

If $i_k\neq 0$ and $k\notin u_t$, then any term that can be written as $J(i_1,\dots,i_K)$ has smaller or the same order than a term that can be written as $J(i_1,\dots,i_{k-1},0,i_{k+1},\dots,i_K)$. If $i_k=0$ and the (t,k)th element of C is one, from (4), $J=0$. Thus it suffices to consider $J(i_1,\dots,i_K)$ with $i_k=0,\dots,t-1$ for $k\in u_t$ and the (t,k)th element of C being zero, $i_k=1,\dots,t-1$ for $k\in u_t$ and the (t,k)th element of C being one and $i_k=0$ for $k\notin u_t$. Clearly, $w\subseteq u_t$ and $c_t\le|w|\le|u_t|$.

Let

$$
\begin{aligned}
G'_{i_1,\dots,i_K}=\left(\prod_{l=1}^{L+1}|D_l|\right)^{-1}&E_{\mathrm{ROA}}\left[\prod_{i=1}^{t-1} f_{u_i}(X_i)\rho(M_{t-1})\right.\\
&\left.\times\left\{\int_{(\prod_{l=1}^{L} D'_l)\times D_{L+1}}\prod_{l=1}^{L+1} f_{v_l}(y_l)\,dy_1\cdots dy_{L+1}\right\}\right],
\end{aligned}
$$

where $v_{L+1}=u_t$ and

$$
D_l^{k\prime}=\begin{cases}\delta_n\big(y_{L+1}^k\big), & \text{if } D_l^k=\delta_n\big(X_t^k\big),\\ D_l^k, & \text{otherwise.}\end{cases}
$$

Then J in (14) can be expressed as

$$
J(i_1,\dots,i_K)=\tilde{b}_t(i_1,\dots,i_K)n^{-|w|}G'_{i_1,\dots,i_K}.
$$

For any $(i_1,\dots,i_K)$, $G'_{i_1,\dots,i_K}$ is a term by (12). Furthermore, the matrix associated with $G'_{i_1,\dots,i_K}$, denoted as $C'_{i_1,\dots,i_K}$, is a $(t-1)\times K$ matrix with equal or fewer elements of ones than the first $t-1$ rows of C. If $i_k=z>0$, the (z,k)th element of $C'_{i_1,\dots,i_K}$ is zero. Other elements of $C'(D_{L+1})$ are the same with that of C. Let c'_i be the number of ones in the ith row of $C'_{i_1,\dots,i_K}$, and let $\theta' = \sum_{i=1}^{t-1} c'_i/|u_i|$, and we have

$$\theta' \geq \theta - c_t/|u_t| - |w|/|u_t|.$$

By induction,

$$G'_{i_1,\dots,i_K} = O\bigl(N^{-(\theta - c_t/|u_t| - |w|/|u_t|)/2}\bigr) = O\bigl(N^{-\theta/2+1}\bigr) \tag{15}$$

and

$$G'_{i_1,\dots,i_K} = O\bigl(N^{-(\theta - c_t/|u_t| - |w|/|u_t|)/2}\bigr) = O\bigl(N^{-\theta/2} n^{|w|}\bigr). \tag{16}$$

Consequently, J in (14) has order $O(N^{-\theta/2})$. This completes the proof. □

The result of Lemma A.1 is improved by Lemma A.2.

LEMMA A.2. *If $c_t > 0$, G has order $o(N^{-\theta/2})$.*

PROOF. It suffices to show J in (14) has order $o(N^{-\theta/2})$. Since $c_t > 0$, (16) becomes

$$G'_{i_1,\dots,i_K} = O\bigl(N^{-\theta/2+|w|/(h+1)}\bigr) = o\bigl(N^{-\theta/2} n^{|w|}\bigr).$$

Therefore, for $|w| \leq h$, $J = o(N^{-\theta/2})$. When $|w| > h$ and $c_t < |u_t|$, (15) becomes

$$G'_{i_1,\dots,i_K} = O\bigl(N^{-(\theta - c_t/|u_t| - |w|/|u_t|)/2}\bigr) = o\bigl(N^{-\theta/2+1}\bigr), \tag{17}$$

and $J = o(N^{-\theta/2})$. When $|w| > h$ and there is a j such that $|w_j| > h$, $b_t(i_1, \dots, i_K)$ in (13) is zero and $J = 0$.

It remains to show $G'_{i_1,\dots,i_K} = o(N^{-\theta/2+1})$ for $c_t = |w| = |u_t|$ and $\max(|w_i|) \leq h$. Let $\{(j_1, k_1), \dots, (j_z, k_z)\}$ denote the elements of $C'_{d_1,\dots,d_K}$ that are different from those of the first $t-1$ rows of C. When $|u_{j_x}| > |u_t|$ for an x with $1 \leq x \leq z$, (15) becomes

$$G'_{d_1,\dots,d_K} = O\bigl(N^{-\{\theta - 1/|u_{j_x}| - (c_t+|w|-1)/|u_t|\}/2}\bigr) = o\bigl(N^{-\theta/2+1}\bigr).$$

When $z < |w|$, (15) becomes

$$G'_{i_1,\dots,i_K} = O\bigl(N^{-(\theta - z/|u_t| - |w|/|u_t|)/2}\bigr) = o\bigl(N^{-\theta/2+1}\bigr).$$

Finally, when $z = |w|$ and $|u_{j_1}| = \cdots = |u_{j_z}| = |u_t|$, since $\max_j\{|w_j|\} \leq h$, $\{j_1, \dots, j_z\}$ are not all equal to each other. Consequently, there is at least one x such that $0 < c'_{j_x} < |u_{j_x}| = |u_t|$. From (17), $G'_{d_1,\dots,d_K} = o(N^{-\theta/2+1})$. Combining all cases, $J = o(N^{-\theta/2})$. This completes the proof. □

We now give the proof of Lemma 3.4.

PROOF. We have argued in (9) that it suffices to show for any $1 \le t \le p$, $|u_1| \ge |u_2| \ge \cdots \ge |u_t| > h$ and continuous functions f,

$$E_{\mathrm{ROA}}\left\{\prod_{i=1}^{t} f_{u_i}(x_i)\right\} = o(N^{-t/2}).$$

$E_{\mathrm{ROA}}\{\prod_{i=1}^{t} f_{u_i}(x_i)\}$ is a term by (12) with $\theta = t$ and $c_t = |u_t| > 0$. From Lemma A.2, $E_{\mathrm{ROA}}\{\prod_{i=1}^{t} f_{u_i}(x_i)\} = o(N^{-t/2})$. This completes the proof. $\square$

A.3. Proof of Lemma 4.1. Similar to the argument in the proof of Lemma 3.2, we have that

$$\begin{aligned} &g_s(d_1, \dots, d_K) \\ &\quad = \begin{cases} 1 + O(n^{-1}), & |w| < h, \\ O(1), & |w| = h, \\ 0, & |w| > h, \max(|w_1|, \dots, |w_{s-1}|) > h, \\ O(n^{|w|}/N), & \text{otherwise.} \end{cases} \end{aligned}$$

However, a special case is when there is a k such that $i_k > s - 1$. From (3), two rows cannot be in the same subdivision with length $1/N$. Thus $g_s = 0$ in this case.

Next, the density is uniform in each of the $D_{i_1}^1 \times \cdots \times D_{i_K}^K$ regions, where $i_1, \dots, i_K = 0, \dots, 2s - 2$. Thus we can write

$$g_s(d_1, \dots, d_K) = \sum_{i_1,\dots,i_K=0}^{2s-2} b_s(i_1, \dots, i_K, M_{s-1}) I(d_1 \in D_{i_1}^1, \dots, d_K \in D_{i_K}^K),$$

where

$$b_s(i_1, \dots, i_K, M_{s-1}) = \begin{cases} 0, & \text{there is a } k \text{ such that } i_k > s-1, \\ 1 + O(n^{-1}), & i_1, \dots, i_K \le s-1, |w| < h, \\ O(1), & i_1, \dots, i_K \le s-1, |w| = h, \\ 0, & |w| > h, \max(|w_1|, \dots, |w_{s-1}|) > h, \\ O(n^{|w|}/N), & \text{otherwise,} \end{cases}$$

and $b_s(\cdot)$ is a deterministic function on $d_1, \dots, d_K$ and M_{s-1}.

A.4. A sketch to prove Lemma 4.3. Suppose G is an arbitrary term given by

$$\begin{aligned} &\left(\prod_{l=1}^{L} |D_l|\right)^{-1} \\ &\quad \times E_{\mathrm{UD}}\left[\prod_{i=1}^{t} f_{u_i}(X_i)\rho(M_t)\left\{\int_{\prod_{l=1}^{L} D_l} \left(\prod_{l=1}^{L} f_{v_l}(y_l)\right) dy_1 \cdots dy_L\right\}\right], \end{aligned} \tag{18}$$

with the following parameters: $\rho(M_t)$ is a deterministic function on M_t which has order $O(1)$ for any M_t, $0 \le t \le p$, $|u_1| \ge |u_2| \ge \cdots \ge |u_t| > h$, L is a nonnegative integer, $v_l \subseteq \{1, \dots, K\}$, $|v_l| > h$, $D_l = D_l^1 \times \cdots \times D_l^K$ and D_l^k is either $[0, 1)$ or $\delta_n(X_i^k)$ with $1 \le i \le t$, or $\delta_n(y_i^k)$ with $l < i \le L$, or $\delta_N(X_i^k)$ with $1 \le i \le t$, or $\delta_N(y_i^k)$ with $l < i \le L$. Suppose that C is an $t \times K$ zero–one matrix with the (i, k)th element being one if and only if $k \in u_i$ and for any $1 \le l \le L$, D_l^k is neither $\delta_n(X_i^k)$ nor $\delta_N(X_i^k)$. Let c_i be the number of ones in the ith row of C, and let $\theta = \sum_{i=1}^t c_i/|u_i|$. The following two lemmas give the order of G.

LEMMA A.3. *The quantity G has order $O(N^{-\theta/2})$.*

PROOF. We show this by induction on t. If $t = 0$, then $\theta = 0$, and the result clearly holds. Next, assume the result holds for $t = 0, \dots, z - 1$ with $z \ge 1$. It suffices to show the result holds for $t = z$. Express

$$
\begin{aligned}
G &= \left(\prod_{l=1}^L |D_l|\right)^{-1} E_{\mathrm{UD}}\left[\prod_{i=1}^t f_{u_i}(X_i)\rho(M_t)\left\{\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\, dy_1 \cdots dy_L\right\}\right] \\
&= \left(\prod_{l=1}^L |D_l|\right)^{-1} \\
&\quad \times E_{\mathrm{UD}}\Bigg[\prod_{i=1}^{t-1} f_{u_i}(X_i) E_{\mathrm{UD}}\Bigg\{\rho(M_t) f_{u_t}(X_t) \\
&\qquad \times \left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\, dy_1 \cdots dy_L\right)\Bigg| \\
&\qquad \{X_1, \dots, X_{t-1}\}\Bigg\}\Bigg].
\end{aligned}
$$

From Lemma 4.1,

$$
\begin{aligned}
&E_{\mathrm{UD}}\left\{\rho(M_t) f_{u_t}(X_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\, dy_1 \cdots dy_L\right)\Big|\{X_1, \dots, X_{t-1}\}\right\} \\
&\quad = \int g(x_t)\rho(M_t) f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t \\
&\quad = \sum_{i_1, \dots, i_K} b_t(i_1, \dots, i_K, M_{t-1}) \int_{D_{L+1}} \rho(M_t) f_{u_t}(x_t) \\
&\qquad \times \left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\, dy_1 \cdots dy_L\right) dx_t,
\end{aligned}
$$

where $g(x_t)$ is the conditional density of X_t, $D_{L+1} = D_{L+1}^1 \times \cdots \times D_{L+1}^K$, $D_{L+1}^k = \delta_n(X_{i_k}^k) \setminus \bigcup_{j=1}^{t-1} \delta_N(X_j^k)$ if $0 < i_k \le t-1$, $D_{L+1}^k = \delta_N(X_{i_k-(t-1)}^k)$ if $i_k > t-1$ and $D_{L+1}^k = [0,1) \setminus \bigcup_{j=1}^{t-1} \delta_n(X_j^k)$ if $i_k = 0$.

In any D_{L+1}, $\rho(M_t)$ is a deterministic function on M_{t-1}. Let $\rho_{i_1,\ldots,i_K}(M_{t-1})$ denote this function. Then for any M_{t-1}, $\rho_{i_1,\ldots,i_K}(M_{t-1}) = O(1)$. Thus

$$G = \sum_{i_1,\ldots,i_K} \left(\prod_{l=1}^L |D_l|\right)^{-1} \times E_{\mathrm{UD}}\left\{\prod_{i=1}^{t-1} f_{u_i}(X_i) b_t(i_1,\ldots,i_K,M_{t-1}) \rho_{i_1,\ldots,i_K}(M_{t-1}) \times \int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t\right\}.$$

If $0 < i_1 \le t-1$, $D_{L+1}^1 = \delta_n(X_{i_1}^1) \setminus \bigcup_{j=1}^{t-1} \delta_N(X_j^1)$. If additionally $k \notin u_t$,

$$\begin{aligned}
&\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t \\
&\quad = \rho_0'(M_{t-1}) \\
&\qquad \times \int_{\delta_n(X_{i_1}^1)\times D_{L+1}^2\times\cdots\times D_{L+1}^K} f_{u_t}(x_t) \\
&\qquad\qquad \times \left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t,
\end{aligned}$$

where $\rho_0'(M_{t-1}) = O(1)$. If $k \in u_t$,

$$\begin{aligned}
&\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t \\
&\quad = \int_{\delta_n(X_{i_1}^1)\times D_{L+1}^2\times\cdots\times D_{L+1}^K} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t \\
&\qquad - \sum_{j=1}^{t-1}\left\{\int_{\delta_N(X_j^1)\times D_{L+1}^2\times\cdots\times D_{L+1}^K} f_{u_t}(x_t) \right. \\
&\qquad\qquad \left. \times \left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right) dx_t\right\}.
\end{aligned}$$

If $i_1 = 0$, $D_{L+1}^1 = [0,1) \setminus \bigcup_{i=1}^{t-1} \delta_n(X_i^1)$. If additionally $k \notin u_t$,

$$\begin{aligned}
&\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t \\
&\qquad = \rho_0'(M_{t-1}) \\
&\qquad\quad \times \int_{[0,1)\times D_{L+1}^2\times\cdots\times D_{L+1}^K} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t,
\end{aligned}$$

where $\rho_0'(M_{t-1}) = O(1)$. If $k \in u_t$,

$$\begin{aligned}
&\int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t \\
&\quad = \int_{[0,1)\times D_{L+1}^2\times\cdots\times D_{L+1}^K} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t \\
&\qquad - \sum_{j=1}^{t-1}\Biggl\{\rho_j'(M_{t-1}) \\
&\qquad\qquad \times \int_{\delta_n(X_j^1)\times D_{L+1}^2\times\cdots\times D_{L+1}^K} f_{u_t}(x_t) \\
&\qquad\qquad\qquad \times \left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t\Biggr\},
\end{aligned}$$

where $\rho_j'(M_{t-1}) = O(1)$ for $j = 1,\ldots,t-1$. Let

$$\tilde{b}_t(i_1,\ldots,i_k) = \begin{cases} 1, & |w| \le h, \\ n^{|w|}/N, & |w| > h. \end{cases}$$

Then $\tilde{b}_t$ is not related to M_{t-1} and $\tilde{b}_t(0,i_2,\ldots,i_K) \le \tilde{b}_t(j,i_2,\ldots,i_K)$ for any $j > 0$.

From arguments above, it suffices to show

$$\begin{aligned}
&J(i_1,\ldots,i_K) \\
&\quad = \tilde{b}_t(i_1,\ldots,i_K)\left(\prod_{l=1}^L |D_l|\right)^{-1} \\
&\qquad \times E_{\mathrm{UD}}\Biggl\{\prod_{i=1}^{t-1} f_{u_i}(X_i)\rho(M_{t-1}) \\
&\qquad\qquad \times \int_{D_{L+1}} f_{u_t}(x_t)\left(\int_{\prod_{l=1}^L D_l} \prod_{l=1}^L f_{v_l}(y_l)\,dy_1\cdots dy_L\right)dx_t\Biggr\}
\end{aligned} \tag{19}$$

has order $O(N^{-\theta/2})$ for any $i_1, \dots, i_K = 0, 1, \dots, t-1$, $\rho(M_{t-1}) = O(1)$, $D_{L+1} = D^1_{L+1} \times \cdots \times D^K_{L+1}$, $D^1_{L+1} = \delta_n(X^1_{i_1})$ if $0 < i_1 \le t-1$, $D^k_{L+1} = \delta_n(X^k_{i_k}) \setminus \bigcup_{j=1}^{t-1} \delta_N(X^k_j)$ if $0 < i_k \le t-1$, $k = 2, \dots, K$, $D^k_{L+1} = \delta_N(X^k_{i_k-(t-1)})$ if $i_k > t-1$, $k = 1, \dots, K$, $D^1_{L+1} = [0, 1)$ if $i_1 = 0$ and $D^k_{L+1} = [0, 1) \setminus \bigcup_{j=1}^{t-1} \delta_n(X^k_j)$ if $i_k = 0$, $k = 2, \dots, K$.

From similar arguments, it suffices to show (19) has order $O(N^{-\theta/2})$ for any $i_1, \dots, i_K = 0, 1, \dots, t-1$, $\rho(M_{t-1}) = O(1)$, $D_{L+1} = D^1_{L+1} \times \cdots \times D^K_{L+1}$, $D^k_{L+1} = \delta_n(X^k_{i_k})$ if $0 < i_k \le t-1$, $D^k_{L+1} = \delta_N(X^k_{i_k-(t-1)})$ if $i_k > t-1$ and $D^k_{L+1} = [0, 1)$ if $i_k = 0$, $k = 1, \dots, K$.

If $i_k \ne 0$ and $k \notin u_t$, then any term that can be written as $J(i_1, \dots, i_K)$ has smaller or the same order than a term that can be written as $J(i_1, \dots, i_{k-1}, 0, i_{k+1}, \dots, i_K)$. If $i_k = 0$ and the (t, k)th element of C is one, from (4), $J = 0$. Thus it suffices to consider $J(i_1, \dots, i_K)$ with $i_k = 0, \dots, 2t-2$ for $k \in u_t$ and the (t, k)th element of C being zero, $i_k = 1, \dots, 2t-2$ for $k \in u_t$ and the (t, k)th element of C being one and $i_k = 0$ for $k \notin u_t$. Clearly, $w \subseteq u_t$ and $c_t \le |w| \le |u_t|$.

Let

$$G'_{i_1,\dots,i_K} = \left(\prod_{l=1}^{L+1} |D_l|\right)^{-1} E_{\mathrm{UD}}\left[\prod_{i=1}^{t-1} f_{u_i}(X_i)\rho(M_{t-1}) \times \left\{\int_{(\prod_{l=1}^{L} D'_l)\times D_{L+1}} \prod_{l=1}^{L+1} f_{v_l}(y_l)\, dy_1 \cdots dy_{L+1}\right\}\right],$$

where $v_{L+1} = u_t$ and

$$D^{k\prime}_l = \begin{cases} \delta_n(y^k_{L+1}), & \text{if } D^k_l = \delta_n(X^k_t), \\ \delta_N(y^k_{L+1}), & \text{if } D^k_l = \delta_N(X^k_t), \\ D^k_l, & \text{otherwise.} \end{cases}$$

Then J in (19) can be expressed as

$$J(i_1, \dots, i_K) = \tilde{b}_t(i_1, \dots, i_K) n^{-|w|} G'_{i_1,\dots,i_K}.$$

For any $(i_1, \dots, i_K)$, $G'_{i_1,\dots,i_K}$ is a term by (18). Furthermore, the matrix associated with $G'_{i_1,\dots,i_K}$, denoted as $C'_{i_1,\dots,i_K}$, is a $(t-1) \times K$ matrix with equal or fewer elements of ones than the first $t-1$ rows of C. If $0 < i_k = z \le t-1$, the (z, k)th element of $C'_{i_1,\dots,i_K}$ is zero. If $i_k = z > t-1$, the $(z-(t-1), k)$th element of $C'_{i_1,\dots,i_K}$ is zero. Other elements of $C'(D_{L+1})$ are the same with that of C. Let c'_i be the number of ones in the ith row of $C'_{i_1,\dots,i_K}$, and let $\theta' = \sum_{i=1}^{t-1} c'_i/|u_i|$, so we have

$$\theta' \ge \theta - c_t/|u_t| - |w|/|u_t|.$$

By induction,

$$G'_{i_1,\dots,i_K} = O\big(N^{-(\theta - c_t/|u_t| - |w|/|u_t|)/2}\big) = O\big(N^{-\theta/2+1}\big) \tag{20}$$

and

$$G'_{i_1,\dots,i_K} = O\big(N^{-(\theta - c_t/|u_t| - |w|/|u_t|)/2}\big) = O\big(N^{-\theta/2} n^{|w|}\big). \tag{21}$$

Consequently, J in (19) has order $O(N^{-\theta/2})$. This completes the proof. $\square$

LEMMA A.4. *If $c_t > 0$, G has order $o(N^{-\theta/2})$.*

The proofs for Lemma A.4 and 4.3 are similar to the proofs for Lemma A.2 and 3.4, respectively, and are omitted.

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