A COMBINATORIAL CENTRAL LIMIT THEOREM FOR RANDOMIZED ORTHOGONAL ARRAY SAMPLING DESIGNS

by

Wei-Liem Loh
Purdue University

Technical Report #94-4

Department of Statistics
Purdue University

March 1994

A COMBINATORIAL CENTRAL LIMIT THEOREM FOR RANDOMIZED ORTHOGONAL ARRAY SAMPLING DESIGNS[1]

By Wei-Liem Loh

Purdue University

Let X be a random vector uniformly distributed on the unit cube and $f : [0,1]^3 \to \mathcal{R}$ be a measurable function. An objective of many computer experiments is to estimate $\mu = E(f \circ X)$ by computing f at a set of points in $[0,1]^3$. There is a design issue in choosing these points. Recently Owen and Tang independently suggested using randomized orthogonal arrays in the choice of such a set. This paper investigates the convergence rate to normality of the sample mean from one of these designs.

1 Introduction

Let d, n and t be positive integers with $t \leq d$. An orthogonal array of strength t is a matrix of n rows and d columns with elements taken from the set $\{0, 1, \ldots, q-1\}$ such that in any n by t submatrix, each of the q^t possible rows occurs the same number of times. The class of all such arrays is denoted by $OA(n, d, q, t)$ and a more detailed description can be found in Raghavarao (1971).

Owen (1992), (1994) and Tang (1993) independently suggested the use of randomized orthogonal arrays in sampling designs for computer experiments on the d-dimensional unit hypercube $[0,1]^d$. The main attraction of these designs is that they, in contrast to simple random sampling, stratify on all t-variate margins simultaneously.

In this paper we shall be concerned with the following orthogonal array based sampling design on the unit cube $[0,1]^3$. Let

(i) π_1, π_2, π_3, be random permutations of $\{0, 1, \ldots, q-1\}$, each uniformly distributed on all the $q!$ possible permutations,

(ii) $U_{i_1,i_2,i_3,j}$, $0 \leq i_1, i_2, i_3 \leq q-1$, $1 \leq j \leq 3$, be $[0,1]$ uniform random variables and

[1]Research supported in part by NSA Grant 904-93-H-3011.

AMS 1980 *subject classifications.* Primary 62E20; secondary 60F05, 62D05.

Key words and phrases. Combinatorial central limit theorem, computer experiment, convergence rate, orthogonal array, sampling design, Stein's method.

(iii) that the $U_{i_1,i_2,i_3,j}$'s and π_k's are all stochastically independent.
An orthogonal array based sample of size q^2 (taken from $[0,1]^3$) is defined to be $\{X(\pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3})) : 1 \leq i \leq q^2\}$ where for all $0 \leq i_1, i_2, i_3 \leq q-1$,

$$\begin{aligned} X_j(i_1, i_2, i_3) &= (i_j + U_{i_1,i_2,i_3,j})/q, \quad \forall 1 \leq j \leq 3, \\ X(i_1, i_2, i_3) &= (X_1(i_1, i_2, i_3), X_2(i_1, i_2, i_3), X_3(i_1, i_2, i_3))', \end{aligned}$$

and $a_{i,j}$ is the (i,j)th element of some $A \in OA(q^2, 3, q, 2)$.

REMARK. The above sampling design is a special case of those proposed by Owen (1992).

Let X be a random vector uniformly distributed on $[0,1]^3$ and f be a measurable function from $[0,1]^3$ to $\mathcal{R}$. An objective of many computer experiments [see for example McKay, Conover and Beckman (1979), Stein (1987), Owen (1992) and Tang (1993)] is to estimate $\mu = E(f \circ X)$ by computing f at a fixed number of points. The estimator for μ that we are concerned with here is one based on an orthogonal array; namely

$$\hat{\mu} = q^{-2} \sum_{i=1}^{q^2} f \circ X(\pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3})), \tag{1}$$

where $\hat{\mu}$ is the mean of the orthogonal array based sample

$$\{f \circ X(\pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3})) : 1 \leq i \leq q^2\}$$

and is an unbiased estimator of μ.

In 1972, Stein introduced a powerful and general method for obtaining an explicit bound for the error in the normal approximation to the distribution of a sum of dependent random variables. Even though since then Stein's method has found considerable applications in combinatorics, probability and statistics [see for example Stein (1986) and the references cited therein], it appears to have largely escaped the attention of researchers in the area of computer experiments. In Section 2 Stein's method is used to investigate the rate of convergence to normality of $\hat{\mu}$. In particular Theorem 2 shows that $\hat{\mu}$ is asymptotically normal (as $q \to \infty$) under the finiteness of rth moments with a corresponding error bound of the order $O(q^{-(r-2)/(2r-2)})$, whenever r is an even integer greater than or equal to 4.

The Appendix contains a number of somewhat technical lemmas that are needed in the proof of Theorem 2.

Throughout this paper, Φ and ϕ denote the cumulative distribution function and probability density function of the standard normal distribution respectively. Given any event B, $I(B)$ denotes its indicator function and if $x \in \mathcal{R}^3$, then x' is the transpose of x.

2 Stein's method

In this section, we shall use Stein's method to investigate the rate of convergence to normality of $\hat{\mu}$ where $\hat{\mu}$ is defined as in (1) with $A \in OA(q^2, 3, q, 2)$. Central to this normal approximation technique is the following lemma.

Lemma 1 (Stein) *Let $z \in \mathcal{R}$. The unique bounded solution $g_z : \mathcal{R} \to \mathcal{R}$ of the differential equation*

$$\frac{d}{dw}g(w) - wg(w) = I(w \leq z) - \Phi(z), \quad \forall w \in \mathcal{R},$$

is given by

$$g_z(w) = \begin{cases} \Phi(w)[1-\Phi(z)]/\phi(w), & \text{if } w \leq z, \\ \Phi(z)[1-\Phi(w)]/\phi(w), & \text{if } w > z, \end{cases}$$

with $0 \leq g_z(w) \leq 1$ and $|dg_z(w)/dw| \leq 1$ for all $w \in \mathcal{R}$.

PROOF. Lemma 1 is due to Stein (1972) and we refer the reader to his paper for a proof. □

Next we state a simple expression for the asymptotic variance of $\hat{\mu}$ due to Owen (1992).

Theorem 1 *Suppose $E(f \circ X)^2 < \infty$. Let $\sigma_{oas}^2 = Var(\hat{\mu})$ with $\hat{\mu}$ as in (1) for some $A \in OA(q^2, 3, q, 2)$. Then as $q \to \infty$, we have*

$$q^2\sigma_{oas}^2 = \int_{[0,1]^3} f_{rem}^2(x)dx + o(1),$$

where for all $x = (x_1, x_2, x_3)' \in [0,1]^3$,

$$\begin{aligned} f_j(x_j) &= \int_{[0,1]^2} [f(x) - \mu] \prod_{k \neq j} dx_k, \quad \forall 1 \leq j \leq 3, \\ f_{k,l}(x_k, x_l) &= \int_0^1 [f(x) - \mu - f_k(x_k) - f_l(x_l)] \prod_{j \neq k,l} dx_j, \\ &\qquad \forall 1 \leq k < l \leq 3, \\ f_{rem}(x) &= f(x) - \mu - \sum_{j=1}^{3} f_j(x_j) - \sum_{1 \leq k < l \leq 3} f_{k,l}(x_k, x_l). \qquad (2) \end{aligned}$$

Assuming that $Var(\hat{\mu}) = \sigma_{oas}^2 > 0$, we define

$$W = \sigma_{oas}^{-1}(\hat{\mu} - \mu).$$

For all $0 \le i_1, i_2, i_3 \le q-1$, we write

$$\begin{aligned}
Ef \circ X(i_1, i_2, i_3) &= \mu(i_1, i_2, i_3), \\
\mu_j(i_j) &= q^{-2} \sum_{k \neq j} \sum_{i_k=0}^{q-1} [\mu(i_1, i_2, i_3) - \mu], \quad \forall 1 \le j \le 3, \\
\mu_{k,l}(i_k, i_l) &= q^{-1} \sum_{j \neq k,l} \sum_{i_j=0}^{q-1} [\mu(i_1, i_2, i_3) - \mu - \mu_k(i_k) - \mu_l(i_l)], \\
& \quad \forall 1 \le k < l \le 3, \\
Y(i_1, i_2, i_3) &= q^{-2} \sigma_{oas}^{-1} [f \circ X(i_1, i_2, i_3) - \mu \\
&\quad - \sum_{j=1}^{3} \mu_j(i_j) - \sum_{1 \le k < l \le 3} \mu_{k,l}(i_k, i_l)], \qquad (3)
\end{aligned}$$

and

$$\tilde{\mu}(i_1, i_2, i_3) = EY(i_1, i_2, i_3). \qquad (4)$$

Since the orthogonal array A has strength 2, a consequence of the above construction is that

$$\sum_{i_j=0}^{q-1} \tilde{\mu}(i_1, i_2, i_3) = 0, \quad \forall 1 \le j \le 3. \qquad (5)$$

We also observe that W can be rewritten as

$$W = \sum_{i=1}^{q^2} Y(\pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3})). \qquad (6)$$

We shall now state and prove the main result of this paper.

Theorem 2 *Let W be as in (6) for some $A \in OA(q^2, 3, q, 2)$. Suppose that $E(f \circ X)^r < \infty$ for some even integer $r \ge 4$, and*

$$\int_{[0,1]^3} f_{rem}^2(x)dx > 0, \qquad (7)$$

with $f_{rem}(x)$ as in (2). Then

$$\sup\{|P(W \le w) - \Phi(w)| : -\infty < w < \infty\} = O(q^{-(r-2)/(2r-2)}),$$

as $q \to \infty$.

PROOF. (7) and Theorem 1 ensure that $\sigma_{oas} > 0$ and hence that W is well defined for sufficiently large q.

Let (J_1, J_2) be a random vector uniformly distributed over the set

$$\{(j_1, j_2) \in \{0, \ldots, q-1\}^2 : j_1 \neq j_2\}.$$

Also we assume that they are independent of all other random quantities previously defined (for example W). Define

$$W^* = \sum_{i=1}^{q^2} Y(\tau_{J_1,J_2} \circ \pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3})),$$

where τ_{J_1,J_2} is a random permutation of $\{0, \ldots, q-1\}$ which transposes J_1 and J_2, leaving all other elements fixed. We observe that (W, W^*) is an exchangeable pair of random variables in that (W, W^*) and (W^*, W) have the same joint distribution.

Since the orthogonal array A is of strength 2, we note that W can be rewritten as

$$W = \sum_{i_1=0}^{q-1} \sum_{i_2=0}^{q-1} Y(i_1, i_2, \rho(i_1, i_2)) \tag{8}$$

where ρ is a function that maps $\{0, \ldots, q-1\}^2$ to $\{0, \ldots, q-1\}$ such that

$$(i_1, i_2, \rho(i_1, i_2)) = (\pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3}))$$

for some $1 \leq i \leq q^2$. Thus it follows from the definition of W^* and (8) that

$$\begin{aligned} W^* &= W - \sum_{i_2=0}^{q-1} Y(J_1, i_2, \rho(J_1, i_2)) - \sum_{i_2=0}^{q-1} Y(J_2, i_2, \rho(J_2, i_2)) \\ &\quad + \sum_{i_2=0}^{q-1} Y(J_2, i_2, \rho(J_1, i_2)) + \sum_{i_2=0}^{q-1} Y(J_1, i_2, \rho(J_2, i_2)) \\ &= W - A_1 - A_2 - A_3 - A_4, \end{aligned} \tag{9}$$

say respectively. For convenience we write

$$V = W - A_1 - A_2.$$

Let $\mathcal{W}$ be the σ-field generated by the random quantities

$$\{(\pi_1(a_{i,1}), \pi_2(a_{i,2}), \pi_3(a_{i,3})), U_{\pi_1(a_{i,1}),\pi_2(a_{i,2}),\pi_3(a_{i,3}),j} : 1 \leq i \leq q^2, 1 \leq j \leq 3\}.$$

We observe that W is $\mathcal{W}$-measurable.

Next let $z \in \mathcal{R}$ and $g_z : \mathcal{R} \to \mathcal{R}$ be as in Lemma 1. From the exchangeability of (W, W^*), we have

$$\begin{aligned} 0 &= E(W^* - W)[g_z(W) + g_z(W^*)] \\ &= 2E[E(W^* - W|\mathcal{W})g_z(W)] + E(W^* - W)[g_z(W^*) - g_z(W)]. \end{aligned}$$

Consequently we observe from Lemma 3 (see Appendix) that

$$\begin{aligned} EWg_z(W) &= (q/4)E(W^* - W)[g_z(W^*) - g_z(W)] - \Delta_1 \\ &= E\int \frac{d}{dw} g_z(V + w)K(w)dw - \Delta_1, \end{aligned} \tag{10}$$

where

$$\Delta_1 = \frac{1}{q-1} E[g_z(W) \sum_{i_1=0}^{q-1} \sum_{i_2=0}^{q-1} \tilde{\mu}(i_1, i_2, \rho(i_1, i_2))],$$

and for all $w \in \mathcal{R}$,

$$K(w) = \begin{cases} (q/4)(W^* - W) & \text{if } W - V < w \leq W^* - V, \\ (q/4)(W - W^*) & \text{if } W^* - V < w \leq W - V, \\ 0 & \text{otherwise.} \end{cases}$$

We further observe that

$$|\Delta_1| \leq \frac{1}{q-1} [Eg_z^2(W)]^{1/2} (EW^2)^{1/2} \leq \frac{1}{q-1}, \tag{11}$$

since $0 \leq g_z(w) \leq 1$ for all $w \in \mathcal{R}$. Now we observe from Lemma 1 and (10) that

$$\begin{aligned} & |P(W \leq z) - \Phi(z)| \\ = \ & |E\{\frac{d}{dw} g_z(W) - W g_z(W)\}| \\ \leq \ & |E\int [\frac{d}{dw} g_z(W) - \frac{d}{dw} g_z(V + w)]K(w)dw| \\ & + |E\frac{d}{dw} g_z(W) E\int K(w)dw - E\frac{d}{dw} g_z(W) \int K(w)dw| \\ & + |E\frac{d}{dw} g_z(W)||1 - E\int K(w)dw| + |\Delta_1|. \end{aligned} \tag{12}$$

Thus to prove Theorem 2, it suffices to obtain appropriate bounds for the terms on the right hand side of (12). This is achieved by (11), (12), and Lemmas 4, 5 and 6 (see Appendix). Hence we conclude that

$$\sup\{|P(W \le w) - \Phi(w)| : -\infty < w < \infty\} = O(q^{-(r-2)/(2r-2)}),$$

as $q \to \infty$. This proves Theorem 2. □

REMARK. We would like to add that the first two terms on the right hand side of (12) have been studied in some detail by Ho and Chen (1978) in the context of investigating the convergence rate of Hoeffding's combinatorial central limit theorem and our proof of Lemma 6 in this paper was motivated by their results.

3 Appendix

Lemma 2 *Let W and A_1 be defined as in (8) and (9) respectively. Then*

$$E(1/q)\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1} Y^2(i_1,i_2,i_3) = 1 + O(1/q), \tag{13}$$

and if $E(f \circ X)^r < \infty$ for some positive even integer r, then

$$E(A_1^r) = O(q^{-r/2}), \tag{14}$$

as $q \to \infty$.

PROOF OF LEMMA 2. We observe from (8) that

$$\begin{aligned}
1 &= EW^2 \\
&= E\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1} Y^2(i_1,i_2,\rho(i_1,i_2)) \\
&\quad + E\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{j_1\ne i_1}\sum_{j_2\ne i_2} \tilde{\mu}(i_1,i_2,\rho(i_1,i_2))\tilde{\mu}(j_1,j_2,\rho(j_1,j_2)) \\
&\quad + E\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{j_2\ne i_2} \tilde{\mu}(i_1,i_2,\rho(i_1,i_2))\tilde{\mu}(i_1,j_2,\rho(i_1,j_2)) \\
&\quad + E\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{j_1\ne i_1} \tilde{\mu}(i_1,i_2,\rho(i_1,i_2))\tilde{\mu}(j_1,i_2,\rho(j_1,i_2))
\end{aligned}$$

$$
\begin{aligned}
&= E\frac{1}{q}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1} Y^2(i_1,i_2,i_3) \\
&\quad +\frac{1}{q(q-1)}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1}\sum_{j_1\neq i_1}\sum_{j_2\neq i_2}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(j_1,j_2,i_3) \\
&\quad +\frac{q-2}{q(q-1)^2}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1}\sum_{j_1\neq i_1}\sum_{j_2\neq i_2}\sum_{j_3\neq i_3}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(j_1,j_2,j_3) \\
&\quad +\frac{1}{q(q-1)}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1}\sum_{j_2\neq i_2}\sum_{j_3\neq i_3}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(i_1,j_2,j_3) \\
&\quad +\frac{1}{q(q-1)}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1}\sum_{j_1\neq i_1}\sum_{j_3\neq i_3}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(j_1,i_2,j_3) \\
&= E\frac{1}{q}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1} Y^2(i_1,i_2,i_3) \\
&\quad +\frac{2q-1}{q(q-1)^2}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1}\tilde{\mu}^2(i_1,i_2,i_3) \\
&= (1/q)(1+O(1/q))E\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1} Y^2(i_1,i_2,i_3),
\end{aligned}
$$

as $q \to \infty$. The second last equality follows from (5). This proves (13).

Next we observe from the definition of A_1 that

$$
\begin{aligned}
E(A_1^r) &= E[\sum_{i_2=0}^{q-1} Y(J_1,i_2,\rho(J_1,i_2))]^r \\
&= E(1/q)\sum_{i_1=0}^{q-1}[\sum_{i_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))]^r. \qquad (15)
\end{aligned}
$$

We observe that on expansion, the right hand side of (15) consists of terms of the form for some $b \geq 1$,

$$
\begin{aligned}
& E(1/q)\sum_{i_1=0}^{q-1}\sum_{(i_{2,1},\ldots,i_{2,b})\in\mathcal{B}(b)}\prod_{a=1}^{b} Y^{r_a}(i_1,i_{2,a},\rho(i_1,i_{2,a})) \\
(16) = \; & \frac{(q-b)!}{q(q!)}\sum_{i_1=0}^{q-1}\sum_{(i_{2,1},\ldots,i_{2,b})\in\mathcal{B}(b)}\sum_{(i_{3,1},\ldots,i_{3,b})\in\mathcal{B}(b)}\prod_{a=1}^{b} E[Y^{r_a}(i_1,i_{2,a},i_{3,a})],
\end{aligned}
$$

where r_a, $1 \le a \le b$, are positive integers such that $\sum_{a=1}^{b} r_a = r$ and $\mathcal{B}(b)$ is the subset of $\{0, \ldots, q-1\}^b$ with all its coordinates different.

If there is an $r_a = 1$, say $r_1 = 1$, then it follows from (4) and (5) that the number of summations on the right hand side of (16) can be reduced by 2, namely the variables $i_{2,1}$ and $i_{3,1}$ can be eliminated. Proceeding in this way, we observe the number of summations in $\sum_{(i_{2,1},\ldots,i_{2,b})\in\mathcal{B}(b)}$ and $\sum_{(i_{3,1},\ldots,i_{3,b})\in\mathcal{B}(b)}$ can be each made to be at most $r/2$. This implies that

$$\begin{aligned} & |\frac{(q-b)!}{q(q!)} \sum_{i_1=0}^{q-1} \sum_{(i_{2,1},\ldots,i_{2,b})\in\mathcal{B}(b)} \sum_{(i_{3,1},\ldots,i_{3,b})\in\mathcal{B}(b)} \prod_{a=1}^{b} E[Y^{r_a}(i_1, i_{2,a}, i_{3,a})]| \\ = & O(q^{(r-6)/2}) \sum_{i_1=0}^{q-1} \sum_{i_2=0}^{q-1} \sum_{i_3=0}^{q-1} E[Y^r(i_1, i_2, i_3)] \\ = & O(q^{-r/2}), \end{aligned}$$

as $q \to \infty$. The last equality follows from Theorem 1 and (3). □

Lemma 3 *With the notations and assumptions of Theorem 2,*

$$\begin{aligned} & E(W^* - W|\mathcal{W}) \\ = & -\frac{2}{q}W - \frac{2}{q(q-1)} E[\sum_{i_1=0}^{q-1} \sum_{i_2=0}^{q-1} \tilde{\mu}(i_1, i_2, \rho(i_1, i_2))|\mathcal{W}]. \end{aligned}$$

Proof of Lemma 3. We observe from (9) that

$$\begin{aligned} & E(W^* - W|\mathcal{W}) \\ = & \frac{2}{q(q-1)} E[\sum_{j_1=0}^{q-1} \sum_{i_2=0}^{q-1} \sum_{j_3\ne j_1} Y(j_1, i_2, \rho(j_3, i_2))|\mathcal{W}] - \frac{2}{q}W \\ = & \frac{2}{q(q-1)} E[\sum_{j_1=0}^{q-1} \sum_{i_2=0}^{q-1} \sum_{j_3\ne j_1} \tilde{\mu}(j_1, i_2, \rho(j_3, i_2))|\mathcal{W}] - \frac{2}{q}W. \qquad (17) \end{aligned}$$

The last equality follows from the observation that given $\mathcal{W}$, $U_{j_1,i_2,\rho(j_3,i_2),k}$ is still a uniform $[0,1]$ random variable whenever $j_1 \ne j_3$ and $1 \le k \le 3$. Lemma 3 follows from (5) and (17). □

Lemma 4 *With the notations and assumptions of Theorem 2, we have*

$$|E\frac{d}{dw} g_z(W)||E \int K(w)dw - 1| \le 1/(q-1).$$

PROOF OF LEMMA 4. Since $|dg_z(w)/dw| \leq 1$ for all $w \in \mathcal{R}$, it suffices only to prove

$$|E\int K(w)dw - 1| \leq 1/(q-1).$$

By replacing $g_z(W)$ by W in (10), we have

$$1 = E(W^2) = E\int K(w)dw - \frac{1}{q-1}E[W\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\tilde{\mu}(i_1, i_2, \rho(i_1, i_2))].$$

Lemma 4 follows since as in (11) we observe that the last term of the above equation is bounded by $1/(q-1)$. □

Lemma 5 *With the notations and assumptions of Theorem 2, we have*

$$|E\frac{d}{dw}g_z(W)E\int K(w)dw - E\frac{d}{dw}g_z(W)\int K(w)dw| = O(q^{-1/2}),$$

as $q \to \infty$ uniformly over $z \in \mathcal{R}$.

PROOF OF LEMMA 5. We observe from (9), Lemma 4 and the definition of $K(w)$ that

$$\begin{aligned}
&|E\frac{d}{dw}g_z(W)E\int K(w)dw - E\frac{d}{dw}g_z(W)\int K(w)dw| \\
\leq\ & E|E[\int K(w)dw - 1|\mathcal{W}]| + 1/(q-1) \\
=\ & (1/4)E|E[q(W^* - W)^2 - 4|\mathcal{W}]| + 1/(q-1) \\
\leq\ & (1/4)\sum_{k=1}^{4} E|E(qA_k^2 - 1|\mathcal{W})| \\
& +(q/2)\sum_{1\leq j<k\leq 4} E|E(A_jA_k|\mathcal{W})| + 1/(q-1). \qquad (18)
\end{aligned}$$

To prove the lemma, it suffices to find appropriate bounds for the terms on the right hand side of (18). For the sake of clarity, we shall break the proof down into 5 steps.

STEP 1. From the Cauchy-Schwarz inequality, we observe that

$$\{E|E(qA_1^2 - 1|\mathcal{W})|\}^2 = \{E|E[q(\sum_{i_2=0}^{q-1} Y(J_1, i_2, \rho(J_1, i_2)))^2 - 1|\mathcal{W}]|\}^2$$

$$\leq E\{\sum_{i_1=0}^{q-1}[\sum_{i_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))]^2\}^2$$

$$-2E\sum_{i_1=0}^{q-1}[\sum_{i_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))]^2+1. \tag{19}$$

We note from (5) and (13) that

$$\begin{aligned} E\sum_{i_1=0}^{q-1}[\sum_{i_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))]^2 &= E(1/q)\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1} Y^2(i_1,i_2,i_3) \\ &\quad +\frac{1}{q(q-1)}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{i_3=0}^{q-1}\tilde{\mu}^2(i_1,i_2,i_3) \\ &= 1+O(1/q), \end{aligned}$$

and similarly (though more tedious),

$$E\{\sum_{i_1=0}^{q-1}[\sum_{i_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))]^2\}^2 = 1+O(1/q),$$

as $q\to\infty$. Thus we conclude from (19) and the symmetry of A_k, $1\leq k\leq 2$, that

$$E|E(qA_1^2-1|\mathcal{W})|+E|E(qA_2^2-1|\mathcal{W})| = O(q^{-1/2}), \tag{20}$$

as $q\to\infty$.

STEP 2. Next, we have

$$\begin{aligned} & E(qA_3^2|\mathcal{W}) \\ =\; & E[q(\sum_{i_2=0}^{q-1} Y(J_2,i_2,\rho(J_1,i_2)))^2|\mathcal{W}] \\ =\; & E[\frac{1}{q-1}\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1} Y^2(i_1,i_2,\rho(j_1,i_2))|\mathcal{W}] \\ & +\frac{1}{q-1}\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{j_2\neq i_2}\tilde{\mu}(i_1,i_2,\rho(j_1,i_2))\tilde{\mu}(i_1,j_2,\rho(j_1,j_2)) \\ =\; & E(A_{3,1}|\mathcal{W})+A_{3,2}, \end{aligned} \tag{21}$$

say respectively. We observe that

$$\{E|E(A_{3,1}-1|\mathcal{W})|\}^2$$

$$
\begin{aligned}
&\leq E(A_{3,1}-1)^2 \\
&= E\{1 - \frac{2}{q-1}\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1} Y^2(i_1,i_2,\rho(j_1,i_2)) \\
&\quad +(\frac{1}{q-1})^2 \sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{a_1=0}^{q-1}\sum_{b_1\neq a_1}\sum_{a_2=0}^{q-1} Y^2(i_1,i_2,\rho(j_1,i_2)) \\
&\quad \times Y^2(a_1,a_2,\rho(b_1,a_2))\}
\end{aligned}
$$

$$
(22) \qquad = O(1/q),
$$

as $q \to \infty$. Also we note from (5) that

$$
\begin{aligned}
& E(A_{3,2}^2) \\
&= E\frac{1}{(q-1)^2}\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{j_2\neq i_2} \tilde{\mu}(i_1,i_2,\rho(j_1,i_2))\tilde{\mu}(i_1,j_2,\rho(j_1,j_2)) \\
&\quad \times \sum_{a_1=0}^{q-1}\sum_{b_1\neq a_1}\sum_{a_2=0}^{q-1}\sum_{b_2\neq a_2} \tilde{\mu}(a_1,a_2,\rho(b_1,a_2))\tilde{\mu}(a_1,b_2,\rho(b_1,b_2))
\end{aligned}
$$

$$
(23) \qquad = O(1/q),
$$

as $q \to \infty$. Thus we conclude from (21), (22), (23) and the symmetry between A_3 and A_4 that

$$
(24) \qquad E|E(qA_3^2 - 1|\mathcal{W})| + E|E(qA_4^2 - 1|\mathcal{W})| = O(q^{-1/2}),
$$

as $q \to \infty$.

STEP 3. We observe that

$$
\begin{aligned}
& qE|E(A_1A_2|\mathcal{W})| \\
&= \frac{1}{q-1}E|\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{j_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))Y(j_1,j_2,\rho(j_1,j_2))| \\
&\leq \frac{1}{q-1}E(W^2) + \frac{1}{q-1}E\sum_{i_1=0}^{q-1}[\sum_{i_2=0}^{q-1} Y(i_1,i_2,\rho(i_1,i_2))]^2
\end{aligned}
$$

$$
(25) \qquad = O(1/q),
$$

as $q \to \infty$.

STEP 4. Now we note from (9) that

$$\begin{aligned} & qE|E(A_3A_4|\mathcal{W})| \\ = \; & \frac{1}{q-1}E|E(\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{j_2=0}^{q-1}\tilde{\mu}(i_1,i_2,\rho(j_1,i_2))\tilde{\mu}(j_1,j_2,\rho(i_1,j_2))|\mathcal{W})| \\ \leq \; & \frac{1}{q(q-1)^2}\sum_{i_3=0}^{q-1}\sum_{j_3\neq i_3}|\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(j_1,i_2,j_3)| \\ & +\frac{q-2}{q(q-1)^3}\sum_{i_3=0}^{q-1}\sum_{j_3\neq i_3}|\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{j_2\neq i_2}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(j_1,j_2,j_3)| \\ & +\frac{q-2}{q(q-1)^3}\sum_{i_3=0}^{q-1}|\sum_{i_1=0}^{q-1}\sum_{j_1\neq i_1}\sum_{i_2=0}^{q-1}\sum_{j_2\neq i_2}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(j_1,j_2,i_3)|. \end{aligned} \tag{26}$$

Thus it follows from (5) and (13) that the right hand side of (26) is bounded by

$$\begin{aligned} & \frac{2q-3}{q(q-1)^3}\sum_{i_3=0}^{q-1}\sum_{j_3\neq i_3}|\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\tilde{\mu}(i_1,i_2,i_3)\tilde{\mu}(i_1,i_2,j_3)| \\ & +\frac{q-2}{q(q-1)^3}\sum_{i_3=0}^{q-1}|\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\tilde{\mu}^2(i_1,i_2,i_3)| \\ = \; & O(1/q), \end{aligned} \tag{27}$$

as $q \to \infty$.

STEP 5. We observe that

$$\begin{aligned} & qE|E(A_1A_3|\mathcal{W})| \\ = \; & \frac{1}{q-1}E|\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\sum_{j_2=0}^{q-1}Y(i_1,i_2,\rho(i_1,i_2))\tilde{\mu}(i_1,j_2,\rho(i_1,j_2))| \\ = \; & O(1/q), \end{aligned}$$

as $q \to \infty$. Thus it follows by symmetry that

$$qE|E(A_1A_3|\mathcal{W})| + qE|E(A_1A_4|\mathcal{W})| = O(1/q), \tag{28}$$

as $q \to \infty$.

Now we conclude from (18) and the results of the above 5 steps, namely (20), (24), (25), (27), and (28) that

$$|E\frac{d}{dw}g_z(W)E\int K(w)dw - E\frac{d}{dw}g_z(W)\int K(w)dw| = O(q^{-1/2}),$$

as $q \to \infty$ uniformly over $z \in \mathcal{R}$. This proves Lemma 5. □

Lemma 6 *With the notations and assumptions of Theorem 2, we have*

$$|E\int[\frac{d}{dw}g_z(W) - \frac{d}{dw}g_z(V+w)]K(w)dw| = O(q^{-(r-2)/(2r-2)}),$$

as $q \to \infty$ uniformly over $z \in \mathcal{R}$.

Proof of Lemma 6. Let $\varepsilon > 0$. We observe as in Ho and Chen (1978), page 247, that

$$\begin{aligned} & E\int|\frac{d}{dw}g_z(W) - \frac{d}{dw}g_z(V+w)|K(w)dw \\ \leq\ & 2E\int_{|w|>2\varepsilon}K(w)dw + 2E\int_{|w|\leq 2\varepsilon}I(|A_1+A_2|>2\varepsilon)K(w)dw \\ & +4\varepsilon E\int_{|w|\leq 2\varepsilon}(|W|+1)K(w)dw \\ & +E\int_{|w|\leq 2\varepsilon}I(z-2\varepsilon\leq V\leq z+2\varepsilon)K(w)dw. \end{aligned} \tag{29}$$

Now to prove Lemma 6, it suffices to get appropriate bounds for the terms on the right hand side of (29). To do so we shall divide the remainder of this proof into 4 steps.

Step 1. First we observe as in Lemma 4.6 of Ho and Chen (1978) that

$$\begin{aligned} E\int_{|w|>2\varepsilon}K(w)dw &\leq 2q\sum_{k=1}^{4}E[A_k^2 I(|A_k|>\varepsilon)] \\ &\leq 8qE[A_1^2 I(|A_1|>\varepsilon)], \end{aligned} \tag{30}$$

since A_k, $1 \leq k \leq 4$, all share the same marginal probability distribution. Hence using Hölder's, Markov's inequalities and (14), the right hand side of (30) is bounded by

$$8q[E(A_1^r)]^{2/r}[P(|A_1|>\varepsilon)]^{(r-2)/r} \leq 8qE(A_1^r)/\varepsilon^{r-2} = \varepsilon^{-(r-2)}O(q^{-(r-2)/2}),$$

as $q \to \infty$ uniformly over $\varepsilon > 0$.

STEP 2. Also by Hölder's and Markov's inequalities, we have

$$\begin{aligned} & E\int_{|w|\le 2\varepsilon} I(|A_1+A_2|>2\varepsilon)K(w)dw \\ \le\ & (q/2)\varepsilon E\{(\sum_{j=1}^{4}|A_j|)[I(|A_1|>\varepsilon)+I(|A_2|>\varepsilon)]\} \\ \le\ & 4q\varepsilon[E(A_1^r)]^{1/r}[P(|A_1|>\varepsilon)]^{(r-1)/r} \\ \le\ & 4qE(A_1^r)/\varepsilon^{r-2} \\ =\ & \varepsilon^{-(r-2)}O(q^{-(r-2)/2}), \end{aligned}$$

as $q \to \infty$ uniformly over $\varepsilon > 0$.

STEP 3. Next we observe from (14) that

$$\begin{aligned} \varepsilon E\int_{|w|\le 2\varepsilon}(|W|+1)K(w)dw &\le q\varepsilon E(|W|+1)(\sum_{k=1}^{4}A_k)^2 \\ &= O(q\varepsilon)[E(A_1^4)]^{1/2} \\ &= O(\varepsilon), \end{aligned}$$

as $q \to \infty$ uniformly over $\varepsilon > 0$.

STEP 4. Define

$$h_z(w) = \begin{cases} -4\varepsilon & \text{if } w \le z-4\varepsilon, \\ w-z & \text{if } z-4\varepsilon \le w \le z+4\varepsilon, \\ 4\varepsilon & \text{if } z+4\varepsilon \le w. \end{cases}$$

Consequently,

$$E\int \frac{d}{dw}h_z(V+w)K(w)dw \ge E\int_{|w|\le 2\varepsilon} I(z-2\varepsilon \le V \le z+2\varepsilon)K(w)dw.$$

Thus we observe as in (10) that

$$\begin{aligned} & E\int_{|w|\le 2\varepsilon} I(z-2\varepsilon \le V \le z+2\varepsilon)K(w)dw \\ \le\ & EWh_z(W) + \frac{1}{q-1}E[h_z(W)\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\tilde{\mu}(i_1,i_2,\rho(i_1,i_2))] \\ \le\ & 4\varepsilon E|W + \frac{1}{q-1}\sum_{i_1=0}^{q-1}\sum_{i_2=0}^{q-1}\tilde{\mu}(i_1,i_2,\rho(i_1,i_2))| \\ =\ & O(\varepsilon), \end{aligned}$$

as $q \to \infty$ uniformly over $\varepsilon > 0$ and $z \in \mathcal{R}$.

Now Lemma 6 follows from (29) and Steps 1 to 4, by taking $\varepsilon = q^{-(r-2)/(2r-2)}$. □

References

[1] HO, S. T. and CHEN, L. H. Y. (1978). An L_p bound for the remainder in a combinatorial central limit theorem. *Ann. Probab.* **6** 231-249.

[2] MCKAY, M. D., CONOVER, W. J. and BECKMAN, R. J. (1979). A comparison of three methods for selecting values of output variables in the analysis of output from a computer code. *Technometrics* **21** 239-245.

[3] OWEN, A. B. (1992). Orthogonal arrays for computer experiments, integration and visualization. *Statist. Sinica* **2** 439-452.

[4] OWEN, A. B. (1994). Lattice sampling revisited: Monte Carlo variance of means over randomized orthogonal arrays. Preprint.

[5] RAGHAVARAO, D. (1971). *Constructions and Combinatorial Problems in Design of Experiments.* Wiley, New York.

[6] STEIN, C. M. (1972). A bound for the error in the normal approximation to the distribution of a sum of dependent random variables. *Proc. Sixth Berkeley Symp. Math. Statist. Probab.* **2** 583-602. Univ. California Press, Berkeley.

[7] STEIN, C. M. (1986). *Approximate Computation of Expectations. IMS Lecture Notes–Monograph Ser.* **7**. IMS, Hayward, California.

[8] STEIN, M. L. (1987). Large sample properties of simulations using Latin hypercube sampling. *Technometrics* **29** 143-151.

[9] TANG, B. (1993). Orthogonal array-based Latin hypercubes. *J. Amer. Statist. Assoc.* **88** 1392-1397.