Bi-directional Sliced Latin Hypercube Designs

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Supplementary Material

This supplementary material includes the detailed proofs of Lemma 1~4 and Theorem 1~2.

Proof of Lemma 1

To prove (1), first note the exchangeability in the construction of BSPV. By symmetry, given any $l = 1, \ldots, n$, $Pr\{\pi(l) = u\}$ takes the same value for all $u = 1, 2, \ldots, n$. Hence $Pr\{\pi(l) = u\} = 1/n$ and (1) holds.

To prove (2), we calculate the joint probability mass function based on the conditional distribution of $\pi(l_2) = v$ given $\pi(l_1) = u$. Here, $u \neq v$ and $l_1 \neq l_2$. The joint probability mass function depends on the relationships between u and v, and also those between $\pi(l_1)$ and $\pi(l_2)$. For convenience, the following proof is carried out based on the relationship between u and v, instead of $\pi(l_1)$ and $\pi(l_2)$ given in the Lemma 1.

Given $\pi(l_1) = u$, assume $\pi(l_1) \in \mathbf{S}_{i_1 j_1}$ and $\pi(l_2) \in \mathbf{S}_{i_2 j_2}$, $i_1, i_2 = 1, \ldots, t$ and $j_1, j_2 = 1, \ldots, s$. The following cases are discussed for the conditional probability of $\pi(l_2) = v$.

(a) If $\gamma_s(u,v) = 1$, then $i_1 \neq i_2$ and $j_1 \neq j_2$ must hold (otherwise $Pr\{\pi(l_2) = v \mid \pi(l_1) = u\} = 0$). By exchangeability, $Pr\{\pi(l_2) = v \mid \pi(l_1) = u\}$ takes the same value for any position $\pi(l_2)$ satisfying $i_1 \neq i_2$ and $j_1 \neq j_2$. As there are $m(s-1)(t-1)$ such locations,

$$Pr\{\pi(l_2) = v \mid \pi(l_1) = u\} = \frac{1}{m(s-1)(t-1)}. \tag{A.1}$$

(b) If $\gamma_s(u,v) = 0$ and $\gamma_t(u,v) = 1$, then $i_1 \neq i_2$ must hold (otherwise $Pr\{\pi(l_2) = v \mid \pi(l_1) = u\} = 0$). By exchangeability, $Pr\{\pi(l_2) = v \mid \pi(l_1) = u\}$ takes the same value for any position $\pi(l_2)$ satisfying $i_1 \neq i_2$. As there are $ms(t-1)$ such locations,

$$Pr\{\pi(l_2)=v \mid \pi(l_1)=u\}=\frac{1}{ms(t-1)}. \tag{A.2}$$

(c) If $\gamma_p(u,v)=0$, then u and v are generated from different $\bar{\mathbf{Q}}_l$ matrices during the Step 2 construction of BSPV. Since $\bar{\mathbf{Q}}_l$ matrices are independently generated, the probability that u and v are at the same location of two $\bar{\mathbf{Q}}_l$ matrices is $1/p$. Thus,

(i) if $i_1 = i_2$ and $j_1 = j_2$,

$$Pr\{\pi(l_2)=v \mid \pi(l_1)=u\}=\frac{1/p}{m-1}=\frac{1}{n-p}, \tag{A.3}$$

(ii) otherwise,

$$Pr\{\pi(l_2)=v \mid \pi(l_1)=u\}=\frac{1/p}{m}=\frac{1}{n}. \tag{A.4}$$

(d) If $\gamma_t(u,v)=0$ and $\gamma_p(u,v)=1$, there are $p-t$ possible choices of v, and the conditional probability of $\pi(l_2) = v$ can be derived by the exchangeability and the regularity of probability. Specifically, we have,

(i) if $i_1 = i_2$ and $j_1 \neq j_2$,

$$Pr\{\pi(l_2)=v \mid \pi(l_1)=u\}=\frac{1-\frac{n-p}{n}}{p-t}=\frac{s}{n(s-1)}; \tag{A.5}$$

(ii) if $i_1 \neq i_2$ and $j_1 = j_2$,

$$Pr\{\pi(l_2)=v \mid \pi(l_1)=u\}=\frac{1-\frac{n-p}{n}-\frac{t-s}{ms(t-1)}}{p-t}=\frac{t}{n(t-1)}; \tag{A.6}$$

(iii) if $i_1 \neq i_2$ and $j_1 \neq j_2$,

$$Pr\{\pi(l_2)=v \mid \pi(l_1)=u\}=\frac{1-\frac{n-p}{n}-\frac{t-s}{ms(t-1)}-\frac{s-1}{m(s-1)(t-1)}}{p-t}=\frac{st-t-s}{n(t-1)(s-1)}. \tag{A.7}$$

Using the γ function defined in (3.3), the proof can be completed by re-classification of the above cases based on the relationships between $\pi(l_1)$ and $\pi(l_2)$, and then multiplying the conditional probability by $Pr\{\pi(l_1) = u\} = 1/n$.

Proof of Lemma 2

(i) Without loss of generality, we focus on $\mathbf{D}_{11}$. By the construction of $\mathbf{D}$, write the entries in $\mathbf{D}_{11}$ as $\pi_k(l)=(\alpha_l^k-1)p+\beta_l^k$, $l = 1,\ldots, m$, $k = 1,\ldots, q$, where $\{\alpha_1^k,\cdots,\alpha_m^k\}$ is a uniform permutation on $\mathbf{Z}_m$, β_l^k's are i.i.d and follow a discrete uniform distribution on $\mathbf{Z}_p$, and α_l^k's are independent with β_l^k's. Then for $l = 1,\ldots, m$, we can rewrite (2.1) as

$$d_{lk} = \frac{(\alpha_l^k - 1)p + \beta_l^k - u_{lk}}{pm} = \frac{\alpha_l^k - \tilde{u}_{lk}}{m}, \tag{A.8}$$

where $\tilde{u}_{lk} = (p - \beta_l^k + u_{lk}) / p$ follows a uniform distribution on (0,1].

(ii) We prove this by showing the equivalence between our construction and that of Qian (2012) for $\mathbf{D}_{1\bullet}$. In our method, note $\mathbf{D}_{1\bullet}$ is constructed based on the first columns of $\bar{\mathbf{Q}}_1, \ldots, \bar{\mathbf{Q}}_m$, or equivalently $\mathbf{W}(:,1)$. Divide $\mathbf{Z}_n$ into r groups of t consecutive numbers, where the ith group is $\mathbf{g}_i = \{a \in \mathbf{Z}_n \mid \lceil a / t \rceil = i\}$, $i = 1,\ldots, r$. For easier interpretation, we replace any number in $\mathbf{g}_i$ with the symbol g_i in our construction. For example, in our numerical example immediately following the construction steps, we can write

$$\bar{\mathbf{Q}}_1 = \mathbf{Q}_1' = \begin{bmatrix} 11 & 5 & 8 & 1 \\ 4 & 12 & 3 & 7 \\ 6 & 2 & 9 & 10 \end{bmatrix} = \begin{bmatrix} g_3 & g_2 & g_2 & g_1 \\ g_1 & g_3 & g_1 & g_2 \\ g_2 & g_1 & g_3 & g_3 \end{bmatrix},$$

where g_i can be viewed as the group index. Based on Step 1 of the construction for a BSPV, it is easy to see that $\bar{\mathbf{Q}}_l(:,1)$ is a uniform permutation on the set $\{g_{(l-1)s+1},\ldots, g_{ls}\}$ and the permutations are independent across l, $l = 1,\ldots, m$. This step produces equivalent outcome to that of Step 1 in Qian (2012).

For the next step in our construction of $\mathbf{D}_{1\bullet}$, first columns of each $\bar{\mathbf{Q}}_l$ are put together, then randomly permuted within each group of m numbers $\mathbf{W}(((j - 1)m + 1) : jm, 1)$ to form $\mathbf{W}(:,1)$, as in Step 3. This procedure is equivalent to carry out independent permutations on each row of the following matrix

$$\left[\bar{\mathbf{Q}}_1(:,1), \bar{\mathbf{Q}}_2(:,1), \ldots, \bar{\mathbf{Q}}_m(:,1)\right],$$

whose lth column is the 1st column of $\bar{\mathbf{Q}}_l$. This step produces equivalent outcome to that of Step 2 in Qian (2012).

Further, from Step 1 in our construction, it is clear that g_i is a uniform random number from $\mathbf{g}_i$. Hence the lth entry in $\mathbf{W}(:,1)$ can be written as $\pi(l) = (\alpha_l - 1)t + \beta_l$, $l = 1,\ldots, r$, where $\{\alpha_1, \cdots, \alpha_r\}$ is a uniform permutation on $\mathbf{Z}_r$ and β_l's are i.i.d uniformly distributed on $\mathbf{Z}_t$. Following the similar idea as that in the proof of part (i) and noting that the q BSPVs are independently generated, it is straightforward that $\mathbf{D}_{1\bullet}$ is equivalent to an SLHD with s slices, each of which contains m runs.

(iii) The proof follows the similar idea as that in part (ii).

Proof of Lemma 3

For any $x_l^k \in (0,1]$, $l = 1,\ldots, n$, $k = 1,\ldots, q$, by (2.1) and Lemma 1,

$$\begin{aligned} p(x_l^k)dx_l^k &= Pr(x_l^k < X_l^k < x_l^k + dx_l^k) \\ &= Pr\{nx_l^k < \pi_k(l) - u_{lk} < n(x_l^k + dx_l^k)\} \\ &= Pr\{\pi_k(l) = \lceil nx_l^k \rceil\} Pr(\lceil nx_l^k \rceil - nx_l^k - ndx_l^k < u_{lk} < \lceil nx_l^k \rceil - nx_l^k) \\ &= \frac{1}{n} ndx_l^k = dx_l^k. \end{aligned} \tag{A.9}$$

So the density of x_l^k satisfies $p(x_l^k) = 1$ for all $x_l^k \in (0,1]$. As x_l^k's are independent across k, $p(\mathbf{x}_l)$ = 1 for all $\mathbf{x}_l \in (0,1]^q$.

Proof of Lemma 4

Similar to the proof in Lemma 3, the joint density can be derived in the same way:

$$\begin{aligned} p(x_{l_1}^k, x_{l_2}^k)dx_{l_1}^k dx_{l_2}^k &= Pr(x_{l_1}^k < X_{l_1}^k < x_{l_1}^k + dx_{l_1}^k, x_{l_2}^k < X_{l_2}^k < x_{l_2}^k + dx_{l_2}^k) \\ &= Pr\{\pi_k(l_1) = \lceil nx_{l_1}^k \rceil, \pi_k(l_2) = \lceil nx_{l_2}^k \rceil\} n^2 dx_{l_1}^k dx_{l_2}^k \end{aligned} \tag{A.10}$$

Then $p(\mathbf{x}_{l_1}, \mathbf{x}_{l_2}) = \prod_{k=1}^q \{n^2 Pr(\pi_k(l_1) = \lceil nx_{l_1}^k \rceil, \pi_k(l_2) = \lceil nx_{l_2}^k \rceil)\}$, and the lemma follows directly from the results in Lemma 1.

Proof of Theorem 1

(i) follows directly from Lemma 2 (i), Lemma 2 in Xiong, Xie, Qian and Wu (2014), Lemma 2 in Qian (2012), and the theorem in McKay, Beckman, and Conover (1979). (ii) follows directly from case (ii) and case (iii) of Lemma 2, Lemma 2 in Xiong, Xie, Qian and Wu (2014), and Theorem 1 in Qian (2012).

Proof of Theorem 2

For (i), by Lemma 2, each $\mathbf{D}_{ij}$ is statistically equivalent to an ordinary LHD with m runs. Then, by Theorem 1 in Stein (1987) or Theorem 1 in Loh (1996), the result in (i) holds.

For (ii), by Lemma 2, each $\mathbf{D}_{i\bullet}$ is statistically equivalent to an SLHD with s slices each of m runs, and each $\mathbf{D}_{\bullet j}$ is statistically equivalent to a SLHD with t slices each of m runs. Then, the result follows directly from Theorem 2 in Qian (2012).

For (iii), by (3.1),

$$\begin{aligned}\mathrm{Var}(\hat{\mu}) &= \mathrm{Var}(\sum_i \sum_j \lambda_{ij}\hat{\mu}_{ij}) \\ &= \sum_{i_1}\sum_{j_1}\sum_{i_2}\sum_{j_2} \mathrm{Cov}(\lambda_{i_1j_1}\hat{\mu}_{i_1j_1}, \lambda_{i_2j_2}\hat{\mu}_{i_2j_2}) \\ &= \sum_i \sum_j \lambda_{ij}^2 \mathrm{Var}(\hat{\mu}_{ij}) + \sum\sum\sum\sum_{(i_1,j_1)\neq(i_2,j_2)} \lambda_{i_1j_1}\lambda_{i_2j_2}\mathrm{Cov}(\hat{\mu}_{i_1j_1}, \hat{\mu}_{i_2j_2})\end{aligned} \tag{A.11}$$

Define the first summation term and second summation term in (A.11) as I_1 and I_2, respectively. Since t and s are fixed integers, and m has the same order with n, we have, by part (i),

$$I_1 = \frac{1}{m}\sum_i\sum_j \lambda_{ij}^2\sigma_{ij}^2 - \frac{1}{m}\sum_i\sum_j\sum_k \lambda_{ij}^2 \int_0^1 \{f_{ij}^{-k}(x)\}^2 dx + o(n^{-1}). \tag{A.12}$$

Next we will show that $I_2 = o(n^{-1})$. Since I_2 is the summation of $p^2 - p$ different terms with p being a fixed number, it suffices to show that when $(i_1, j_1) \neq (i_2, j_2)$,

$$\mathrm{Cov}(\hat{\mu}_{i_1j_1}, \hat{\mu}_{i_2j_2}) = o(n^{-1}). \tag{A.13}$$

As $\hat{\mu}_{ij}$ defined in (3.1), we have

$$\mathrm{Cov}(\hat{\mu}_{i_1j_1}, \hat{\mu}_{i_2j_2}) = \frac{1}{m^2} \sum_{\mathbf{x}_{l_1}\in\mathbf{D}_{i_1j_1}, \mathbf{x}_{l_2}\in\mathbf{D}_{i_2j_2}} \mathrm{Cov}\{f_{i_1j_1}(\mathbf{x}_{l_1}), f_{i_2j_2}(\mathbf{x}_{l_2})\}. \tag{A.14}$$

Now we will show that when $(i_1, j_1) \neq (i_2, j_2)$,

$$\mathrm{Cov}\{f_{i_1j_1}(\mathbf{x}_{l_1}), f_{i_2j_2}(\mathbf{x}_{l_2})\} = o(n^{-1}). \tag{A.15}$$

To prove this, we first introduce the following lemma.

Lemma A1. Let $f(\cdot)$ and $g(\cdot)$ be two integrable functions defined on (0, 1], n is a positive integer, and $\delta_n(x, y)$ is defined in (3.4). Then we have, when $n \to \infty$,

$$\int_0^1\int_0^1 f(x_1)g(x_2)\delta_n(x_1, x_2)dx_1dx_2 = \frac{1}{n}\int_0^1 f(x)g(x)dx + o(n^{-1}). \tag{A.16}$$

Proof. Let $J_i = (\frac{i-1}{n}, \frac{i}{n}]$, $i = 1, \ldots, n$, we have

$$\delta_n(x_1, x_2) = \sum_{i=1}^n I\{x_1 \in J_i\} I\{x_2 \in J_i\}, \tag{A.17}$$

where $I(\cdot)$ is the indicator function. Therefore, when $n \to \infty$,

$$\begin{aligned}
&\int_0^1\int_0^1 f(x_1)g(x_2)\delta_n(x_1,x_2)dx_1dx_2 \\
&=\sum_{i=1}^{n}\int_0^1\int_0^1 f(x_1)g(x_2)I\{x_1\in J_i\}I\{x_2\in J_i\}dx_1dx_2 \\
&=\sum_{i=1}^{n}\int_{J_i} f(x)dx\int_{J_i} g(x)dx \\
&=\frac{1}{n}\int_0^1 f(x)g(x)dx+o(n^{-1}).
\end{aligned} \tag{A.18}$$

Now we go back to prove (A.15). The condition $(i_1, j_1) \neq (i_2, j_2)$ contains the three following cases, each corresponds to one case in Lemma 4.

(i) If $i_1 = i_2 = i$ and $j_1 \neq j_2$, it corresponds to the case (ii) in Lemma 4. Thus,

$$\begin{aligned}
&\mathrm{Cov}\{f_{ij_1}(\mathbf{x}_{l_1}), f_{ij_2}(\mathbf{x}_{l_2})\} \\
&=\int \{f_{ij_1}(\mathbf{x}_{l_1})-\mu_{ij_1}\}\{f_{ij_2}(\mathbf{x}_{l_2})-\mu_{ij_2}\}p(\mathbf{x}_{l_1},\mathbf{x}_{l_2})d\mathbf{x}_{l_1}d\mathbf{x}_{l_2} \\
&=\int \{f_{ij_1}(\mathbf{x}_{l_1})-\mu_{ij_1}\}\{f_{ij_2}(\mathbf{x}_{l_2})-\mu_{ij_2}\}\left\{1+\frac{1}{s-1}\sum_{k=1}^{q}\left[\delta_m(x_{l_1}^k,x_{l_2}^k)-s\delta_r(x_{l_1}^k,x_{l_2}^k)\right]\right\}d\mathbf{x}_{l_1}d\mathbf{x}_{l_2}+o(m^{-1}) \\
&=\frac{1}{s-1}\sum_{k=1}^{q}\int f_{ij_1}^{-k}(x_{l_1}^k)f_{ij_2}^{-k}(x_{l_2}^k)\delta_m(x_{l_1}^k,x_{l_2}^k)dx_{l_1}^k dx_{l_2}^k \\
&\quad-\frac{s}{s-1}\sum_{k=1}^{q}\int f_{ij_1}^{-k}(x_{l_1}^k)f_{ij_2}^{-k}(x_{l_2}^k)\delta_r(x_{l_1}^k,x_{l_2}^k)dx_{l_1}^k dx_{l_2}^k+o(m^{-1}) \\
&=\frac{1}{s-1}(\frac{1}{m}-\frac{s}{r})\sum_{k=1}^{q}\int f_{ij_1}^{-k}(x)f_{ij_2}^{-k}(x)dx+o(m^{-1}) \\
&=o(n^{-1}).
\end{aligned} \tag{A.19}$$

(ii) If $i_1 \neq i_2$ and $j_1 = j_2 = j$, it corresponds to the case (iii) in Lemma 4. By the same argument in part (ii), we have

$$\mathrm{Cov}\{f_{i_1j}(\mathbf{x}_{l_1}), f_{i_2j}(\mathbf{x}_{l_2})\}=o(n^{-1}). \tag{A.20}$$

(iii) If $i_1 \neq i_2$ and $j_1 \neq j_2$, it corresponds to the case (iv) in Lemma 4. Thus,

$$
\begin{aligned}
&\mathrm{Cov}\{f_{i_1j_1}(\mathbf{x}_{l_1}), f_{i_2j_2}(\mathbf{x}_{l_2})\} \\
&= \int \{f_{i_1j_1}(\mathbf{x}_{l_1}) - \mu_{i_1j_1}\}\{f_{i_2j_2}(\mathbf{x}_{l_2}) - \mu_{i_2j_2}\} p(\mathbf{x}_{l_1}, \mathbf{x}_{l_2}) d\mathbf{x}_{l_1} d\mathbf{x}_{l_2} \\
&= \int \{f_{i_1j_1}(\mathbf{x}_{l_1}) - \mu_{i_1j_1}\}\{f_{i_2j_2}(\mathbf{x}_{l_2}) - \mu_{i_2j_2}\} \\
&\quad \left\{1 + (s-1)^{-1}(t-1)^{-1}\sum_{k=1}^{q}\left[-\delta_m(x_{l_1}^k, x_{l_2}^k) + s\delta_r(x_{l_1}^k, x_{l_2}^k) + t\delta_h(x_{l_1}^k, x_{l_2}^k) - p\delta_n(x_{l_1}^k, x_{l_2}^k)\right]\right\} d\mathbf{x}_{l_1} d\mathbf{x}_{l_2} + o(n^{-1}) \\
&= (s-1)^{-1}(t-1)^{-1}\sum_{k=1}^{q}\int f_{i_1j_1}^{-k}(x_{l_1}^k) f_{i_2j_2}^{-k}(x_{l_2}^k) \\
&\quad [-\delta_m(x_{l_1}^k, x_{l_2}^k) + s\delta_r(x_{l_1}^k, x_{l_2}^k) + t\delta_h(x_{l_1}^k, x_{l_2}^k) - p\delta_n(x_{l_1}^k, x_{l_2}^k)] dx_{l_1}^k dx_{l_2}^k + o(n^{-1}) \\
&= (s-1)^{-1}(t-1)^{-1}(-\frac{1}{m} + \frac{s}{r} + \frac{t}{h} - \frac{p}{n})\sum_{k=1}^{q}\int f_{i_1j_1}^{-k}(x) f_{i_2j_2}^{-k}(x) dx + o(n^{-1}) \\
&= o(n^{-1}).
\end{aligned}
\tag{A.21}
$$

This proves (A.15) and completes the proof of Theorem 2.