

Design for sequential follow-up experiments in computer emulations (Supplements)

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APPENDIX A: Sampling Properties of SDs.

We now provide some sampling properties for SDs. Lehmann (1966) introduced the concept of negatively quadrant dependent variables. Two random variables τ_1 and τ_2 are negatively quadrant dependent if $P(\tau_1 \leq v_1, \tau_2 \leq v_2) \leq P(\tau_1 \leq v_1)P(\tau_2 \leq v_2)$ for any v_1 and v_2 . Under some conditions, negatively quadrant dependent variables have a negative covariance. The following Lemma gives the joint distribution of two design points from different stages of an experiment. For $0 \leq r_1, r_2 \leq 1$ and a positive integer p , define $\delta_p(r_1, r_2) = 1$ if $\lceil pr_1 \rceil = \lceil pr_2 \rceil$ and $\delta_p(r_1, r_2) = 0$ if $\lceil pr_1 \rceil \neq \lceil pr_2 \rceil$.

Lemma 1 *For an $SD(n_1, n_2)$ constructed in (2), we have*

(i) *the joint density function of $X_{i_1} \in D_1$ and $X_{i_2} \in D_A$ is*

$$\left(\frac{n_1 + L}{L}\right)^m \prod_{k=1}^m \left[\frac{L}{n_1 + L} + \frac{n_1}{n_1 + L} \delta_{n_1}(x_{i_1,k}, x_{i_2,k}) - \delta_{n_1+L}(x_{i_1,k}, x_{i_2,k}) \right], \quad (\text{A.1})$$

where $X_{i_1} = (x_{i_1,1}, \dots, x_{i_1,m})$ and $X_{i_2} = (x_{i_2,1}, \dots, x_{i_2,m})$;

(ii) $X_{i_1,k}$ and $X_{i_2,k}$ are negatively quadrant dependent for $k \in Z_m$;

(iii) D_A is statistically equivalent to an n_A -run ordinary LHD when n_A divides n_1 .

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Proof. (i) Because each column is independently generated, we only consider one dimensional projection. Let $X_{i_1} = (X_{i_1,1}, \dots, X_{i_1,m})$ and $X_{i_2} = (X_{i_2,1}, \dots, X_{i_2,m})$. Consider the joint density function of $X_{i_1,1}$ and $X_{i_2,1}$. Let $\rho(x_{i_1,1})$ denote the density function of $X_{i_1,1}$. The conditional density function of $X_{i_2,1}$ given $X_{i_1,1}$ is denoted by $\rho(x_{i_2,1}|x_{i_1,1})$. Because each point from an LHD follows the uniform distribution on $[0, 1]^m$, we have $\rho(x_{i_1,1}) = 1$ for $x_{i_1,1} \in [0, 1]$. Consider $\rho(x_{i_2,1}|x_{i_1,1})$. Given \mathcal{D}_1 , $X_{i_2,1}$ is uniformly distributed on $R_1^{(\mathcal{D}_1)}$. The density function of $X_{i_2,1}$ is $(L + n_1)L^{-1}$ on $R_1^{(\mathcal{D}_1)}$. Let $\mathcal{D}_{1,1}$ denote the first column of \mathcal{D}_1 . $\mathcal{D}_{1,1}$ is random given $x_{i_1,1}$. Then

$$\rho(x_{i_2,1}|x_{i_1,1}) = \frac{L + n_1}{L} P(X_{i_2,1} \notin R_1^{(\mathcal{D}_1)} | x_{i_1,1} \in R_1^{(\mathcal{D}_1)}). \quad (\text{A.2})$$

Let $a_1 = \lceil (n_1 + L)x_{i_1,1} \rceil$. For $a \in Z_{n_1+L}$, a simple calculation reveals that (i) $P(a \notin \mathcal{D}_{1,1} | a_1 \in \mathcal{D}_{1,1}) = 0$ if $a = a_1$; (ii) $P(a \notin \mathcal{D}_{1,1} | a_1 \in \mathcal{D}_{1,1}) = 1$ if $a \neq a_1$ and $\lceil a_1/n_1 \rceil = \lceil a/n_1 \rceil$; and (iii) $P(a \notin \mathcal{D}_{1,1} | a_1 \in \mathcal{D}_{1,1}) = L/(n_1 + L)$ otherwise. Thus, the one dimensional joint distribution of $X_{i_1,1}$ and $X_{i_2,1}$ is

$$\frac{n_1 + L}{L} \left[\frac{L}{n_1 + L} + \frac{n_1}{n_1 + L} \delta_{n_1}(x_{i_1,1}, x_{i_2,1}) - \delta_{n_1+L}(x_{i_1,1}, x_{i_2,1}) \right].$$

The m dimensions are generated independently, and (A.1) follows.

(ii) Consider the case that $X_{i_1} \in D_1$ and $X_{i_2} \in D_A$. Without loss of generality, assume $v_1 \leq v_2$. Then $P(X_{i_1,k} \leq v_1, X_{i_2,k} \leq v_2) - P(X_{i_1,k} \leq v_1)P(X_{i_2,k} \leq v_2)$ can be calculated as

$$\int_0^{v_1} \int_0^{v_2} \left[\frac{n_1}{L + n_1} \delta_{n_1}(x_{i_1,1}, x_{i_2,1}) - \delta_{n_1+L}(x_{i_1,1}, x_{i_2,1}) \right] dx_{i_1,1} dx_{i_2,1}. \quad (\text{A.3})$$

Let $\lambda = \lfloor n_1 v_1 \rfloor$, where $\lfloor r \rfloor$ is the largest integer not greater than r . Let $v_{1,0} = v_1 - n_1^{-1}\lambda$ and $v_{2,0} = v_2 - n_1^{-1}\lambda$. Then integral (A.3) becomes

$$\int_0^{v_{1,0}} \int_0^{v_{2,0}} \left[\frac{n_1}{L + n_1} \delta_{n_1}(x_{i_1,1}, x_{i_2,1}) - \delta_{n_1+L}(x_{i_1,1}, x_{i_2,1}) \right] dx_{i_1,1} dx_{i_2,1}. \quad (\text{A.4})$$

Case 1. $v_{2,0} \geq \frac{1}{n_1}$. The integral equals 0.

Case 2. $0 \leq v_{2,0} \leq \frac{1}{n_1}$ and $\lceil (n_1 + L)x_{i_1,1} \rceil \neq \lceil (n_1 + L)x_{i_2,1} \rceil$.

The integral equals $\frac{n_1}{L+n_1} v_{1,0}(v_{2,0} - n_1^{-1}) \leq 0$.

Case 3. $0 \leq v_{2,0} \leq \frac{1}{n_1}$ and $\lceil (n_1 + L)x_{i_1,1} \rceil = \lceil (n_1 + L)x_{i_2,1} \rceil$.

Let $p = \lfloor (n_1 + L)v_{2,0} \rfloor = \lfloor (n_1 + L)v_{1,0} \rfloor$, $t_1 = (n_1 + L)v_{1,0} - p$ and $t_2 = (n_1 + L)v_{2,0} - p$. The integral becomes $\frac{(t_1+p)(t_2+p)n_1}{(n_1+L)^3} - \frac{p+t_1 t_2}{(n_1+L)^2}$. Note that $\frac{L+n_1}{n_1} \geq p + 1$. The integral is no greater than $-\frac{p(1-t_1)(1-t_2)}{(p+1)(n_1+L)^2} \leq 0$. Thus, integral (A.4) is no greater than 0, which completes the proof.

(iii) When n_A divides n_1 , $L(n_1, n_A) = n_1$. Consider a one-dimensional projection. Note that $X_{1,j}, \dots, X_{n_1,j}$ form the j th column of a randomized LHD. It is obvious that $z_{1,j}, \dots, z_{n_1,j}$ are n_1 independent random variables. For $i = 1, \dots, n_A$, let \mathcal{S}_i denote the random set of $\{z_{(i-1)\lambda_0+1,j}, \dots, z_{i\lambda_0,j}\}$ where $\lambda_0 = n_1/n_A$. Then \mathcal{S}_i are independent and

$P(k_i \in \mathcal{S}_i) = \frac{1}{2}$ for any $\frac{i-1}{n_A} \cdot 2n_1 < k_i \leq \frac{i}{n_A} \cdot 2n_1$. Thus, in Step 2 of the construction (2), $P(a_{n_1+i,j} = k_i) = \frac{n_A}{2n_1}$ and a_{n_1+i} are n_A independent random variables for $i = 1, \dots, n_A$. Thus, $(2n_1)^{-1}(a_{n_1+i} - \varepsilon_{i,j})$ follows the uniform distribution on $[\frac{i-1}{n_A}, \frac{i}{n_A})$ and the result immediately follows.

When n_A divides n_1 , the following proposition compares the variance formula of $\hat{\mu}_2$ for the three schemes.

Proposition 1 *Suppose that (i) $f(x)$ is monotonic in each argument; or (ii) $f(x) = \mu + \sum_{k=1}^m f_k(x_k)$. When n_A divides n_1 , for the three design schemes IID(n_2), IL(n_1, n_2) and SD(n_1, n_2) constructed in (2), we have*

$$\text{Var}_{\text{IID}}(\hat{\mu}_2) \geq \text{Var}_{\text{IL}}(\hat{\mu}_2) \geq \text{Var}_{\text{SD}}(\hat{\mu}_2).$$

Proof. For both SDs and ILs, decompose the variance of $\hat{\mu}_2$ as

$$\text{Var}(\hat{\mu}_2) = E(\hat{\mu}_2 - \mu)^2 = \frac{n_1^2}{n_2^2} E(\hat{\mu}_1 - \mu)^2 + \frac{n_A^2}{n_2^2} E(\hat{\mu}_A - \mu)^2 + 2 \frac{n_1 n_A}{n_2^2} \text{Cov}(\hat{\mu}_1, \hat{\mu}_A). \quad (\text{A.5})$$

When n_A divides n_1 , the first two items in equation (A.5) are the same as those of the ILs. So it is sufficient to show that the third item of equation (A.5), which is 0 for ILs, is negative. (i) From Lemma 1 (ii), the third item of (A.5) is negative for SDs when the function is monotonic in each argument. (ii) When $f(x) = \mu + \sum_{k=1}^m f_k(x_k)$, given \mathcal{D}_1 , D_1 and D_A are independent. For $k = 1, \dots, m$, let $W_k^{\mathcal{D}_1} = [0, 1] \setminus R_k^{\mathcal{D}_1}$. We have

$$E(\hat{\mu}_1 - \mu | \mathcal{D}_1) = \left(\frac{n_1 + L}{n_1} \right)^m \sum_{k=1}^m \int_{W_k^{\mathcal{D}_1}} f_k(x_k) dx_k,$$

and

$$E(\hat{\mu}_A - \mu | \mathcal{D}_1) = \left(\frac{n_1 + L}{L} \right)^m \sum_{k=1}^m \int_{R_k^{\mathcal{D}_1}} f_k(x_k) dx_k.$$

Noting that $\int_{R_k^{\mathcal{D}_1} \cup W_k^{\mathcal{D}_1}} f_k(x_k) dx_k = 0$, we have

$$\left(\frac{n_1 + L}{n_1} \right)^{-m} \cdot E(\hat{\mu}_1 - \mu | \mathcal{D}_1) + \left(\frac{n_1 + L}{L} \right)^{-m} \cdot E(\hat{\mu}_A - \mu | \mathcal{D}_1) = 0,$$

and consequently

$$E(\hat{\mu}_1 - \mu | \mathcal{D}_1) \times E(\hat{\mu}_A - \mu | \mathcal{D}_1) \leq 0.$$

The third item of equation (A.5) can be calculated as

$$\text{Cov}(\hat{\mu}_1, \hat{\mu}_A) = E_{\mathcal{D}_1}[E(\hat{\mu}_1 - \mu | \mathcal{D}_1) \cdot E(\hat{\mu}_A - \mu | \mathcal{D}_1)] < 0,$$

which completes the proof. Note that a one-stage sequentially refined LHD in Xu et al. (2015) reduces to an ordinary LHD. Theorem 3 in Xu et al. (2015) shows that the variance of $\hat{\mu}$ based on a one-stage sequentially refined LHD is smaller than that based on an IID sample with the same sample size in conditions (i) or (ii). Thus, $\text{Var}_{\text{LHD}}(\hat{\mu}_1) \leq \text{Var}_{\text{IID}}(\hat{\mu}_1)$, $\text{Var}_{\text{LHD}}(\hat{\mu}_A) \leq \text{Var}_{\text{IID}}(\hat{\mu}_A)$, and $\text{Var}_{\text{IID}}(\hat{\mu}_2) \geq \text{Var}_{\text{IL}}(\hat{\mu}_2)$ immediately follows.

Similarly, we can obtain the following Proposition 2 by analogous argument to the proof of Proposition 1.

Proposition 2 Suppose that $f_H(x)$ and $f_L(x)$ are either both increasing or both decreasing in each argument of x . When n_A divides n_1 , for the variance of $\hat{\eta}$, we have

$$\text{Var}_{\text{IID}}(\hat{\eta}) \geq \text{Var}_{\text{IL}}(\hat{\eta}) \geq \text{Var}_{\text{SD}}(\hat{\eta}).$$

APPENDIX B: Proofs of Theorems.

Proof of Theorem 1

For an $SD(n_1, n_2)$ constructed in (2), define $f_{\mathcal{D}_1} : (0, 1]^m \rightarrow R$ as $f_{\mathcal{D}_1}(x) = f(\Phi_{(\mathcal{D}_1)}(x))$. Then $\hat{\mu}_A = n_A^{-1} \sum_{i=n_1+1}^{n_2} f_{\mathcal{D}_1}(\Phi_{(\mathcal{D}_1)}^{-1}(X_i))$. Recall the definition of $\phi_j^{(\mathcal{D}_1)}$ given in (3). Let $\lambda = L/n_1$. It is trivial that for any $k = 1, \dots, n_1$ and $x \in [\frac{k-1}{n_1}, \frac{k}{n_1})$, $\phi_j^{(\mathcal{D}_1)}(x) \in [\frac{\tau_{(k-1)\lambda+1,j}^{(\mathcal{D}_1)-1}}{n_1+L}, \frac{\tau_{k\lambda,j}^{(\mathcal{D}_1)}}{n_1+L})$. From the definition of $\tau_{i,j}^{(\mathcal{D}_1)}$, we have $\tau_{(k-1)\lambda+1,j}^{(\mathcal{D}_1)} - 1 \geq (k-1)\frac{n_1+L}{n_1}$ and $\tau_{k\lambda,j}^{(\mathcal{D}_1)} \leq k\frac{n_1+L}{n_1}$. It follows immediately that $|\phi_j^{(\mathcal{D}_1)}(x) - x| \leq n_1^{-1}$. By recalling the definition of the mapping $\Phi_{(\mathcal{D}_1)} : (0, 1]^m \rightarrow \prod_{j=1}^m R_j^{(\mathcal{D}_1)}$, we know that for any $x \in (0, 1]^m$, $\|\Phi_{(\mathcal{D}_1)}(x) - x\| \leq m^{1/2}n_1^{-1}$. Because f is Lipschitz continuous, there exists a constant c_0 such that $|f(x) - f(\Phi_{(\mathcal{D}_1)}(x))| \leq c_0n_1^{-1}$ and

$$|n_A^{-1} \sum_{i=n_1+1}^{n_2} [f(\Phi_{(\mathcal{D}_1)}^{-1}(X_i)) - f_{\mathcal{D}_1}(\Phi_{(\mathcal{D}_1)}^{-1}(X_i))]| \leq n_A^{-1}c_0r, \quad (\text{A.6})$$

where $r = n_A/n_1$ is bounded as $n_1 \rightarrow \infty$. Define

$$\hat{\mu}_A^* = \frac{1}{n_A} \sum_{i=n_1+1}^{n_2} f(\Phi_{(\mathcal{D}_1)}^{-1}(X_i)).$$

Note that the D_A^* generated from equation (4) is an n_A -run ordinary LHD on $[0, 1)^m$ independent from D_1 . From Theorem 1 in Owen (1992), for any two positive real numbers ω_1 and ω_A , we have

$$\omega_1\hat{\mu}_1 + \omega_A\hat{\mu}_A^* \rightarrow N\left(0, \int_{[0,1]^m} \frac{\omega_1^2}{n_1}r^2(x) + \frac{\omega_A^2}{n_A}r^2(x)dx\right).$$

From equation (A.6), it is easy to prove that

$$\omega_A\hat{\mu}_A^* - \omega_A\hat{\mu}_A = O(n_A^{-1}).$$

So Slutsky's theorem shows that

$$\omega_1\hat{\mu}_1 + \omega_A\hat{\mu}_A \rightarrow N\left(0, \int_{[0,1]^m} \frac{\omega_1^2}{n_1}r^2(x) + \frac{\omega_A^2}{n_A}r^2(x)dx\right).$$

Thus, when $\omega_1 = n_1/n_2$ and $\omega_A = n_A/n_2$, the asymptotic normal distribution of $\hat{\mu}_2$ immediately follows.

Proof of Theorem 3

Denote the greatest common divisor of n_1, \dots, n_u by $G = G(n_1, \dots, n_u)$. Let $n_k = G \cdot p_k$ for $k = 1, \dots, u$. From the construction of multi-stage SDs, it is easily seen that G is also a common divisor of N_1, \dots, N_u . Note that n_{i+1}/n_i is fixed for any $1 \leq i < u$ as $n_1 \rightarrow \infty$, and n_1, \dots, n_u are integers. Simple algebra shows that the above condition is equivalent to $G \rightarrow \infty$ with p_k fixed.

Let $|\mathcal{S}|$ denote the number of different elements in an arbitrary set \mathcal{S} . When z_1 divides z_2 , we write $z_1|z_2$ for convenience. For $j = 1, \dots, m$ and $k \geq 1$, denote the set $\{\frac{\lfloor nX_{1,j} \rfloor}{n}, \dots, \frac{\lfloor nX_{n_k,j} \rfloor}{n}\}$ by $\frac{\lfloor nD_k^{(j)} \rfloor}{n}$. For any $k \geq 1$, we have (i) $G|n_k$ and $G|N_k$, and (ii) $N_k|N_{k+1}$. It is obvious that for any $g = 1, \dots, G$ and $t > 1$,

$$\left| \frac{\lfloor N_t D_1^{(j)} \rfloor}{N_t} \cap \left[\frac{g-1}{G}, \frac{g}{G} \right) \right| = \frac{n_1}{G}.$$

Assume that for any $g = 1, \dots, G$ and $t > k - 1$,

$$\left| \frac{\lfloor N_t D_{k-1}^{(j)} \rfloor}{N_t} \cap \left[\frac{g-1}{G}, \frac{g}{G} \right) \right| = \frac{n_{k-1}}{G}.$$

From the definitions of N_k and G , we know $G|(n_k - n_{k-1})$ and $(n_k - n_{k-1})|(N_k - n_{k-1})$. With these results, for the construction of multi-stage SDs, we have $|\mathcal{B}_k^{(j)} \cap [\frac{g-1}{G}, \frac{g}{G})| = \frac{N_k - n_{k-1}}{G}$ and, for any $x \in [\frac{g-1}{G}, \frac{g}{G})$,

$$\phi_{\mathcal{A}_k^{(j)}, l_k}(x) \in \bigcup_{r \in \mathcal{B}_k^{(j)} \cap [\frac{g-1}{G}, \frac{g}{G})} \left[r, r + \frac{1}{N_k} \right) \subset \left[\frac{g-1}{G}, \frac{g}{G} \right). \quad (\text{A.7})$$

It can be verified that for any $g = 1, \dots, G$ and $t > k$,

$$\left| \frac{\lfloor N_t D_k^{(j)} \rfloor}{N_t} \cap \left[\frac{g-1}{G}, \frac{g}{G} \right) \right| = \frac{n_k}{G}.$$

It should be noted that $\phi_{\mathcal{A}_1^{(j)}, l_1}(x) = x$ and so, from the result given by (A.7), we have $|\phi_{\mathcal{A}_k^{(j)}, l_k}(x) - x| \leq G^{-1}$ for any $1 \leq j \leq m$ and $k \geq 1$. For $x = (x_1, \dots, x_m) \in [0, 1]^m$, let

$$\Phi_{(\mathcal{D}_{k-1})}(x) = \left(\phi_{\mathcal{A}_k^{(1)}, l_k}(x_1), \dots, \phi_{\mathcal{A}_k^{(m)}, l_k}(x_m) \right).$$

It follows that $\|\Phi_{(\mathcal{D}_{k-1})}(x) - x\| \leq m^{1/2}G^{-1}$ for any $x \in [0, 1]^m$. Note that $G = O(n_1)$ and $\{\Phi_{(\mathcal{D}_{k-1})}^{-1}(X) : X \in D_k \setminus D_{k-1}\}$ is statistically equivalent to an ordinary LHD of $n_k - n_{k-1}$ runs. The proof of the final result can be given recursively, which is analogous to the proof of Theorem 1 where $k = 2$.

APPENDIX C: Figures.

Comparison of MSEs for SD, IL and SS

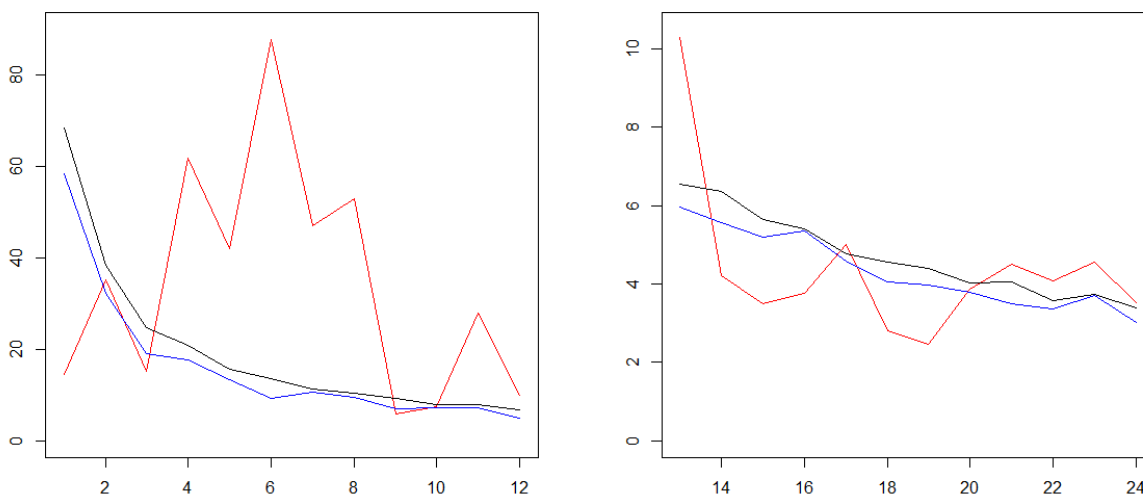


Figure 1: MSEs of $\hat{\mu}$ given $n_1 = 6$ in Example 3 for SD (blue), IL (black), and SS (red) with different choices of n_A (abscissa).

Comparison of MSEs for SD, IL and SS

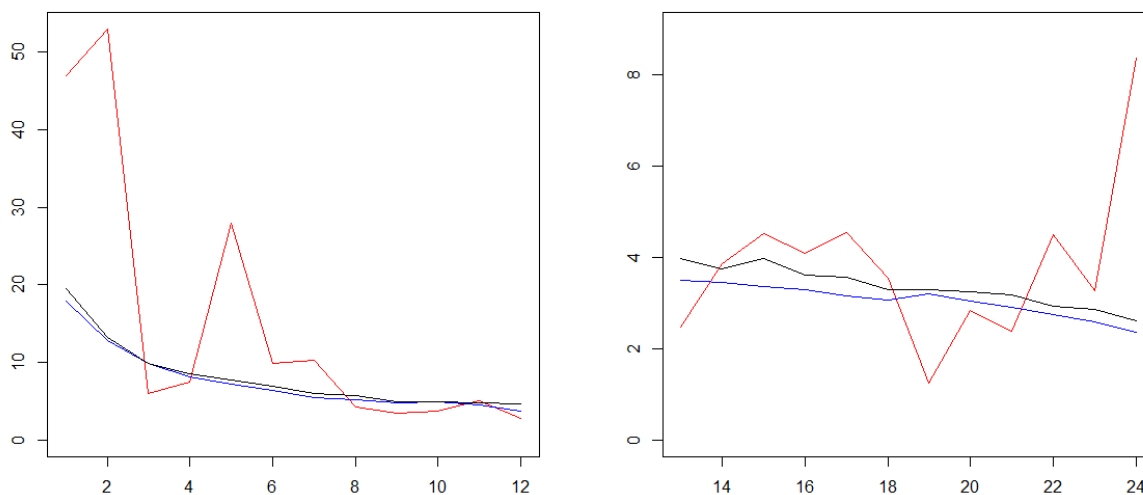


Figure 2: MSEs of $\hat{\mu}$ given $n_1 = 12$ in Example 3 for SD (blue), IL (black), and SS (red) with different choices of n_A (abscissa).

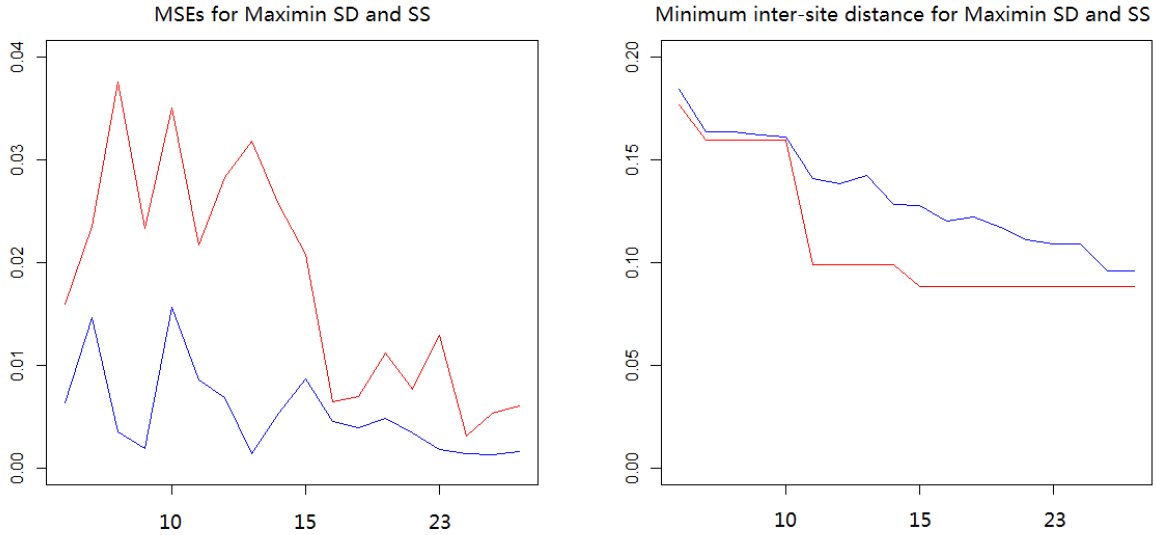


Figure 3: Plots of MSEs of $\hat{\mu}$ (left) and minimum inter-site distance (right) for the maximin SD (blue) and SS (red) in Example 5 with different choices of n_A (abscissa).

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