OPTIMAL DESIGNS FOR 2^k FACTORIAL EXPERIMENTS WITH BINARY RESPONSE

Jie Yang[1], Abhyuday Mandal[2] and Dibyen Majumdar[1]

[1] *University of Illinois at Chicago and* [2] *University of Georgia*

Supplementary Materials

Connection between General Equivalence Theorem and Theorem 3.1.1:

Extending the notations of this paper, we consider the problem when a design $\xi = \{(\mathbf{x}_i, p_i),\ i = 1, \ldots, 2^k\}$ maximizes the D-criterion $|M(\xi)| = |X'WX|$, where $\mathbf{x}_i$ is the ith row of X and X is the $2^k \times (d+1)$ model matrix.

General Equivalence Theorem (see, for example, Atkinson et al. (2007)): ξ maximizes $|M(\xi)|$ (or equivalently minimizes $\Psi\{M(\xi)\} = -\log|M(\xi)|$) if and only if

$$w_i \mathbf{x}_i'(X'WX)^{-1}\mathbf{x}_i \leq d+1$$

for each $i = 1, \ldots, 2^k$ and equality holds if $p_i > 0$.

Here's the outline of the proof of the General Equivalence Theorem described in Atkinson et al. (2007, §9.2, page 122): For each $i = 1, \ldots, 2^k$, let $\bar{\xi}_i$ be the design supported only on $\mathbf{x}_i$, or in other words, it puts unit mass at the point $\mathbf{x}_i$ and let $\xi_i' = (1-\alpha)\xi + \alpha\bar{\xi}_i$. The derivative of Ψ in the direction $\bar{\xi}_i$ or $\mathbf{x}_i$ is

$$\phi(\mathbf{x}_i, \xi) = \lim_{\alpha \to 0^+} \frac{1}{\alpha}[\Psi(M(\xi_i')) - \Psi(M(\xi))] = (d+1) - w_i \mathbf{x}_i'(X'WX)^{-1}\mathbf{x}_i \ .$$

Then ξ is D-optimal if and only if $\min_i \phi(\mathbf{x}_i, \xi) = 0$ and $\phi(\mathbf{x}_i, \xi) = 0$ if $p_i > 0$. Comparing with our proof of Theorem 3.1.1, $\xi_i' = (1-\alpha)\xi + \alpha\bar{\xi}_i = \xi + \alpha(\bar{\xi}_i - \xi)$ corresponds to our $\mathbf{p}_r + u\boldsymbol{\delta}_i^{(r)}$ with u replaced by α and $\boldsymbol{\delta}_i^{(r)}$ replaced by $\bar{\xi}_i - \xi$. Therefore, $\phi(\mathbf{x}_i, \xi)$ is equal to $\left.\frac{\partial f^{(r)}(\mathbf{p}_r + u\boldsymbol{\delta}_i^{(r)})}{\partial u}\right|_{u=0}$ and the if and only if condition comparing Atkinson et al. (2007) becomes

$$\left.\frac{\partial f^{(r)}(\mathbf{p}_r + u\boldsymbol{\delta}_i^{(r)})}{\partial u}\right|_{u=0} \begin{array}{lll} = & 0 & \text{if } p_i > 0; \\ \leq & 0 & \text{otherwise.} \end{array}$$

The major difference between the general equivalence theorem and Theorem 3.11 is that the general equivalence theorem ends up with the inverse of $X'WX$, while we expressed the same set of conditions in terms of determinants with the aid of Lemma 3.1.1, as well as Lemma S1.2 and Lemma S1.3. $\square$

Additional Results for Example 4.1: Consider a 2^3 main-effects model with logit link. Suppose $\beta_1 = 0$. As a corollary of Theorem 4.1.4, the regular fractions $\{1,4,6,7\}$, $\{2,3,5,8\}$ are D-optimal half-fractions if and only

$$4\,\nu\left(|\beta_0|+|\beta_2|+|\beta_3|\right) \geq \nu\left(|\beta_0|+|\beta_2|+|\beta_3| - 2\max_{0\leq i\leq 3}|\beta_i|\right).$$

Note that $\nu(\eta) = \frac{1}{2+e^{\eta}+e^{-\eta}}$ for logit link, which is symmetric about 0. To simplify the notations, let $\beta_{2\vee 3} = \max\{|\beta_2|,|\beta_3|\}$ and $\beta_{2\wedge 3} = \min\{|\beta_2|,|\beta_3|\}$. The regular fractions $\{1,4,6,7\}$, $\{2,3,5,8\}$ are D-optimal half-fractions if and only if one of three conditions below is satisfied:

$$\text{(i)} \qquad |\beta_2|+|\beta_3| \leq \log 2; \tag{S.1}$$

$$\begin{aligned}
&\text{(ii)} && |\beta_2|+|\beta_3| > \log 2,\ \beta_{2\vee 3} \leq \log\left(1+e^{-\beta_{2\wedge 3}}+\left[1+e^{-\beta_{2\wedge 3}}+e^{-2\beta_{2\wedge 3}}\right]^{1/2}\right),\\
& && \text{and } |\beta_0| \leq \log\left(\frac{2\exp\{|\beta_2|+|\beta_3|\}-1}{\exp\{|\beta_2|+|\beta_3|\}-2}\right);\\
&\text{(iii)} && \beta_{2\vee 3} > \log\left(1+e^{-\beta_{2\wedge 3}}+\left[1+e^{-\beta_{2\wedge 3}}+e^{-2\beta_{2\wedge 3}}\right]^{1/2}\right),\\
& && |\beta_{2\vee 3}| \leq \log\left(\frac{2e^{|\beta_{2\wedge 3}|}-1}{e^{|\beta_{2\wedge 3}|}-2}\right) \text{ and } |\beta_0| \leq \log\left(\frac{2e^{\beta_{2\vee 3}}-1}{e^{\beta_{2\vee 3}}-2}\right) - \beta_{2\wedge 3}.
\end{aligned}$$

The above result is displayed in the right panel of Figure 4.2. In the x- and y-axis, we have plotted β_2 and β_3 respectively. The rhomboidal region at the center (marked as ∞) represents the region where the regular fractions will always be D-optimal, irrespective of the values of β_0. The contours outside this region are for the upper bound of $|\beta_0|$. Regular fractions will be D-optimal if the values of $|\beta_0|$ will be smaller than the upper bound with β_2 and β_3 falling inside the region outlined by the contour.

Proofs

We need two lemmas before the proof of Theorem 3.1.1.

Lemma S1.2 *Suppose* $\mathbf{p} = (p_1, \ldots, p_{2^k})'$ *satisfies* $f(\mathbf{p}) > 0$. *Given* $i = 1, \ldots, 2^k$,

$$f_i(z) = a_i z(1-z)^d + b_i(1-z)^{d+1}, \tag{S.2}$$

for some constants a_i *and* b_i. *If* $p_i > 0$, $b_i = f_i(0)$, $a_i = \frac{f(\mathbf{p}) - b_i(1-p_i)^{d+1}}{p_i(1-p_i)^d}$; *otherwise,* $b_i = f(\mathbf{p})$, $a_i = f_i\left(\frac{1}{2}\right) \cdot 2^{d+1} - b_i$. *Note that* $a_i \geq 0$, $b_i \geq 0$, *and* $a_i + b_i > 0$. □

Lemma S1.3 *Let* $h(z) = az(1-z)^d + b(1-z)^{d+1}$ *with* $0 \leq z \leq 1$ *and* $a \geq 0, b \geq 0, a + b > 0$. *If* $a > b(d+1)$, *then* $\max_z h(z) = \left(\frac{d}{a-b}\right)^d \left(\frac{a}{d+1}\right)^{d+1}$ *at* $z = \frac{a - b(d+1)}{(a-b)(d+1)} < 1$. *Otherwise,* $\max_z h(z) = b$ *at* $z = 0$. □

Proof of Theorem 3.1.1: Note that $f(\mathbf{p}) > 0$ implies $0 \leq p_i < 1$ for each $i = 1, \ldots, 2^k$. Since $\sum_i p_i = 1$, without any loss of generality, we assume $p_{2^k} > 0$. Define $\mathbf{p}_r = (p_1, \ldots, p_{2^k-1})'$, and $f^{(r)}(\mathbf{p}_r) = f(p_1, \ldots, p_{2^k-1}, 1 - \sum_{i=1}^{2^k-1} p_i)$.

For $i = 1, \ldots, 2^k - 1$, let $\boldsymbol{\delta}_i^{(r)} = (-p_1, \ldots, -p_{i-1}, 1 - p_i, -p_{i+1}, \ldots, -p_{2^k-1})'$. Then $f_i(z) = f^{(r)}(\mathbf{p}_r + u\boldsymbol{\delta}_i^{(r)})$ with $u = \frac{z - p_i}{1 - p_i}$. Since the determinant $|(\boldsymbol{\delta}_1^{(r)}, \ldots, \boldsymbol{\delta}_{2^k-1}^{(r)})| = p_{2^k} \neq 0$, $\boldsymbol{\delta}_1^{(r)}, \ldots, \boldsymbol{\delta}_{2^k-1}^{(r)}$ are linearly independent and thus may serve as a new basis of

$$S_r = \{(p_1, \ldots, p_{2^k-1})' \mid \sum_{i=1}^{2^k-1} p_i \leq 1, \text{ and } p_i \geq 0, i = 1, \ldots, 2^k - 1\}. \tag{S.3}$$

Since $\log f^{(r)}(\mathbf{p}_r)$ is concave, $\mathbf{p}_r$ maximizes $f^{(r)}$ if and only if along each direction $\boldsymbol{\delta}_i^{(r)}$,

$$\left.\frac{\partial f^{(r)}(\mathbf{p}_r + u\boldsymbol{\delta}_i^{(r)})}{\partial u}\right|_{u=0} = 0 \text{ if } p_i > 0; \quad \leq 0 \text{ otherwise.}$$

That is, $f_i(z)$ attains its maximum at $z = p_i$, for each $i = 1, \ldots, 2^k - 1$ (and thus for $i = 2^k$). Based on Lemma S1.2 and Lemma S1.3, it implies one of the two cases:

(i) $p_i = 0$ and $f_i\left(\frac{1}{2}\right) \cdot 2^{d+1} - f(\mathbf{p}) \leq f(\mathbf{p})(d+1)$;

(ii) $p_i > 0$, $a > b(d+1)$, and $a - b(d+1) = p_i(a-b)(d+1)$, where $b = f_i(0)$, and $a = \frac{f(\mathbf{p}) - b(1-p_i)^{d+1}}{p_i(1-p_i)^d}$.

The conclusion needed can be obtained by simplifying those two cases above. $\square$

Proof of Theorem 3.1.2: Let $\mathbf{p}_I$ be the minimally supported design satisfying $p_{i_1} = p_{i_2} = \cdots = p_{i_{d+1}} = \frac{1}{d+1}$. Note that if $|X[i_1, i_2, \ldots, i_{d+1}]| = 0$, $\mathbf{p}_I$ can not be D-optimal. Suppose $|X[i_1, i_2, \ldots, i_{d+1}]| \neq 0$, $\mathbf{p}_I$ is D-optimal if and only if $\mathbf{p}_I$ satisfies the conditions of Theorem 3.1.1. By Lemma 3.1.1, $f(\mathbf{p}_I) = (d+1)^{-(d+1)}|X[i_1, i_2, \ldots, i_{d+1}]|^2 w_{i_1} w_{i_2} \cdots w_{i_{d+1}}$.

For $i \in \mathbf{I}$, $p_i = \frac{1}{d+1}$, $f_i(0) = 0$. By case (ii) of Theorem 3.1.1, $p_i = \frac{1}{d+1}$ maximizes $f_i(x)$. For $i \notin \mathbf{I}$, $p_i = 0$,

$$\begin{aligned} f_i\left(\frac{1}{2}\right) &= [2(d+1)]^{-(d+1)}|X[i_1, \ldots, i_{d+1}]|^2 w_{i_1} \cdots w_{i_{d+1}} \\ &+ 2^{-(d+1)}(d+1)^{-d} w_i \cdot w_{i_1} \cdots w_{i_{d+1}} \sum_{j \in \mathbf{I}} \frac{|X[\{i\} \cup \mathbf{I} \setminus \{j\}]|^2}{w_j}. \end{aligned}$$

Then $p_i = 0$ maximizes $f_i(x)$ if and only if $f_i\left(\frac{1}{2}\right) \leq f(\mathbf{p}) \frac{d+2}{2^{d+1}}$, which is equivalent to

$$\sum_{j \in \mathbf{I}} \frac{|X[\{i\} \cup \mathbf{I} \setminus \{j\}]|^2}{w_j} \leq \frac{|X[i_1, i_2, \ldots, i_{d+1}]|^2}{w_i}.$$

$\square$

Proof of Theorem 3.3.3: Suppose the lift-one algorithm or its modified version converges at $\mathbf{p}^* = (p_1^*, \ldots, p_{2^k}^*)'$. According to the algorithm, $|X'WX| > 0$ at $\mathbf{p}^*$ and $p_i^* < 1$ for $i = 1, \ldots, 2^k$. The proof of Theorem 3.1.1 guarantees that $\mathbf{p}^*$ maximizes $f(\mathbf{p}) = |X'WX|$.

Now we show that the modified lift-one algorithm must converge to the maximum value $\max_{\mathbf{p}} |X'WX|$. Based on the algorithm, we obtain a sequence of designs $\{\mathbf{p}_n\}_{n \geq 0} \subset S_r$ defined in (S.3) such that $|X'WX| > 0$. We only need to check the case when the sequence is infinite. To simplify the notation, here we still denote $f(\mathbf{p}) = f(p_1, \ldots, p_{2^k-1}, 1 - \sum_{i=1}^{2^k-1} p_i)$ for $\mathbf{p} = (p_1, \ldots, p_{2^k-1})' \in S_r$. Since that $f(\mathbf{p})$ is bounded from above on S_r and $f(\mathbf{p}_n)$ strictly increases with n, then $\lim_{n \to \infty} f(\mathbf{p}_n)$ exists.

Suppose $\lim_{n\to\infty} f(\mathbf{p}_n) < \max_{\mathbf{p}} |X'WX|$. Since S_r is compact, there exists a $\mathbf{p}_* = (p_1^*, \ldots, p_{2^k-1}^*)' \in S_r$ and a subsequence $\{\mathbf{p}_{n_s}\}_{s\geq 1} \subset \{\mathbf{p}_{10m}\}_{m\geq 0} \subset \{\mathbf{p}_n\}_{n\geq 0}$ such that

$$0 < f(\mathbf{p}_*) = \lim_{n\to\infty} f(\mathbf{p}_n) = \lim_{s\to\infty} f(\mathbf{p}_{n_s}) \text{ and } \|\mathbf{p}_{n_s} - \mathbf{p}_*\| \longrightarrow 0 \text{ as } s \to \infty,$$

where "$\|\cdot\|$" represents the Euclidean distance. Since $\mathbf{p}_*$ is not a solution maximizing $|X'WX|$, by the proof of Theorem 3.1.1 and the modified algorithm, there exists a $\boldsymbol{\delta}_i^{(r)}$ at $\mathbf{p}_*$ and an optimal $u_* \neq 0$ such that $\mathbf{p}_* + u_*\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_*) \in S_r$ and $\Delta := f\left(\mathbf{p}_* + u_*\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_*)\right) - f(\mathbf{p}_*) > 0$.

As $s \to \infty$, $\mathbf{p}_{n_s} \to \mathbf{p}_*$, its ith direction $\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_{n_s})$ determined by the algorithm $\to \boldsymbol{\delta}_i^{(r)}(\mathbf{p}_*)$, and the optimal $u(\mathbf{p}_{n_s}) \to u_*$. Thus $\mathbf{p}_{n_s} + u(\mathbf{p}_{n_s})\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_{n_s}) \longrightarrow \mathbf{p}_* + u_*\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_*)$ and

$$f\left(\mathbf{p}_{n_s} + u(\mathbf{p}_{n_s})\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_{n_s})\right) - f(\mathbf{p}_{n_s}) \longrightarrow f\left(\mathbf{p}_* + u_*\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_*)\right) - f(\mathbf{p}_*) = \Delta.$$

For all large enough s, $f\left(\mathbf{p}_{n_s} + u(\mathbf{p}_{n_s})\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_{n_s})\right) - f(\mathbf{p}_{n_s}) > \Delta/2 > 0$. However,

$$f\left(\mathbf{p}_{n_s} + u(\mathbf{p}_{n_s})\boldsymbol{\delta}_i^{(r)}(\mathbf{p}_{n_s})\right) - f(\mathbf{p}_{n_s}) \leq f(\mathbf{p}_{n_s+1}) - f(\mathbf{p}_{n_s}) \leq f(\mathbf{p}_*) - f(\mathbf{p}_{n_s}) \to 0$$

The contradiction implies that $\lim_{n\to\infty} f(\mathbf{p}_n) = \max_{\mathbf{p}} |X'WX|$. □

Proof of Theorem 4.1.4: Given $\beta_1 = 0$, we have $w_1 = w_5 = \nu(\beta_0 + \beta_2 + \beta_3)$, $w_2 = w_6 = \nu(\beta_0 + \beta_2 - \beta_3)$, $w_3 = w_7 = \nu(\beta_0 - \beta_2 + \beta_3)$, $w_4 = w_8 = \nu(\beta_0 - \beta_2 - \beta_3)$. The goal is to find a half-fraction $\mathbf{I} = \{i_1, i_2, i_3, i_4\}$ which maximizes $s(\mathbf{I}) := |X[i_1, i_2, i_3, i_4]|^2 w_{i_1} w_{i_2} w_{i_3} w_{i_4}$. For regular half-fractions $\mathbf{I} = \{1, 4, 6, 7\}$ or $\{2, 3, 5, 8\}$, $s(\mathbf{I}) = 256 w_1 w_2 w_3 w_4$. Note that $|X[i_1, i_2, i_3, i_4]|^2 = 0$ for 12 half-fractions identified by $1 = \pm A$, $1 = \pm B$, $1 = \pm C$, $1 = \pm AB$, $1 = \pm AC$, or $1 = \pm BC$; and $|X[i_1, i_2, i_3, i_4]|^2 = 64$ for all other 56 cases.

Without any loss of generality, suppose $w_1 \geq w_2 \geq w_3 \geq w_4$. Note that the half-fraction $\{1, 5, 2, 6\}$ identified by $1 = B$ leads to $s(\mathbf{I}) = 0$. Then the competitive half-fractions consist of both 1 and 5, one element from the second block $\{2, 6\}$, and one element from the third block $\{3, 7\}$. The corresponding $s(\mathbf{I}) = 64 w_1^2 w_2 w_3$. In this case, the regular fractions are optimal ones if and only if $4w_4 \geq w_1$. $\square$

We need the lemma below for Theorem 5.1.6:

Lemma S1.4 *Suppose $k \geq 3$ and $d(d+1) \leq 2^{k+1} - 4$. For any index set $\mathbf{I} = \{i_1, \ldots, i_{d+1}\} \subset \{1, \ldots, 2^k\}$, there exists another index set $\mathbf{I'} = \{i'_1, \ldots, i'_{d+1}\}$ such that*

$$|X[i_1, \ldots, i_{d+1}]|^2 = |X[i'_1, \ldots, i'_{d+1}]|^2 \text{ and } \mathbf{I} \cap \mathbf{I'} = \emptyset. \tag{S.4}$$

Proof of Lemma S1.4: Note that $k \geq 3$ and $d(d+1) \leq 2^{k+1} - 4$ imply $d+1 \leq 2^{k-1}$ and $\frac{d(d+1)}{2} < 2^k - 1$. Let $\mathbf{I} = \{i_1, \ldots, i_{d+1}\} \subset \{1, \ldots, 2^k\}$ be the given index set. It can be verified that there exists a nonempty subset $\mathbf{J} \subset \{1, 2, \ldots, k\}$, such that (i) the i_1th, $\ldots$, i_{d+1}th rows of the matrix $[C_1, C_2, \ldots, C_k]$ are same as the i'_1th, $\ldots$, i'_{d+1}th rows of the matrix $[A_1, A_2, \ldots, A_k]$, where $A_1, \ldots, A_k$ are the columns of X corresponding to the main effects, $C_i = -A_i$ if $i \in \mathbf{J}$ and $C_i = A_i$ otherwise; (ii) $\mathbf{I'} = \{i'_1, \ldots, i'_{d+1}\}$ satisfies conditions (S.4). Actually, the index set $\mathbf{I'}$ satisfying (i) always exists once $\mathbf{J}$ is given, since the 2^k rows of matrix $[A_1, \ldots, A_k]$ contain all possible vectors in $\{-1, 1\}^k$. Then $|X[i_1, \ldots, i_{d+1}]|^2 = |X[i'_1, \ldots, i'_{d+1}]|^2$ is guaranteed once $\mathbf{I'}$ satisfies (i). If $\mathbf{I} \cap \mathbf{I'} \neq \emptyset$, then there exists an $i'_a \in \mathbf{I} \cap \mathbf{I'}$ ($a \in \{1, \ldots, d+1\}$). Thus $i_a \in \mathbf{I}$ and the i_ath row of $[C_1, \ldots, C_k]$ is same as the i'_ath row of $[A_1, \ldots, A_k]$. Based on the definitions of $C_1, \ldots, C_k$, the i_ath and i'_ath rows of $[A_1, \ldots, A_k]$ have the same entries at A_i for all $i \notin \mathbf{J}$ but different entries at A_i for all $i \in \mathbf{J}$. On the other hand, once the index pair $\{i_a, i'_a\} \subset \mathbf{I}$ is given, it uniquely determines the subset $\mathbf{J} \subset \{1, \ldots, k\}$. Note that there are $2^k - 1$ possible nonempty $\mathbf{J}$ but only $\frac{d(d+1)}{2}$ possible pairs in $\mathbf{I}$. Since $\frac{d(d+1)}{2} < 2^k - 1$, there is at least one $\mathbf{J}$ such that there is no pair in $\mathbf{I}$ corresponding to it. For such a $\mathbf{J}$, we must have $\mathbf{I} \cap \mathbf{I'} = \emptyset$. $\square$

Proof of Theorem 5.1.6: Fixing any row index set $I = \{i_1, \ldots, i_{d+1}\}$ of X such that $|X[i_1, i_2, \ldots, i_{d+1}]|^2 > 0$, among all the $(d+1)$-row fractional designs satisfying $p_i = 0, \forall i \notin \mathbf{I}$, $|X'WX|$ attains its maximum $\left(\frac{1}{d+1}\right)^{d+1} w_{i_1} \cdots w_{i_{d+1}} \times |X[i_1, i_2, \ldots, i_{d+1}]|^2$ at $\mathbf{p}_I$ satisfying $p_{i_1} = \cdots = p_{i_{d+1}} = \frac{1}{d+1}$. Given any other index set $\mathbf{I'} = \{i'_1, \ldots, i'_{d+1}\}$ with minimally supported design $\mathbf{p}_{I'}$ satisfying $p_{i'_1} = \cdots = p_{i'_{d+1}} = \frac{1}{d+1}$, the loss of efficiency of $\mathbf{p}_I$ with respect to $\mathbf{p}_{I'}$ given $\mathbf{w}_{I'} =$

$(w_1, \ldots, w_{2^k})'$ is

$$\begin{aligned} R_{I'}(I) &= 1 - \left(\frac{\psi(\mathbf{p}_I, \mathbf{w}_{I'})}{\psi(\mathbf{p}_{I'}, \mathbf{w}_{I'})}\right)^{\frac{1}{d+1}} = 1 - \left(\frac{w_{i_1}\cdots w_{i_{d+1}}|X[i_1,\ldots,i_{d+1}]|^2}{w_{i'_1}\cdots w_{i'_{d+1}}|X[i'_1,\ldots,i'_{d+1}]|^2}\right)^{\frac{1}{d+1}} \\ &\le 1 - \frac{a}{b}\cdot\left(\frac{|X[i_1,\ldots,i_{d+1}]|^2}{|X[i'_1,\ldots,i'_{d+1}]|^2}\right)^{\frac{1}{d+1}}. \end{aligned}$$

By Lemma S1.4, there always exists an index set $\mathbf{I}' = \{i'_1, \ldots, i'_{d+1}\}$ such that $|X[i'_1, \ldots, i'_{d+1}]|^2 = |X[i_1, \ldots, i_{d+1}]|^2$ and $\mathbf{I} \cap \mathbf{I}' = \emptyset$. Let $\mathbf{w}_{I'} = (w_1, \ldots, w_{2^k})'$ satisfy $w_i = b, \forall i \in \mathbf{I}'$ and $w_i = a, \forall i \in \mathbf{I}$ (here we assume $(w_1, \ldots, w_{2^k})$ can take any point in $[a, b]^{2^k}$). Then the loss of efficiency of $\mathbf{p}_I$ with respect to this $\mathbf{w}_{I'}$ is at least $1 - a/b$. If we choose $\mathbf{I} = \{i_1, \ldots, i_{d+1}\}$ which maximizes $X[i_1, \ldots, i_{d+1}]|^2$, then the corresponding $\mathbf{p}_I$ attains the minimum value $1 - a/b$ of the maximum loss in efficiency compared to other minimally supported designs. □

We need two lemmas for the exchange algorithm for integer-valued allocations.

Lemma S1.5 *Let $g(z) = Az(m - z) + Bz + C(m - z) + D$ for real numbers $A > 0, B \ge 0, C \ge 0, D \ge 0$, and integers $m > 0, 0 \le z \le m$. Let Δ be the integer closest to $\frac{mA+B-C}{2A}$.*

(i) If $0 \le \Delta \le m$, then $\max_{0\le z\le m} g(z) = mC + D + (mA + B - C)\Delta - A\Delta^2$ at $z = \Delta$.

(ii) If $\Delta < 0$, then $\max_{0\le z\le m} = mC + D$ at $z = 0$.

(iii) If $\Delta > m$, then $\max_{0\le z\le m} = mB + D$ at $z = m$.

Lemma S1.6 *Let $\mathbf{n} = (n_1, \ldots, n_{2^k})'$, $W_n = \mathrm{diag}\{n_1 w_1, \ldots, n_{2^k} w_{2^k}\}$, $f(\mathbf{n}) = |X' W_n X|$. Fixing $1 \le i < j \le 2^k$, let*

$$\begin{aligned} f_{ij}(z) &= f(n_1, \ldots, n_{i-1}, z, n_{i+1}, \ldots, n_{j-1}, m - z, n_{j+1}, \ldots, n_{2^k}) \\ &\triangleq Az(m - z) + Bz + C(m - z) + D, \end{aligned} \tag{S.5}$$

where $m = n_i + n_j$. Then (i) $D > 0 \Longrightarrow B > 0$ and $C > 0$; (ii) $B > 0$ or $C > 0 \Longrightarrow A > 0$; (iii) $f(\mathbf{n}) > 0 \Longrightarrow A > 0$; (iv) $D = f(n_1, \ldots, n_{i-1}, 0, n_{i+1}, \ldots, n_{j-1}, 0, n_{j+1}, \ldots, n_{2^k})$. (v) Suppose $m > 0$, then $A = \frac{2}{m^2}\left(2f_{ij}\left(\frac{m}{2}\right) - f_{ij}(0) - f_{ij}(m)\right)$, $B = \frac{1}{m}(f_{ij}(m) - D)$, $C = \frac{1}{m}(f_{ij}(0) - D)$.

Exchange algorithm for real-valued allocations

Lemma S1.7 *Let $g(z) = Az(e-z)+Bz+C(e-z)+D$ for nonnegative constants A, B, C, D, e. Define $\Delta = \frac{eA+B-C}{2A}$.*

(i) If $0 \leq \Delta \leq e$, then $\max_{0\leq z\leq e} g(z) = eC + D + \frac{(eA+B-C)^2}{4A}$ at $z = \Delta$.

(ii) If $\Delta < 0$, then $\max_{0\leq z\leq e} = eC + D$ at $z = 0$.

(iii) If $\Delta > e$, then $\max_{0\leq z\leq e} = eB + D$ at $z = e$.

Lemma S1.8 *Let $\mathbf{p} = (p_1, \ldots, p_{2^k})'$, $f(\mathbf{p}) = |X'WX|$, and*

$$\begin{aligned} f_{ij}(z) &:= f\left(p_1, \ldots, p_{i-1}, z, p_{i+1}, \ldots, p_{j-1}, e-z, p_{j+1}, \ldots, p_{2^k}\right) \\ &\stackrel{\triangle}{=} Az(e-z) + Bz + C(e-z) + D, \end{aligned}$$

where $1 \leq i < j \leq 2^k$ and $e = p_i + p_j$. Then (i) $D > 0 \Longrightarrow B > 0$ and $C > 0$; (ii) $B > 0$ or $C > 0 \Longrightarrow A > 0$; (iii) $f(\mathbf{p}) > 0 \Longrightarrow A > 0$; (iv) $D = f(p_1, \ldots,\ p_{i-1}, 0, p_{i+1}, \ldots,\ p_{j-1}, 0, p_{j+1}, \ldots,\ p_{2^k})$; (v) Suppose $e > 0$, then $A = \frac{2}{e^2}\left(2f_{ij}\left(\frac{e}{2}\right) - f_{ij}(0) - f_{ij}(e)\right)$, $B = \frac{1}{e}\left(f_{ij}(e) - D\right)$, $C = \frac{1}{e}\left(f_{ij}(0) - D\right)$.

Exchange algorithm for maximizing $f(\mathbf{p}) = f(p_1, \ldots, p_{2^k}) = |X'WX|$

1° Start with an arbitrary design $\mathbf{p}^{(0)} = (p_1^{(0)}, \ldots, p_{2^k}^{(0)})'$ such that $f(\mathbf{p}^{(0)}) > 0$.

2° Set up a random order of (i, j) going through all pairs

$$\{(1,2), (1,3), \ldots, (1, 2^k), (2,3), \ldots, (2^k - 1, 2^k)\}.$$

3° For each (i, j), if $e := p_i^{(0)} + p_j^{(0)} = 0$, let $\mathbf{p}^{(1)} = \mathbf{p}^{(0)}$ and jump to 5°. Otherwise, let

$$\begin{aligned} f_{ij}(z) &= f\left(p_1^{(0)}, \ldots, p_{i-1}^{(0)}, z, p_{i+1}^{(0)}, \ldots, p_{j-1}^{(0)}, e-z, p_{j+1}^{(0)}, \ldots, p_{2^k}^{(0)}\right) \\ &= Az(e-z) + Bz + C(e-z) + D \end{aligned}$$

with nonnegative constants A, B, C, D determined by Lemma S1.8.

4° Define $\mathbf{p}^{(1)} = \left(p_1^{(0)}, \ldots, p_{i-1}^{(0)}, z_*, p_{i+1}^{(0)}, \ldots, p_{j-1}^{(0)}, e - z_*, p_{j+1}^{(0)}, \ldots, p_{2^k}^{(0)}\right)'$ where z_* maximizes $f_{ij}(z)$ with $0 \leq z \leq e$ (see Lemma S1.7). Note that $f(\mathbf{p}^{(1)}) = f_{ij}(z_*) \geq f(\mathbf{p}^{(0)}) > 0$.

5° Repeat $2^\circ \sim 4^\circ$ until convergence (no more increase in terms of $f(\mathbf{p})$ by any pairwise adjustment).

Theorem S1.7 *If the exchange algorithm converges, the converged* $\mathbf{p}$ *maximizes* $|X'WX|$.

Proof of Theorem S1.7: Suppose the exchange algorithm converges at $\mathbf{p}^* = (p_1^*, \ldots, p_{2^k}^*)'$. According to the algorithm, $|X'WX| > 0$ at $\mathbf{p}^*$. Without any loss of generality, assume $p_{2^k}^* > 0$. Let $\mathbf{p}_r^* = (p_1^*, \ldots, p_{2^k-1}^*)$, $l_r(\mathbf{p}_r) = \log f_r(\mathbf{p}_r)$, and $f_r(\mathbf{p}_r) = f(p_1, \ldots, p_{2^k-1}, 1 - \sum_{i=1}^{2^k-1} p_i)$. Then for $i = 1, \ldots, 2^k - 1$, $\left.\frac{\partial l_r}{\partial p_i}\right|_{p_r^*} = \frac{1}{f(\mathbf{p}^*)} \cdot \left.\frac{\partial f_r}{\partial p_i}\right|_{p_r^*} = 0$, if $p_i^* > 0$; $\quad \le 0$, otherwise. Thus $\mathbf{p}^*$ (or $\mathbf{p}_r^*$) locally maximizes $l(\mathbf{p})$ (or $l_r(\mathbf{p}_r)$), and $\mathbf{p}^*$ attains the global maximum of $f(\mathbf{p})$ on S. □

Similar to the lift-one algorithm, we may modify the exchange algorithm so that $\mathbf{p}^{(0)}$ won't be updated until all potential pairwise exchanges among p_i's have been checked. It can be verified that the modified exchange algorithm must converge.