D-OPTIMAL DESIGNS WITH ORDERED CATEGORICAL DATA

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Supplementary Materials

S.1 Commonly Used Link Functions for Cumulative Link Models

Link function	$g(\gamma)$	$g^{-1}(\eta)$	$(g^{-1})'(\eta)$
logit	$\log\left(\frac{\gamma}{1-\gamma}\right)$	$\frac{e^\eta}{1+e^\eta}$	$\frac{e^\eta}{(1+e^\eta)^2}$
probit	$\Phi^{-1}(\gamma)$	$\Phi(\eta)$	$\phi(\eta)$
log-log	$-\log[-\log(\gamma)]$	$\exp\{-e^{-\eta}\}$	$\exp\{-\eta - e^{-\eta}\}$
c-log-log	$\log[-\log(1-\gamma)]$	$1-\exp\{-e^{\eta}\}$	$\exp\{\eta - e^{\eta}\}$
cauchit	$\tan[\pi(\gamma-\frac{1}{2})]$	$\frac{1}{\pi}\arctan(\eta)+\frac{1}{2}$	$\frac{1}{\pi(1+\eta^2)}$

where $\Phi^{-1}(\cdot)$ is the cumulative distribution function of $N(0,1)$, $\phi(\cdot)$ is the probability density function of $N(0,1)$, and "c-log-log" stands for complementary log-log.

Example 1 (*continued*) For logit link g, $g^{-1}(\eta) = e^\eta/(1+e^\eta)$ and $(g^{-1})' = g^{-1}(1-g^{-1})$. Thus $g_{ij} = (g^{-1})'(\theta_j - \mathbf{x}_i^T\boldsymbol{\beta}) = \gamma_{ij}(1-\gamma_{ij})$. With $J=3$, we have $\pi_{i1}+\pi_{i2}+\pi_{i3} = 1$ for $i = 1,\ldots,m$. Then for $i=1,\ldots,m$, $g_{i1} = \pi_{i1}(\pi_{i2}+\pi_{i3})$, $g_{i2} = (\pi_{i1}+\pi_{i2})\pi_{i3}$, $b_{i2} = \pi_{i1}\pi_{i3}\pi_{i2}^{-1}(\pi_{i1}+\pi_{i2})(\pi_{i2}+\pi_{i3})$, $u_{i1} = \pi_{i1}\pi_{i2}^{-1}(\pi_{i1}+\pi_{i2})(\pi_{i2}+\pi_{i3})^2$, $u_{i2} = \pi_{i3}\pi_{i2}^{-1}(\pi_{i1}+\pi_{i2})^2(\pi_{i2}+\pi_{i3})$, $c_{i1} = \pi_{i1}(\pi_{i1}+\pi_{i2})(\pi_{i2}+\pi_{i3})$, $c_{i2} = \pi_{i3}(\pi_{i1}+\pi_{i2})(\pi_{i2}+\pi_{i3})$, $e_i = (\pi_{i1}+\pi_{i2})(\pi_{i1}+\pi_{i3})(\pi_{i2}+\pi_{i3})$.
□

S.2 Additional Lemmas

For Section 2: Since $(Y_{i1},\ldots,Y_{iJ}), i = 1,\ldots,m$ are m independent random vectors, the log-likelihood function (up to a constant) of the cumulative link model is

$$l(\beta_1,\ldots,\beta_d,\theta_1,\ldots,\theta_{J-1}) = \sum_{i=1}^m\sum_{j=1}^J Y_{ij}\log(\pi_{ij})$$

where $\pi_{ij} = \gamma_{ij} - \gamma_{i,j-1}$ with $\gamma_{ij} = g^{-1}(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta})$ for $j = 1, \ldots, J-1$ and $\gamma_{i0} = 0$, $\gamma_{iJ} = 1$, $i = 1, \ldots, m$. For $s = 1, \ldots, d$, $t = 1, \ldots, J-1$,

$$\begin{aligned}
\frac{\partial l}{\partial \beta_s} &= \sum_{i=1}^m (-x_{is}) \cdot \Bigg\{ \frac{Y_{i1}}{\pi_{i1}} \cdot (g^{-1})'(\theta_1 - \mathbf{x}_i^T \boldsymbol{\beta}) \\
&\quad + \frac{Y_{i2}}{\pi_{i2}} \cdot \left[(g^{-1})'(\theta_2 - \mathbf{x}_i^T \boldsymbol{\beta}) - (g^{-1})'(\theta_1 - \mathbf{x}_i^T \boldsymbol{\beta}) \right] \\
&\quad + \cdots + \frac{Y_{iJ}}{\pi_{iJ}} \left[-(g^{-1})'(\theta_{J-1} - \mathbf{x}_i^T \boldsymbol{\beta}) \right] \Bigg\} \\
\frac{\partial l}{\partial \theta_t} &= \sum_{i=1}^m (g^{-1})'(\theta_t - \mathbf{x}_i^T \boldsymbol{\beta}) \left(\frac{Y_{it}}{\pi_{it}} - \frac{Y_{i,t+1}}{\pi_{i,t+1}} \right)
\end{aligned}$$

Since Y_{ij}'s come from multinomial distributions, we know $E(Y_{ij}) = n_i \pi_{ij}$, $E(Y_{ij}^2) = n_i(n_i - 1)\pi_{ij}^2 + n_i \pi_{ij}$, and $E(Y_{is} Y_{it}) = n_i(n_i - 1)\pi_{is}\pi_{it}$ when $s \neq t$. Then we have the following lemma:

Lemma S.1. *Let* $\mathbf{F} = (F_{st})$ *be the* $(d+J-1) \times (d+J-1)$ *Fisher information matrix.*

(i) For $1 \le s \le d$, $1 \le t \le d$,

$$F_{st} = E\left(\frac{\partial l}{\partial \beta_s} \frac{\partial l}{\partial \beta_t} \right) = \sum_{i=1}^m n_i x_{is} x_{it} \sum_{j=1}^J \frac{(g_{ij} - g_{i,j-1})^2}{\pi_{ij}}$$

where $g_{ij} = (g^{-1})'(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta}) > 0$ *for* $j = 1, \ldots, J-1$ *and* $g_{i0} = g_{iJ} = 0$.

(ii) For $1 \le s \le d$, $1 \le t \le J-1$,

$$F_{s,d+t} = E\left(\frac{\partial l}{\partial \beta_s} \frac{\partial l}{\partial \theta_t} \right) = \sum_{i=1}^m n_i (-x_{is}) g_{it} \left(\frac{g_{it} - g_{i,t-1}}{\pi_{it}} - \frac{g_{i,t+1} - g_{it}}{\pi_{i,t+1}} \right)$$

(iii) For $1 \le s \le J-1$, $1 \le t \le d$,

$$F_{d+s,t} = E\left(\frac{\partial l}{\partial \theta_s} \frac{\partial l}{\partial \beta_t} \right) = \sum_{i=1}^m n_i (-x_{it}) g_{is} \left(\frac{g_{is} - g_{i,s-1}}{\pi_{is}} - \frac{g_{i,s+1} - g_{is}}{\pi_{i,s+1}} \right)$$

(iv) For $1 \le s \le J-1$, $1 \le t \le J-1$,

$$F_{d+s,d+t} = E\left(\frac{\partial l}{\partial \theta_s} \frac{\partial l}{\partial \theta_t} \right) = \begin{cases} \sum_{i=1}^m n_i g_{is}^2 (\pi_{is}^{-1} + \pi_{i,s+1}^{-1}), & \text{if } s = t \\ \sum_{i=1}^m n_i g_{is} g_{it} (-\pi_{i,s \vee t}^{-1}), & \text{if } |s-t| = 1 \\ 0, & \text{if } |s-t| \ge 2 \end{cases}$$

where $s \vee t = \max\{s, t\}$.

Perevozskaya et al. (2003) obtained a detailed form of Fisher information matrix for logit link and one predictor. Our expressions here are good for fairly general link and d predictors. To simplify the notations, we denote for $i = 1, \ldots, m$,

$$e_i = \sum_{j=1}^{J} \frac{(g_{ij} - g_{i,j-1})^2}{\pi_{ij}} > 0 \tag{S.1}$$

$$c_{it} = g_{it} \left(\frac{g_{it} - g_{i,t-1}}{\pi_{it}} - \frac{g_{i,t+1} - g_{it}}{\pi_{i,t+1}} \right), \quad t = 1, \ldots, J-1 \tag{S.2}$$

$$u_{it} = g_{it}^2 (\pi_{it}^{-1} + \pi_{i,t+1}^{-1}) > 0, \quad t = 1, \ldots, J-1 \tag{S.3}$$

$$b_{it} = g_{i,t-1} g_{it} \pi_{it}^{-1} > 0, \quad t = 2, \ldots, J-1 \text{ (if } J \geq 3) \tag{S.4}$$

Note that g_{ij} is defined in Lemma S.1 (i). Then we obtain the following lemma which plays a key role in calculating $|\mathbf{F}|$.

Lemma S.2. *$c_{it} = u_{it} - b_{it} - b_{i,t+1}$, $i = 1, \ldots, m; t = 1, \ldots, J-1$; $e_i = \sum_{t=1}^{J-1} c_{it} = \sum_{t=1}^{J-1} (u_{it} - 2b_{it})$, $i = 1, \ldots, m$, where $b_{i1} = b_{iJ} = 0$ for $i = 1, \ldots, m$.*

Lemma S.3. Rank$((\mathbf{A}_{i1}\, \mathbf{A}_{i2})) \leq 1$ *where "=" is true if and only if* $\mathbf{x}_i \neq 0$.

Based on Lemmas 1 and S.3, we obtain the two lemmas below on $c_{\alpha_1,\ldots,\alpha_m}$ which significantly simplify the structure of $|\mathbf{F}|$ as a polynomial of $(n_1, \ldots, n_m)$.

Lemma S.4. *If $\max_{1 \leq i \leq m} \alpha_i \geq J$, then $|\mathbf{A}_\tau| = 0$ for any $\tau \in (\alpha_1, \ldots, \alpha_m)$ and thus $c_{\alpha_1,\ldots,\alpha_m} = 0$.*

Proof of Lemma S.4: Without any loss of generality, we assume $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_m$. Then $\max_{1 \leq i \leq m} \alpha_i \geq J$ implies $\alpha_1 \geq J$. In this case, for any $\tau \in (\alpha_1, \ldots, \alpha_m)$, $\tau^{-1}(1) := \{i \mid \tau(i) = 1\} \subset \{1, \ldots, d+J-1\}$ and $|\tau^{-1}(1)| = \alpha_1$. If $|\tau^{-1}(1) \cap \{1, \ldots, d\}| \geq 2$, then $|A_\tau| = 0$ due to Lemma S.3; otherwise $\{d+1, \ldots, d+J-1\} \subset \tau^{-1}(1)$ and thus $|A_\tau| = 0$ due to Lemma 1. Thus $c_{\alpha_1,\ldots,\alpha_m} = 0$ according to (2.3) provided in Theorem 2. □

Lemma S.5. *If $\#\{i : \alpha_i \geq 1\} \leq d$, then $|\mathbf{A}_\tau| = 0$ for any $\tau \in (\alpha_1, \ldots, \alpha_m)$ and thus $c_{\alpha_1,\ldots,\alpha_m} = 0$.*

Proof of Lemma S.5: Without any loss of generality, we assume $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_m$. Then $\#\{i : \alpha_i \geq 1\} \leq d$ indicates $\alpha_{d+1} = \cdots = \alpha_m = 0$. Let $\tau : \{1, 2, \ldots, d+J-1\} \to \{1, \ldots, m\}$ satisfy $\tau \in (\alpha_1, \ldots, \alpha_m)$. Then the $(d+J-1) \times (d+J-1)$ matrix A_τ can be written as

$$\begin{pmatrix} A_{\tau 1} & A_{\tau 2} \\ A_{\tau 3} & A_{\tau 4} \end{pmatrix}$$

$$= \begin{pmatrix} (e_{\tau(s)} x_{\tau(s)s} x_{\tau(s)t})_{s=1,\ldots d; t=1,\ldots,d} & (-x_{\tau(s)s} c_{\tau(s)t})_{s=1,\ldots,d; t=1,\ldots,J-1} \\ (-c_{\tau(d+s)s} x_{\tau(d+s)t})_{s=1,\ldots,J-1; t=1,\ldots,d} & A_{\tau 4} \end{pmatrix}$$

where the $(J-1)\times(J-1)$ matrix $A_{\tau 4}$ is either a single entry $u_{\tau(d+1)1}$ (if $J = 2$) or symmetric tri-diagonal with diagonal entries $u_{\tau(d+1)1}, \ldots, u_{\tau(d+J-1),J-1}$, upper off-diagonal entries $-b_{\tau(d+1)2}, \ldots, -b_{\tau(d+J-2),J-1}$, and lower off-diagonal entries $-b_{\tau(d+2)2}, \ldots, -b_{\tau(d+J-1),J-1}$. Note that A_τ is asymmetric in general.

If $\#\{i : \alpha_i \geq 1\} \leq d-1$, then there exists an i_0 such that $1 \leq i_0 \leq d$ and $|\tau^{-1}(i_0) \cap \{1, \ldots, d\}| \geq 2$. In this case, $|A_\tau| = 0$ according to Lemma S.3.

If $\#\{i : \alpha_i \geq 1\} = d$, we may assume $|\tau^{-1}(i) \cap \{1, \ldots, d\}| = 1$ for $i = 1, \ldots, d$ (otherwise $|A_\tau| = 0$ according to Lemma S.3). Suppose $\alpha_1 \geq \alpha_2 \geq \cdots \geq \alpha_k \geq 2 > \alpha_{k+1}$. Then $\{d+1, \ldots, d+J-1\} \subset \cup_{i=1}^{k} \tau^{-1}(i)$ and $\sum_{i=1}^{k}(\alpha_i - 1) = J - 1$. In order to show $|A_\tau| = 0$, we first replace $A_{\tau 1}$ with $A_{\tau 1}^{(1)} = (e_{\tau(s)} x_{\tau(s)t})_{s=1,\ldots d;\ t=1,\ldots,d}$ and replace $A_{\tau 2}$ with $A_{\tau 2}^{(1)} = (-c_{\tau(s)t})_{s=1,\ldots,d;\ t=1,\ldots,J-1}$. It changes A_τ into a new matrix $A_\tau^{(1)}$. Note that $|A_\tau| = \prod_{s=1}^{d} x_{\tau(s)s} \cdot |A_\tau^{(1)}|$. According to Lemma S.2, the sum of the columns of $A_{\tau 2}^{(1)}$ is $(-e_{\tau(1)}, \ldots, -e_{\tau(d)})^T$, and the elementwise sum of the columns of $A_{\tau 4}$ is $(c_{\tau(d+1)1}, c_{\tau(d+2)2}, \ \ldots, \ c_{\tau(d+J-1),J-1})^T$. Secondly, for $t = 1, \ldots, d$, we add $x_{1t}(-e_{\tau(1)}, \ldots, -e_{\tau(d)}, c_{\tau(d+1)1}, \ \ldots, \ c_{\tau(d+J-1),J-1})^T$ to the tth column of $A_\tau^{(1)}$. We denote the resulting matrix by $A_\tau^{(2)}$. Note that $|A_\tau^{(1)}| = |A_\tau^{(2)}|$. We consider the sub-matrix $A_{\tau d}^{(2)}$ which consists of the first d columns of $A_\tau^{(2)}$. For $s \in \tau^{-1}(1)$, the sth row of $A_{\tau d}^{(2)}$ is simply 0. For $i = 2, \ldots, k$, the jth row of $A_{\tau d}^{(2)}$ is proportional to $(x_{i1} - x_{11}, x_{i2} - x_{12}, \ldots, x_{id} - x_{1d})$ if $j \in \tau^{-1}(i)$. Therefore, $\text{Rank}(A_{\tau d}^{(2)}) \leq (d + J - 1) - \alpha_1 - \sum_{i=2}^{k}(\alpha_i - 1) = d - 1$, which leads to $|A_\tau^{(2)}| = 0$ and thus $|A_\tau^{(1)}| = 0$, $|A_\tau| = 0$. According to (2.3) in Theorem 2, $c_{\alpha_1,\ldots,\alpha_m} = 0$. □

Lemma S.6. $\mathbf{F} = \mathbf{F}(\mathbf{p})$ *is always positive semi-definite. It is positive definite if and only if* $\mathbf{p} \in S_+$. *Furthermore,* $\log f(\mathbf{p})$ *is concave on* S.

For Section 5.2: The procedure seeking for analytic solutions here follows Tong, Volkmer, and Yang (2014). As a direct conclusion of the Karush-Kuhn-Tucker conditions (see also Theorem 10), a necessary condition for (p_1, p_2, p_3) to maximize $f(p_1, p_2, p_3)$ in (5.5) is (5.6), which are equivalent to $\partial f/\partial p_1 = \partial f/\partial p_3$ and $\partial f/\partial p_2 = \partial f/\partial p_3$. In terms of p_i, w_i's, they are

$$(p_3 - p_1)(p_1 w_1 + p_2 w_2 + p_3 w_3) = (w_3 - w_1) p_1 p_3 \quad \text{(S.5)}$$
$$(p_3 - p_2)(p_1 w_1 + p_2 w_2 + p_3 w_3) = (w_3 - w_2) p_2 p_3 \quad \text{(S.6)}$$

Denote $y_1 = p_1/p_3 > 0$ and $y_2 = p_2/p_3 > 0$. Since $p_1 + p_2 + p_3 = 1$, it implies $p_3 = 1/(y_1+y_2+1)$, $p_1 = y_1/(y_1+y_2+1)$, and $p_2 = y_2/(y_1+y_2+1)$. In terms of y_1, y_2, (S.5) and (S.6) are equivalent to

$$(1-y_1)(y_1w_1 + y_2w_2 + w_3) = (w_3 - w_1)y_1 \tag{S.7}$$
$$(1-y_2)(y_1w_1 + y_2w_2 + w_3) = (w_3 - w_2)y_2 \tag{S.8}$$

Lemma S.7. *Suppose* $0 < w_3 < w_2 < w_1$. *If* (p_1, p_2, p_3) *maximizes* $f(p_1, p_2, p_3)$ *in (5.5) under the constrains* $p_1, p_2, p_3 \geq 0$ *and* $p_1+p_2+p_3 = 1$, *then* $0 < p_3 \leq p_2 \leq p_1 < 1$.

The proof of the lemma above is straightforward, because otherwise one could exchange p_i, p_j to strictly improve $f(p_1, p_2, p_3)$. Now we are ready to get solutions to equations (S.7) and (S.8) case by case.

(i) $w_1 = w_3$. In that case, (S.7) implies $y_1 = 1$. After plugging it into (S.8), the only positive solution is $y_2 = (-3w_1 + 2w_2 + \sqrt{9w_1^2 - 4w_1w_2 + 4w_2^2})/(2w_2)$.

(ii) $w_2 = w_3$. In that case, (S.8) implies $y_2 = 1$. After plugging it into (S.7), the only positive solution is $y_1 = (2w_1 - 3w_2 + \sqrt{4w_1^2 - 4w_1w_2 + 9w_2^2})/(2w_1)$.

(iii) $w_1 = w_2$ but $w_1 \neq w_3$. The ratio of (S.7) and (S.8) leads to $y_1 = y_2$. After plugging it into (S.7), the only positive solution is $y_1 = (3w_1 - 2w_3 + \sqrt{9w_1^2 - 4w_1w_3 + 4w_3^2})/(4w_1)$.

(iv) w_1, w_2, w_3 are distinct. Without any loss of generality, we assume $0 < w_3 < w_2 < w_1$, because otherwise the previous elimination procedure in the order of p_3, p_2, p_1 could be easily changed accordingly. Based on Lemma S.7, if (p_1, p_2, p_3) maximizes f_4, then $0 < p_3 \leq p_2 \leq p_1 < 1$ and thus $y_1 \geq y_2 \geq 1$. The ratio of (S.7) and (S.8) leads to $(1-y_1)/(1-y_2) = (w_3 - w_1)/(w_3 - w_2) \cdot y_1/y_2$, which implies

$$y_2 = \frac{(w_1 - w_3)y_1}{(w_2 - w_3) + (w_1 - w_2)y_1} \ . \tag{S.9}$$

Note that $(w_2 - w_3) + (w_1 - w_2)y_1 \geq w_1 - w_3 > 0$. After plugging (S.9) into (S.7), we get

$$c_0 + c_1y_1 + c_2y_1^2 + c_3y_1^3 = 0 \tag{S.10}$$

where $c_0 = w_3(w_2 - w_3) > 0$, $c_1 = 3w_1w_2 - w_1w_3 - 4w_2w_3 + 2w_3^2 > 0$, $c_2 = 2w_1^2 - 4w_1w_2 - w_1w_3 + 3w_2w_3$, $c_3 = w_1(w_2 - w_1) < 0$.

Lemma S.8. *Suppose* $0 < w_3 < w_2 < w_1$ *. Then equation (S.10) has one and only one solution* $y_1^* \geq 1$*. Furthermore,* $y_1^* > 1$*.*

Proof of Lemma S.8: In order to locate the roots of equation (S.10), we let $f_1(y_1) = c_0 + c_1 y_1 + c_2 y_1^2 + c_3 y_1^3$. Then $f_1(1) = c_0 + c_1 + c_2 + c_3 = (w_1 - w_3)^2 > 0$.

On the other hand, the first derivative of f_1 is $f_1'(y_1) = a_0 + a_1 y_1 + a_2 y_1^2$, where $a_0 = 3w_1w_2 - w_1w_3 - 4w_2w_3 + 2w_3^2 = w_1(w_2 - w_3) + 2(w_1 - w_2)w_2 + 2(w_2 - w_3)^2 > 0$, $a_1 = 2(2w_1^2 - 4w_1w_2 - w_1w_3 + 3w_2w_3)$, and $a_2 = 3w_1(w_2 - w_1) < 0$. Therefore, $a_1^2 - 4a_0a_2 > a_1^2 \geq 0$ and $f_1'(y_1) = a_2(y_1 - y_{11})(y_1 - y_{12})$, where

$$y_{11} = \frac{-a_1 + \sqrt{a_1^2 - 4a_0a_2}}{2a_2} < 0, \quad y_{12} = \frac{-a_1 - \sqrt{a_1^2 - 4a_0a_2}}{2a_2} > y_{11}$$

It can be verified that $y_{12} < 1$ if and only if $w_1 < 2(w_2 + w_3)$. There are two cases: *Case (i)*: If $y_{12} < 1$, then $f_1'(y_1) < 0$ for all $y_1 > 1$. That is, $f_1(y_1)$ strictly decreases after $y_1 = 1$. Since $f_1(1) > 0$ and $f_1(\infty) = -\infty$, then there is one and only one solution in $(1, \infty)$; *Case (ii)*: If $y_{12} \geq 1$, then $f_1'(y_1) \geq 0$ for $y_1 \in [1, y_{12}]$ and $f_1'(y_1) < 0$ for $y_1 \in (y_{12}, \infty)$. That is, $f_1(y_1)$ increases in $[1, y_{12}]$ and then strictly decreases in (y_{12}, ∞). Again, due to $f_1(1) > 0$ and $f_1(\infty) = -\infty$, there is one and only one solution in $(1, \infty)$. In either case, the conclusion is justified. □

S.3 Additional Proofs

Proof of Theorem 1 It is a direct conclusion of Lemmas S.1 and S.2. □

Examples of $\mathbf{A}_{i3}$ in Theorem 1 include (u_{i1}),

$$\begin{pmatrix} u_{i1} & -b_{i2} \\ -b_{i2} & u_{i2} \end{pmatrix}, \begin{pmatrix} u_{i1} & -b_{i2} & 0 \\ -b_{i2} & u_{i2} & -b_{i3} \\ 0 & -b_{i3} & u_{i3} \end{pmatrix}, \begin{pmatrix} u_{i1} & -b_{i2} & 0 & 0 \\ -b_{i2} & u_{i2} & -b_{i3} & 0 \\ 0 & -b_{i3} & u_{i3} & -b_{i4} \\ 0 & 0 & -b_{i4} & u_{i4} \end{pmatrix}$$

for $J = 2$, 3, 4, or 5 respectively.

Proof of Theorem 2 To study the structure of $|\mathbf{F}|$ as a polynomial function of $(n_1, \ldots, n_m)$, we denote the (k, l)th entry of $\mathbf{A}_i$ by $a_{kl}^{(i)}$. Given a row map $\tau : \{1, 2, \ldots, d + J - 1\} \to \{1, \ldots, m\}$, we define a $(d + J - 1) \times (d + J - 1)$ matrix $\mathbf{A}_\tau = \left(a_{kl}^{(\tau(k))}\right)$ whose kth row is given by the kth row of

$\mathbf{A}_{\tau(k)}$. For a power index $(\alpha_1, \ldots, \alpha_m)$ with $\alpha_i \in \{0, 1, \ldots, d+J-1\}$ and $\sum_{i=1}^m \alpha_i = d + J - 1$, we denote

$$\tau \in (\alpha_1, \ldots, \alpha_m)$$

if $\alpha_i = \#\{j : \tau(j) = i\}$ for each $i = 1, \ldots, m$. In terms of the construction of $\mathbf{A}_\tau$, it says that α_i rows of $\mathbf{A}_\tau$ are from the matrix $\mathbf{A}_i$.

According to the Leibniz formula for the determinant,

$$|\mathbf{F}| = \left|\sum_{i=1}^m n_i \mathbf{A}_i\right| = \sum_{\sigma \in S_{d+J-1}} (-1)^{\mathrm{sgn}(\sigma)} \prod_{k=1}^{d+J-1} \sum_{i=1}^m n_i a_{k,\sigma(k)}^{(i)}$$

where σ is a permutation of $\{1, 2, \ldots, d+J-1\}$, and $\mathrm{sgn}(\sigma)$ is the sign or signature of σ. Therefore,

$$\begin{aligned} c_{\alpha_1,\ldots,\alpha_m} &= \sum_{\sigma \in S_{d+J-1}} (-1)^{\mathrm{sgn}(\sigma)} \sum_{\tau \in (\alpha_1,\ldots,\alpha_m)} \prod_{k=1}^{d+J-1} a_{k,\sigma(k)}^{(\tau(k))} \\ &= \sum_{\tau \in (\alpha_1,\ldots,\alpha_m)} \sum_{\sigma \in S_{d+J-1}} (-1)^{\mathrm{sgn}(\sigma)} \prod_{k=1}^{d+J-1} a_{k,\sigma(k)}^{(\tau(k))} \\ &= \sum_{\tau \in (\alpha_1,\ldots,\alpha_m)} |\mathbf{A}_\tau| \end{aligned}$$

□

Proof of Lemma 2 To simplify the notations, we let $i_s = s + 1$, $s = 0, \ldots, d$. That is, $\alpha_1 = J - 1$, $\alpha_2 = \cdots = \alpha_{d+1} = 1$. There are only two types of $\tau \in (\alpha_1, \ldots, \alpha_m)$, such that, $|\mathbf{A}_\tau|$ may not be 0.

τ of type I: There exist $1 \le k \le d$, $2 \le l \le d+1$, and $1 \le q \le J-1$, such that, $\tau(k) = 1$ and $\tau(d+q) = l$. Following a similar procedure as in the proof of Lemma S.5, we obtain

$$|\mathbf{A}_\tau| = \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X_1}[1, 2, \ldots, d+1]| \cdot (-1)^{\mathrm{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s} \cdot \frac{c_{lq}}{e_l}$$

τ of type II: $\tau(d+1) = \cdots = \tau(d+J-1) = 1$ and $\{\tau(1), \ldots, \tau(d)\} = \{2, \ldots, d+1\}$. It can be verified that

$$|\mathbf{A}_\tau| = \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X_1}[1, 2, \ldots, d+1]| \cdot (-1)^{\mathrm{sgn}(\tau)} \prod_{s=1}^d x_{\tau(s)s}$$

According to Theorem 2,

$$
\begin{aligned}
c_{\alpha_1,\ldots,\alpha_m} &= \sum_{\tau \text{ of type I}} |\mathbf{A}_\tau| + \sum_{\tau \text{ of type II}} |\mathbf{A}_\tau| \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X_1}[1,2,\ldots,d+1]| \cdot \left(\sum_{k=1}^{d} \sum_{l=2}^{d+1} \sum_{\tau \in S_{d+1}:\tau(k)=1,\tau(d+1)=l} \right. \\
&\quad \left. (-1)^{\mathrm{sgn}(\tau)} \prod_{s=1}^{d} x_{\tau(s)s} \sum_{q=1}^{J-1} \frac{c_{lq}}{e_l} + \sum_{\tau \in S_{d+1}:\tau(d+1)=1} (-1)^{\mathrm{sgn}(\tau)} \prod_{s=1}^{d} x_{\tau(s)s} \right) \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X_1}[1,2,\ldots,d+1]| \cdot \sum_{\tau \in S_{d+1}} (-1)^{\mathrm{sgn}(\tau)} \prod_{s=1}^{d} x_{\tau(s)s} \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot (-1)^d |\mathbf{X_1}[1,2,\ldots,d+1]| \cdot (-1)^d |\mathbf{X_1}[1,2,\ldots,d+1]| \\
&= \prod_{i=2}^{d+1} e_i \cdot |\mathbf{A}_{13}| \cdot |\mathbf{X_1}[1,2,\ldots,d+1]|^2
\end{aligned}
$$

where S_{d+1} is the set of permutations of $\{1,\ldots,d+1\}$. The general case with $i_0, i_1, \ldots, i_d$ can be obtained similarly. □

Proof of Theorem 4 Suppose $\mathrm{Rank}(\mathbf{X_1}) = d+1$. Then there exist $i_0, \ldots, i_d \in \{1,\ldots,m\}$, such that, $|\mathbf{X_1}[i_0, i_1, \ldots, i_d]| \neq 0$. According to Lemma S.4, $f(\mathbf{p})$ can be regarded as an order-$(J-1)$ polynomial of p_{i_0}. Let $p_{i_0} = x \in (0,1)$ and $p_i = (1-x)/(m-1)$ for $i \neq i_0$. Based on Lemma 2, $f(\mathbf{p})$ can be written as

$$
\begin{aligned}
f_{i_0}(x) &= a_{J-1} x^{J-1} \left(\frac{1-x}{m-1}\right)^d + a_{J-2} x^{J-2} \left(\frac{1-x}{m-1}\right)^{d+1} \\
&\quad + \cdots + a_1 x \left(\frac{1-x}{m-1}\right)^{d+J-2} + a_0 \left(\frac{1-x}{m-1}\right)^{d+J-1}, \text{ where} \\
a_{J-1} &= |\mathbf{A}_{i_0 3}| \sum_{\{i'_1,\ldots,i'_d\} \subset \{1,\ldots,m\} \setminus \{i_0\}} \prod_{s=1}^{d} e_{i'_s} \, |\mathbf{X_1}[i_0, i'_1, \ldots, i'_d]|^2 > 0
\end{aligned}
$$

Therefore, $\lim_{x \to 1^-} (1-x)^{-d} x^{1-J} f_{i_0}(x) = (m-1)^{-d} a_{J-1} > 0$. That is, $f(\mathbf{p}) > 0$ for $p_{i_0} = x$ close enough to 1 and $p_i = (1-x)/(m-1)$ for $i \neq i_0$.

In order to justify that the condition $\text{Rank}(\mathbf{X_1}) = d+1$ is also necessary, we only need to show that $f(\mathbf{p}) \equiv 0$ if $\text{Rank}(\mathbf{X_1}) \le d$. Actually, for any $\tau : \{1, \ldots, d + J - 1\} \to \{1, \ldots, m\}$, we construct $\mathbf{A}_\tau^{(1)}$ as in the proof of Lemma S.5. Then $|\mathbf{A}_\tau| = \prod_{s=1}^{d} x_{\tau(s)s} \cdot |\mathbf{A}_\tau^{(1)}|$. Similar as in the proof of Lemma S.5, for $t = 1, \ldots, d$, we add $x_{\tau(1)t}(-e_{\tau(1)}, \ldots, -e_{\tau(d)}, c_{\tau(d+1)1}, \ldots, c_{\tau(d+J-1),J-1})^T$ to the tth column of $\mathbf{A}_\tau^{(1)}$. We denote the resulting matrix by $\mathbf{A}_\tau^{(3)}$. Note that $|\mathbf{A}_\tau^{(1)}| = |\mathbf{A}_\tau^{(3)}|$. We consider the sub-matrix $\mathbf{A}_{\tau d}^{(3)}$ which consists of the first d columns of $\mathbf{A}_\tau^{(3)}$. For $s \in \tau^{-1}(\tau(1))$, the sth row of $\mathbf{A}_{\tau d}^{(3)}$ is simply 0. For $s = 2, \ldots, k$, the sth row of $\mathbf{A}_{\tau d}^{(3)}$ is $e_{\tau(s)}(x_{\tau(s)1} - x_{\tau(1)1}, \ldots, x_{\tau(s)d} - x_{\tau(1)d})$. For $s = 1, \ldots, J - 1$, the $(d + s)$th row of $\mathbf{A}_{\tau d}^{(3)}$ is $-c_{\tau(d+s)s}(x_{\tau(d+s)1} - x_{\tau(1)1}, \ldots, x_{\tau(d+s)d} - x_{\tau(1)d})$. We claim that $\text{Rank}(\mathbf{A}_{\tau d}^{(3)}) \le d - 1$. Otherwise, if $\text{Rank}(\mathbf{A}_{\tau d}^{(3)}) = d$, then there exist $i_1, \ldots, i_d \in \{2, \ldots, d + J - 1\}$, such that, the sub-matrix consisting of the i_1th$, \ldots, i_d$th rows of $\mathbf{A}_{\tau d}^{(3)}$ is nonsingular. Then the sub-matrix consisting of the $\tau(1)$th$, \tau(i_1)$th$, \ldots, \tau(i_d)$th rows of $\mathbf{X_1}$ is nonsingular, which implies $\text{Rank}(\mathbf{X_1}) = d + 1$. The contradiction implies $\text{Rank}(\mathbf{A}_{\tau d}^{(3)}) \le d - 1$. Then $|\mathbf{A}_\tau^{(3)}| = 0$ and thus $|\mathbf{A}_\tau| = 0$ for each τ. Based on Theorem 2, $|\mathbf{F}| \equiv 0$ and thus $f(\mathbf{p}) \equiv 0$. □

Proof of Theorem 5 Combining Theorem 1 and Theorem 4, it is straightforward that $f(\mathbf{p}) = 0$ if $\text{Rank}(\ \mathbf{X_1}[\{i \mid p_i > 0\}]) \le d$. We only need to show that $f(\mathbf{p}) > 0$ if $\text{Rank}(\mathbf{X_1}[\{i \mid p_i > 0\}]) = d + 1$. Due to Theorem 1, we only need to verify the case $p_i > 0, i = 1, \ldots, m$, because otherwise we may simply remove all support points with $p_i = 0$.

Suppose $p_i > 0, i = 1, \ldots, m$ and $\text{Rank}(\mathbf{X_1}) = d + 1$. Then there exist $i_0, \ldots, i_d \in \{1, \ldots, m\}$, such that, $|\mathbf{X_1}[i_0, \ldots, i_d]| \ne 0$. According to the proof of Theorem 4, for each $i \in \{i_0, \ldots, i_d\}$, there exists an $\epsilon_i \in (0, 1)$, such that, $f(\mathbf{p}) > 0$ as long as $p_i = x \in (1 - \epsilon_i, 1)$ and $p_j = (1 - x)/(m - 1)$ for $j \ne i$. On the other hand, for each $i \notin \{i_0, \ldots, i_d\}$, if we denote the jth row of $\mathbf{X_1}$ by α_j, $j = 1, \ldots, m$, then $\alpha_i = a_0\alpha_{i_0} + \cdots + a_d\alpha_{i_d}$ for some real numbers $a_0, \ldots, a_d$. Since $\alpha_i \ne 0$, then at least one $a_i \ne 0$. Without any loss of generality, we assume $a_0 \ne 0$. Then it can be verified that $|\mathbf{X_1}[i, i_1, \ldots, i_d]| \ne 0$ too. Following the proof of Theorem 4 again, for such an $i \notin \{i_0, \ldots, i_d\}$, there also exists an $\epsilon_i \in (0, 1)$, such that, $f(\mathbf{p}) > 0$ as long as $p_i = x \in (1 - \epsilon_i, 1)$ and $p_j = (1 - x)/(m - 1)$ for $j \ne i$. Let $\epsilon_* = \min\{\min_i \epsilon_i, (m - 1)\min_i p_i, 1 - 1/m\}/2$. For $i = 1, \ldots, m$, denote $\delta_i = (\delta_{i1}, \ldots, \delta_{im})^T \in S$ with $\delta_{ii} = 1 - \epsilon_*$ and $\delta_{ij} = \epsilon_*/(m - 1)$ for $j \ne i$. It can be verified that $\mathbf{p} = a_1\delta_1 + \cdots + a_m\delta_m$ with $a_i = (p_i - \epsilon_*/(m - 1))/(1 -$

$m\epsilon_*/(m-1))$. By the choice of ϵ_*, $f(\delta_i) > 0$, $a_i > 0, i = 1, \ldots, m$, and $\sum_i a_i = 1$. Then $f(\mathbf{p}) > 0$ according to Lemma S.6. □

Proof of Corollary 3 In order to check when a minimally supported design supported only on $\{x_1, x_2\}$ is D-optimal, we add one more support point, that is, x_3 . According to Theorem 2, Lemmas S.4, S.5, and 2, the objective function for a D-optimal approximate design on $\{x_1, x_2, x_3\}$ is $f(p_1, p_2, p_3) = p_1p_2(c_{210}p_1 + c_{120}p_2) + p_1p_3(c_{201}p_1 + c_{102}p_3) + p_2p_3(c_{021}p_2 + c_{012}p_3) + c_{111}p_1p_2p_3$, where

$$
\begin{aligned}
c_{210} &= e_2 g_{11}^2 g_{12}^2 (\pi_{11}\pi_{12}\pi_{13})^{-1}(x_1 - x_2)^2 > 0 \\
c_{120} &= e_1 g_{21}^2 g_{22}^2 (\pi_{21}\pi_{22}\pi_{23})^{-1}(x_1 - x_2)^2 > 0 \\
c_{201} &= e_3 g_{11}^2 g_{12}^2 (\pi_{11}\pi_{12}\pi_{13})^{-1}(x_1 - x_3)^2 > 0 \\
c_{102} &= e_1 g_{31}^2 g_{32}^2 (\pi_{31}\pi_{32}\pi_{33})^{-1}(x_1 - x_3)^2 > 0 \\
c_{021} &= e_3 g_{21}^2 g_{22}^2 (\pi_{21}\pi_{22}\pi_{23})^{-1}(x_2 - x_3)^2 > 0 \\
c_{012} &= e_2 g_{31}^2 g_{32}^2 (\pi_{31}\pi_{32}\pi_{33})^{-1}(x_2 - x_3)^2 > 0 \\
c_{111} &= e_1(u_{22}u_{31} + u_{21}u_{32} - 2b_{22}b_{32})(x_1 - x_2)(x_1 - x_3) + \\
&\quad\; e_2(u_{12}u_{31} + u_{11}u_{32} - 2b_{12}b_{32})(x_2 - x_1)(x_2 - x_3) + \\
&\quad\; e_3(u_{12}u_{21} + u_{11}u_{22} - 2b_{12}b_{22})(x_3 - x_1)(x_3 - x_2)
\end{aligned}
$$

Based on Theorem 10, the design $\mathbf{p} = (p_1^*, p_2^*, 0)^T$ is D-optimal if and only if

$$\partial f(\mathbf{p})/\partial f(p_1) = \partial f(\mathbf{p})/\partial f(p_2) \geq \partial f(\mathbf{p})/\partial f(p_3)$$

Similar conclusions could be justified for $x_4, \ldots, x_m$ if $m \geq 4$. □

Proof of Theorem 12 According to the solutions provided by the software `Mathematica`, the largest root of equation (S.10) after simplification is

$$y_1 = -\frac{b_2}{3} - \frac{2^{1/3}(3b_1 - b_2^2)}{3A^{1/3}} + \frac{A^{1/3}}{3 \times 2^{1/3}} \tag{S.11}$$

where $A = -27b_0 + 9b_1b_2 - 2b_2^3 + 3^{3/2}(27b_0^2 + 4b_1^3 - 18b_0b_1b_2 - b_1^2b_2^2 + 4b_0b_2^3)^{1/2}$, and $b_i = c_i/c_3$, $i = 0, 1, 2$. Note that the calculation of A and thus y_1 should be regarded as operations among complex numbers since the expression under square root could be negative. Nevertheless, y_1 at the end would be a real number. Thus we are able to provide the analytic solution maximizing $f(p_1, p_2, p_3)$. □

Proof of Corollary 5 In order to check when a minimally supported design is D-optimal, we first add the four design points, that is, we consider four design points (x_{i1}, x_{i2}), $i = 1, 2, 3, 4$ and check when the D-optimal design could be constructed on the first three design points. Let $\mathbf{X_1}$ be defined as in Lemma 2. In this case, $\mathbf{X_1}$ is a 4×3 matrix. Following Theorem 2, Lemmas S.4, S.5, and 2, the objective function for a minimally supported design at $(d, J, m) = (2, 3, 4)$ is

$$\begin{aligned} f(p_1, p_2, p_3, p_4) &= c_{1111} p_1 p_2 p_3 p_4 \\ &+ |\mathbf{X_1}[1,2,3]|^2 e_1 e_2 e_3 \cdot p_1 p_2 p_3 (w_1 p_1 + w_2 p_2 + w_3 p_3) \\ &+ |\mathbf{X_1}[1,2,4]|^2 e_1 e_2 e_4 \cdot p_1 p_2 p_4 (w_1 p_1 + w_2 p_2 + w_4 p_4) \\ &+ |\mathbf{X_1}[1,3,4]|^2 e_1 e_3 e_4 \cdot p_1 p_3 p_4 (w_1 p_1 + w_3 p_3 + w_4 p_4) \\ &+ |\mathbf{X_1}[2,3,4]|^2 e_2 e_3 e_4 \cdot p_2 p_3 p_4 (w_2 p_2 + w_3 p_3 + w_4 p_4) \end{aligned}$$

where $e_i = u_{i1} + u_{i2} - 2b_{i2}$, $w_i = e_i^{-1} g_{i1}^2 g_{i2}^2 (\pi_{i1}\pi_{i2}\pi_{i3})^{-1}$, $i = 1, 2, 3, 4$, and

$$c_{1111} = \sum_{1 \le i < j \le 4} e_i e_j (u_{k1} u_{l2} + u_{k2} u_{l1} - 2 b_{k2} b_{l2}) \cdot |\mathbf{X_1}[i,j,k]| \cdot |\mathbf{X_1}[i,j,l]| \quad \text{(S.12)}$$

with $\{i, j, k, l\} = \{1, 2, 3, 4\}$ given $1 \le i < j \le 4$.

According to Theorem 10, a minimally supported design $\mathbf{p} = (p_1^*, p_2^*, p_3^*, 0)^T$ in this case is D-optimal if and only if $\partial f/\partial p_1 = \partial f/\partial p_2 = \partial f/\partial p_3 \ge \partial f/\partial p_4$ at $\mathbf{p}$. Then $\partial f/\partial p_1 = \partial f/\partial p_2 = \partial f/\partial p_3$ at $\mathbf{p}$ is equivalent to (1) of Corollary 5, and $\partial f/\partial p_4 \le \partial f/\partial p_1$ at $\mathbf{p}$ leads to (2) of Corollary 5 since the forms of $\partial f/\partial p_i$ at $\mathbf{p}$, $i = 1, 2, 3$ will not change if more than four design points (i.e., $m > 4$) are added into consideration. Note that $|\mathbf{X_1}[1,2,3]|^2 e_1 e_2 e_3 p_2^* p_3^* (2w_1 p_1^* + w_2 p_2^* + w_3 p_3^*)$ in (2) of Corollary 5 is equal to $\partial f/\partial p_1$ at $\mathbf{p}$. It could be replaced with $|\mathbf{X_1}[1,2,3]|^2 e_1 e_2 e_3 p_1^* p_3^* (w_1 p_1^* + 2w_2 p_2^* + w_3 p_3^*)$ (i.e., $\partial f/\partial p_2$), or $|\mathbf{X_1}[1,2,3]|^2 e_1 e_2 e_3 p_1^* p_2^* (w_1 p_1^* + w_2 p_2^* + 2w_3 p_3^*)$ (i.e., $\partial f/\partial p_3$), since these three are all equal. $\square$

S.4 Maximization of $f_i(z)$ in Section 3

According to Theorem 6, $f_i(z)$ is an order-$(d + J - 1)$ polynomial of z. In other to determine its coefficients $a_0, a_1, \ldots, a_{J-1}$ as in (3.2), we need to calculate $f_i(0)$, $f_i(1/2)$, $f_i(1/3)$, $\ldots$, $f_i(1/J)$, which are J determinants defined in (3.1).

Note that $\mathbf{B}_{J-1}^{-1}$ is a matrix determined by $J - 1$ only. For example, $B_1^{-1} = 1$ for $J = 2$,

$$B_2^{-1} = \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}, B_3^{-1} = \begin{pmatrix} 3 & -3 & 1 \\ -\frac{5}{2} & 4 & -\frac{3}{2} \\ \frac{1}{2} & -1 & \frac{1}{2} \end{pmatrix},$$

$$B_4^{-1} = \begin{pmatrix} 4 & -6 & 4 & -1 \\ -\frac{13}{3} & \frac{19}{2} & -7 & \frac{11}{6} \\ \frac{3}{2} & -4 & \frac{7}{2} & -1 \\ -\frac{1}{6} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{6} \end{pmatrix}$$

for $J = 3$, 4, or 5 respectively.

Once $a_0, \ldots, a_{J-1}$ in (3.2) are determined, the maximization of $f_i(z)$ on $z \in [0, 1]$ is numerically straightforward since it is a polynomial and its derivative $f_i'(z)$ is given by

$$(1-z)^d \sum_{j=1}^{J-1} j a_j z^{j-1}(1-z)^{J-1-j} - (1-z)^{d-1} \sum_{j=0}^{J-1} (d+J-1-j) a_j z^j (1-z)^{J-1-j} \tag{S.13}$$

S.5 Exchange algorithm for D-optimal exact allocation in Section 4

Exchange algorithm for D-optimal allocation $(n_1, \ldots, n_m)^T$ *given* $n > 0$*:*

1° Start with an initial design $\mathbf{n} = (n_1, \ldots, n_m)^T$ such that $f(\mathbf{n}) > 0$.

2° Set up a random order of (i, j) going through all pairs $\{(1, 2), (1, 3), \ldots, (1, m), (2, 3), \ldots, (m-1, m)\}$.

3° For each (i, j), let $c = n_i + n_j$. If $c = 0$, let $\mathbf{n}_{ij}^* = \mathbf{n}$. Otherwise, there are two cases. *Case one:* $0 < c \leq J$, we calculate $f_{ij}(z)$ as defined in (4.1) for $z = 0, 1, \ldots, c$ directly and find z^* which maximizes $f_{ij}(z)$. *Case two:* $c > J$, we first calculate $f_{ij}(z)$ for $z = 0, 1, \ldots, J$; secondly determine $c_0, c_1, \ldots, c_J$ in (4.2) according to Theorem 9; thirdly calculate $f_{ij}(z)$ for $z = J+1, \ldots, c$ based on (4.2); fourthly find z^* maximizing $f_{ij}(z)$ for $z = 0, \ldots, c$. For both cases, we define

$$\mathbf{n}_{ij}^* = (n_1, \ldots, n_{i-1}, z^*, n_{i+1}, \ldots, n_{j-1}, c - z^*, n_{j+1}, \ldots, n_m)^T$$

Note that $f(\mathbf{n}_{ij}^*) = f_{ij}(z^*) \geq f(\mathbf{n}) > 0$. If $f(\mathbf{n}_{ij}^*) > f(\mathbf{n})$, replace $\mathbf{n}$ with $\mathbf{n}_{ij}^*$, and $f(\mathbf{n})$ with $f(\mathbf{n}_{ij}^*)$.

4° Repeat 2° ∼ 3° until convergence, that is, $f(\mathbf{n}_{ij}^*) = f(\mathbf{n})$ in step 3° for any (i, j).

S.6 More on Example 6: Polysilicon Deposition Study

Table S.1 shows the list of experimental settings for the polysilicon deposition study. The factors are `decomposition temperature`(A), `decomposition pressure`(B), `nitrogen flow` (C), `silane flow`(D), `setting time`(E), `cleaning method`(F). Column 1 provides original indices of experimental settings out of 729 distinct ones. For each experimental setting labelled "1" in a design, 9 responses are collected (Phadke (1989)) and assumed to be independent.

Table S.1: Polysilicon Deposition Study: Experimental Settings for the Original, Rounded Approximate, and D-optimal Exact Designs

Index	A	B	C	D	E	F	Original	Rounded	D-optimal
1	1	1	1	1	1	1	1	0	0
76	1	1	3	3	2	1	1	0	0
89	1	2	1	1	3	2	1	0	0
98	1	2	1	2	3	2	0	0	1
111	1	2	2	1	1	3	0	0	1
116	1	2	2	1	3	2	0	1	0
122	1	2	2	2	2	2	1	0	0
130	1	2	2	3	2	1	0	0	1
167	1	3	1	1	2	2	0	0	1
181	1	3	1	3	1	1	0	1	0
199	1	3	2	2	1	1	0	1	1
201	1	3	2	2	1	3	1	0	0
243	1	3	3	3	3	3	1	0	1
258	2	1	1	2	2	3	1	0	0
286	2	1	2	2	3	1	0	1	0
290	2	1	2	3	1	2	1	0	0
291	2	1	2	3	1	3	0	1	0
294	2	1	2	3	2	3	0	0	1
299	2	1	3	1	1	2	0	0	1
301	2	1	3	1	2	1	0	1	0
313	2	1	3	2	3	1	0	0	1
331	2	2	1	1	3	1	0	1	1
336	2	2	1	2	1	3	0	1	1
339	2	2	1	2	2	3	0	1	0
350	2	2	1	3	3	2	0	1	0
365	2	2	2	2	2	2	0	0	1
376	2	2	2	3	3	1	1	0	0
384	2	2	3	1	2	3	1	0	0
394	2	2	3	2	3	1	0	1	0
399	2	2	3	3	1	3	0	1	0
407	2	3	1	1	1	2	0	0	1
421	2	3	1	2	3	1	1	0	0
461	2	3	3	1	1	2	1	1	0
464	2	3	3	1	2	2	0	1	0
495	3	1	1	1	3	3	0	1	0
501	3	1	1	2	2	3	0	0	1
505	3	1	1	3	1	1	0	0	1
521	3	1	2	1	3	2	0	0	1
522	3	1	2	1	3	3	1	0	0
536	3	1	2	3	2	2	0	1	0
557	3	1	3	2	3	2	1	0	0
558	3	1	3	2	3	3	0	1	0
569	3	2	1	1	1	2	0	1	0
588	3	2	1	3	1	3	1	0	0
625	3	2	3	1	2	1	0	0	1
631	3	2	3	2	1	1	1	0	0
641	3	2	3	3	1	2	0	0	1
671	3	3	1	3	2	2	1	0	0
679	3	3	2	1	2	1	1	0	0

Table S.2 shows the model matrix for the D-optimal design $\mathbf{n}_o$ found for the polysilicon deposition study. In this table, each 3-level factor is represented by its linear component and quadratic component. Thus there are level combinations of 12 predictors.

Table S.2: Polysilicon Deposition Study: Model Matrix for the D-optimal Design

Index	A_1	A_2	B_1	B_2	C_1	C_2	D_1	D_2	E_1	E_2	F_1	F_2
98	−1	1	0	−2	−1	1	0	−2	1	1	0	−2
111	−1	1	0	−2	0	−2	−1	1	−1	1	1	1
130	−1	1	0	−2	0	−2	1	1	0	−2	−1	1
167	−1	1	1	1	−1	1	−1	1	0	−2	0	−2
199	−1	1	1	1	0	−2	0	−2	−1	1	−1	1
243	−1	1	1	1	1	1	1	1	1	1	1	1
294	0	−2	−1	1	0	−2	1	1	0	−2	1	1
299	0	−2	−1	1	1	1	−1	1	−1	1	0	−2
313	0	−2	−1	1	1	1	0	−2	1	1	−1	1
331	0	−2	0	−2	−1	1	−1	1	1	1	−1	1
336	0	−2	0	−2	−1	1	0	−2	−1	1	1	1
365	0	−2	0	−2	0	−2	0	−2	0	−2	0	−2
407	0	−2	1	1	−1	1	−1	1	−1	1	0	−2
501	1	1	−1	1	−1	1	0	−2	0	−2	1	1
505	1	1	−1	1	−1	1	1	1	−1	1	−1	1
521	1	1	−1	1	0	−2	−1	1	1	1	0	−2
625	1	1	0	−2	1	1	−1	1	0	−2	−1	1
641	1	1	0	−2	1	1	1	1	−1	1	0	−2