Supplement to "Bayesian D-Optimal Design of Experiments with Quantitative and Qualitative Responses"

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S1 Proofs and Derivations

Proof of (3.3)

Proof.

$$\begin{aligned}\Psi(\boldsymbol{X}|\mu_0,\sigma^2) &= \int p(\boldsymbol{y},\boldsymbol{z}|\mu_0,\sigma^2)\int \log\left(p(\boldsymbol{\beta}^{(1)},\boldsymbol{\beta}^{(2)},\boldsymbol{\eta}|\boldsymbol{y},\boldsymbol{z},\mu_0,\sigma^2)\right) \\ &\qquad p(\boldsymbol{\beta}^{(1)},\boldsymbol{\beta}^{(2)},\boldsymbol{\eta}|\boldsymbol{y},\boldsymbol{z},\mu_0,\sigma^2)\mathrm{d}\boldsymbol{\beta}^{(1)}\mathrm{d}\boldsymbol{\beta}^{(2)}\mathrm{d}\boldsymbol{\eta}\mathrm{d}\boldsymbol{y}\mathrm{d}\boldsymbol{z} \\ &= \int p(\boldsymbol{y},\boldsymbol{z}|\mu_0,\sigma^2)\left\{\int \log\left(p(\boldsymbol{\eta}|\boldsymbol{z})\right)p(\boldsymbol{\eta}|\boldsymbol{z})\mathrm{d}\boldsymbol{\eta}\right. \\ &\qquad \left. + \sum_{i=1}^{2}\int \log\left(p(\boldsymbol{\beta}^{(i)}|\boldsymbol{y},\boldsymbol{z},\mu_0,\sigma^2)\right)p(\boldsymbol{\beta}^{(i)}|\boldsymbol{y},\boldsymbol{z},\mu_0,\sigma^2)\mathrm{d}\boldsymbol{\beta}^{(i)}\right\}\mathrm{d}\boldsymbol{y}\mathrm{d}\boldsymbol{z} \\ &= \int p(\boldsymbol{y},\boldsymbol{z}|\mu_0,\sigma^2)\left\{\int \log\left(p(\boldsymbol{\eta}|\boldsymbol{z})\right)p(\boldsymbol{\eta}|\boldsymbol{z})\mathrm{d}\boldsymbol{\eta}\right. \\ &\qquad \left. - \frac{1}{2}\sum_{i=1}^{2}\log\det\{\sigma^{-2}(\boldsymbol{F}'\boldsymbol{V}_i\boldsymbol{F})^{-1}\} - n\log(2\pi) - n\right\}\mathrm{d}\boldsymbol{y}\mathrm{d}\boldsymbol{z} \\ &= \int \log(p(\boldsymbol{\eta}|\boldsymbol{z}))p(\boldsymbol{\eta}|\boldsymbol{z})p(\boldsymbol{z})\mathrm{d}\boldsymbol{\eta}\mathrm{d}\boldsymbol{z} \\ &\qquad - \frac{1}{2}\sum_{i=1}^{2}\int \log\det\{\sigma^{-2}(\boldsymbol{F}'\boldsymbol{V}_i\boldsymbol{F})^{-1}\}p(\boldsymbol{z})\mathrm{d}\boldsymbol{z} + \text{constant} \\ &= \int \log(p(\boldsymbol{\eta}|\boldsymbol{z}))p(\boldsymbol{z},\boldsymbol{\eta})\mathrm{d}\boldsymbol{\eta}\mathrm{d}\boldsymbol{z} \\ &\qquad + \frac{1}{2}\sum_{i=1}^{2}\int \log\det\{(\boldsymbol{F}'\boldsymbol{V}_i\boldsymbol{F})\}p(\boldsymbol{z}|\boldsymbol{\eta})p(\boldsymbol{\eta})\mathrm{d}\boldsymbol{z}\mathrm{d}\boldsymbol{\eta} + \text{constant}.\end{aligned}$$

Write the integration into the form of expectation,

$$\begin{aligned}\Psi(\boldsymbol{X}|\mu_0,\sigma^2) &= \mathbb{E}_{\boldsymbol{z},\boldsymbol{\eta}}\left\{\log(p(\boldsymbol{\eta}|\boldsymbol{z}))\right\} \\ &\qquad + \frac{1}{2}\sum_{i=1}^{2}\mathbb{E}_{\boldsymbol{\eta}}\mathbb{E}_{\boldsymbol{z}|\boldsymbol{\eta}}\left\{\log\det(\boldsymbol{F}'\boldsymbol{V}_i\boldsymbol{F})\right\} + \text{constant}.\end{aligned}$$

□

Proof of Theorem 1

Proof. To show (3.6), we just need to show that $\mathbb{E}_{\boldsymbol{z}|\boldsymbol{\eta}}(\log\det(\boldsymbol{F}'\boldsymbol{V}_i\boldsymbol{F})) \leq \log\det(\boldsymbol{F}'\boldsymbol{W}_i\boldsymbol{F}')$ for $i = 1, 2$.

First we need to show that $\log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F}) = \log\det(\sum_{i=1}^{n} a_i \boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)')$ with $\boldsymbol{A} = \text{diag}\{a_1, \ldots, a_n\}$ is a concave function of $\boldsymbol{a} = (a_1, \ldots, a_n)'$ for $\boldsymbol{a} \in [0,1]^n$. Denote $\boldsymbol{B} = \text{diag}\{b_1, \ldots, b_n\}$ for $\boldsymbol{b} = (b_1, \ldots, b_n)' \in [0,1]^n$. We assume that $\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F}$ is nonsingular, thus $\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F}$ is positive definite. For any scalar value of t, define function $g(t)$

$$
\begin{aligned}
g(t) &= \log\det\left(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \boldsymbol{F}'(t\boldsymbol{B})\boldsymbol{F}\right) \\
&= \log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F}) + \log\det(\boldsymbol{I}_q + t(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F})^{-1/2}(\boldsymbol{F}'\boldsymbol{B}\boldsymbol{F})(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F})^{-1/2}) \\
&= \log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F}) + \sum_{i=1}^{q}\log(1 + t\lambda_i),
\end{aligned}
$$

where λ_i's are the eigenvalues of the positive definite matrix $(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F})^{-1/2}(\boldsymbol{F}'\boldsymbol{B}\boldsymbol{F})(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F})^{-1/2}$. Thus $g(t)$ is a concave function in t for any choice of $\boldsymbol{a}$, which is the sufficient and necessary condition that $\log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F})$ is a concave function of $\boldsymbol{a}$. According to Jensen's inequality, if $\pi(\boldsymbol{x}_i, \boldsymbol{\eta}) \in (0,1)$ for $i = 1, \ldots, n$, then

$$
\begin{aligned}
\mathbb{E}_{\boldsymbol{z}|\boldsymbol{\eta}}\left(\log\det(\boldsymbol{F}'\boldsymbol{V}_1\boldsymbol{F})\right) &\leq \log\det\left(\sum_{i=1}^{n}\mathbb{E}(Z_i|\boldsymbol{\eta})\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'\right) \\
&= \log\det\left(\sum_{i=1}^{n}\pi(\boldsymbol{x}_i, \boldsymbol{\eta})\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'\right), \\
\mathbb{E}_{\boldsymbol{z}|\boldsymbol{\eta}}\left(\log\det(\boldsymbol{F}'\boldsymbol{V}_2\boldsymbol{F})\right) &\leq \log\det\left(\sum_{i=1}^{n}\mathbb{E}((1 - Z_i)|\boldsymbol{\eta})\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'\right) \\
&= \log\det\left(\sum_{i=1}^{n}(1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'\right).
\end{aligned}
$$

So we have proved (3.6). □

Proof of Proposition 1

Proof.

$$
m = \sum_{i=1}^{m} I\left(0 < \sum_{j=1}^{n_i} Z_{ij} < n_i\right) + \sum_{i=1}^{m} I\left(\sum_{j=1}^{n_i} Z_{ij} = 0\right) + \sum_{i=1}^{m} I\left(\sum_{j=1}^{n_i} Z_{ij} = n_i\right) \geq q
$$

If $m = q$, (3.7) is equivalent to $I\left(0 < \sum_{j=1}^{n_i} Z_{ij} < n_i\right) = 1$ for $i = 1, 2, \ldots, m$. A sufficient condition for any $\Pr\left(0 < \sum_{j=1}^{n_i} Z_{ij} < n_i\right) \geq \kappa$ can be derived as follows.

$$\Pr\left(0 < \sum_{j=1}^{n_i} Z_{ij} < n_i\right) = 1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} - (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} \geq \kappa$$
$$\iff \quad \pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} + (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} \leq 1 - \kappa.$$

Next develop an upper bound for $\pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} + (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i}$. If $\pi(\boldsymbol{x}_i, \boldsymbol{\eta}) \geq 1/2$, denote $a = (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))/\pi(\boldsymbol{x}_i, \boldsymbol{\eta})$ and $a \leq 1$. Then

$$\pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} + (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} = \frac{1 + a^{n_i}}{(1+a)^{n_i}} \leq \frac{1+a}{(1+a)^{n_i}}.$$

If

$$\frac{1+a}{(1+a)^{n_i}} \leq 1 - \kappa \quad \iff \quad n_i \geq 1 + \frac{\log(1-\kappa)}{\log \pi(\boldsymbol{x}_i, \boldsymbol{\eta})},$$

then $\pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} + (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} \leq 1 - \kappa$. If $\pi(\boldsymbol{x}_i, \boldsymbol{\eta}) < 1/2$, denote $a = \pi(\boldsymbol{x}_i, \boldsymbol{\eta})/(1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))$ and $a < 1$. Then

$$\pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} + (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} = \frac{1 + a^{n_i}}{(1+a)^{n_i}} < \frac{1+a}{(1+a)^{n_i}}.$$

The sufficient condition becomes

$$\frac{1+a}{(1+a)^{n_i}} \leq 1 - \kappa \quad \iff \quad n_i \geq 1 + \frac{\log(1-\kappa)}{\log(1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))}.$$

Combining the two cases, the sufficient condition on n_i for $i = 1, \ldots, m$ is (3.8). It is known that

$$2\left(\pi(\boldsymbol{x}_i, \boldsymbol{\eta})(1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta})\right)^{n_i/2} \leq \pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} + (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} \leq 1 - \kappa.$$

The necessary condition is

$$2\left(\pi(\boldsymbol{x}_i, \boldsymbol{\eta})(1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta})\right)^{n_i/2} \leq 1 - \kappa \quad \iff \quad n_i \geq \frac{2\log\left(\frac{1-\kappa}{2}\right)}{\log \pi(\boldsymbol{x}_i, \boldsymbol{\eta}) + \log(1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))}.$$

□

Proof of Proposition 2

Proof. If $m > q$, (3.7) is equivalent to

$$\sum_{i=1}^{m} I\left(\sum_{j=1}^{n_i} Z_{ij} = 0\right) \leq m - q, \text{ and } \sum_{i=1}^{m} I\left(\sum_{j=1}^{n_i} Z_{ij} = n_i\right) \leq m - q.$$

For the two inequalities to hold with large probability,

$$\sum_{i=1}^{m} \mathbb{E}\left\{ I\left(\sum_{j=1}^{n_i} Z_{ij} = 0 \right) \right\} = \sum_{i=1}^{m} (1 - \pi(\boldsymbol{x}_i, \boldsymbol{\eta}))^{n_i} \le m - q, \tag{1}$$

$$\text{and } \sum_{i=1}^{m} \mathbb{E}\left\{ I\left(\sum_{j=1}^{n_i} Z_{ij} = n_i \right) \right\} = \sum_{i=1}^{m} \pi(\boldsymbol{x}_i, \boldsymbol{\eta})^{n_i} \le m - q. \tag{2}$$

It is known that

$$m\left(\prod_{i=1}^{m}(1-\pi_{\max})^{n_i}\right)^{1/m} \le \sum_{i=1}^{m}(1-\pi_{\max})^{n_i} \le \sum_{i=1}^{m}(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))^{n_i} \le \sum_{i=1}^{m}(1-\pi_{\min})^{n_i} \le m(1-\pi_{\min})^{n_0}.$$

Thus one sufficient condition for (1) is

$$m(1-\pi_{\min})^{n_0} \le m - q \quad \Longleftrightarrow \quad n_0 \ge \frac{\log(1-q/m)}{\log(1-\pi_{\min})}.$$

One necessary condition for (1) is

$$m\left(\prod_{i=1}^{m}(1-\pi_{\max})^{n_i}\right)^{1/m} \le m - q \quad \Longleftrightarrow \sum_{i=1}^{m} n_i \ge m\frac{\log(1-q/m)}{\log(1-\pi_{\max})}.$$

Similarly,

$$m\left(\prod_{i=1}^{m}\pi_{\min}^{n_i}\right)^{1/m} \le \sum_{i=1}^{m}\pi_{\min}^{n_i} \le \sum_{i=1}^{m}\pi(\boldsymbol{x}_i,\boldsymbol{\eta})^{n_i} \le \sum_{i=1}^{m}\pi_{\max}^{n_i} \le m\cdot\pi_{\max}^{n_0}.$$

Thus one sufficient condition for (2) is

$$m\cdot\pi_{\max}^{n_0} \le m - q \quad \Longleftrightarrow \quad n_0 \ge \frac{\log(1-q/m)}{\log \pi_{\max}}.$$

One necessary condition for (2) is

$$m\left(\prod_{i=1}^{m}\pi_{\min}^{n_i}\right)^{1/m} \le m - q \quad \Longleftrightarrow \sum_{i=1}^{m} n_i \ge m\frac{\log(1-q/m)}{\log \pi_{\min}}.$$

Thus the sufficient condition for (1) and (2) derived here is

$$n_0 \ge \max\left\{1, \frac{\log(1-q/m)}{\log(1-\pi_{\min})}, \frac{\log(1-q/m)}{\log \pi_{\max}}\right\},$$

or equivalently,

$$\sum_{i=1}^{m} n_i \ge m\cdot n_0 \ge m\cdot\max\left\{1, \frac{\log(1-q/m)}{\log(1-\pi_{\min})}, \frac{\log(1-q/m)}{\log \pi_{\max}}\right\}.$$

The necessary condition for (1) and (2) derived here is

$$\sum_{i=1}^{n} n_i \geq m \cdot \max\left\{1, \frac{\log(1-q/m)}{\log(1-\pi_{\max})}, \frac{\log(1-q/m)}{\log \pi_{\min}}\right\}.$$

It is easy to see that this lower bound in the necessary condition is smaller than the one in the sufficient condition,

$$\sum_{i=1}^{m} n_i \geq m \cdot n_0 \geq m \cdot \max\left\{1, \frac{\log(1-q/m)}{\log(1-\pi_{\min})}, \frac{\log(1-q/m)}{\log \pi_{\max}}\right\}.$$

□

Proof of Theorem 2

Proof. We only need to show that $\log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1}) = \log\det(\sum_{i=1}^{n} a_i \boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)' + \rho\boldsymbol{R}_i^{-1})$ with $\boldsymbol{A} = \mathrm{diag}\{a_1, \ldots, a_n\}$ is a concave function of $\boldsymbol{a} = (a_1, \ldots, a_n)'$ for $\boldsymbol{a} \in [0,1]^n$. Denote $\boldsymbol{B} = \mathrm{diag}\{b_1, \ldots, b_n\}$ for $\boldsymbol{b} = (b_1, \ldots, b_n)' \in [0,1]^n$ and $\boldsymbol{K} = \boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1}$. Define $g(t)$ as follows.

$$\begin{aligned}
g(t) &= \log\det\left(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1} + \boldsymbol{F}'(t\boldsymbol{B})\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1}\right) \\
&= \log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1}) \\
&+ \log\det(\boldsymbol{I}_q + (\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1})^{-1/2}(\boldsymbol{F}'t\boldsymbol{B}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1})(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1})^{-1/2}) \\
&= \log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1}) \\
&+ \log\det(\boldsymbol{I}_q + t\boldsymbol{K}^{-1/2}\boldsymbol{F}'\boldsymbol{B}\boldsymbol{F}\boldsymbol{K}^{-1/2} + \rho\boldsymbol{K}^{-1/2}\boldsymbol{R}_i^{-1}\boldsymbol{K}^{-1/2}) \\
&= \log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1}) + \log\det(\boldsymbol{I}_q + \rho\boldsymbol{K}^{-1/2}\boldsymbol{R}_i^{-1}\boldsymbol{K}^{-1/2}) + \sum_{i=1}^{q}\log(1+t\lambda_i),
\end{aligned}$$

where λ_i's are the eigenvalues of

$$(\boldsymbol{I}_q + \rho\boldsymbol{K}^{-1/2}\boldsymbol{R}_i^{-1}\boldsymbol{K}^{-1/2})^{-1/2}\boldsymbol{K}^{-1/2}\boldsymbol{F}'\boldsymbol{B}\boldsymbol{F}\boldsymbol{K}^{-1/2}(\boldsymbol{I}_q + \rho\boldsymbol{K}^{-1/2}\boldsymbol{R}_i^{-1}\boldsymbol{K}^{-1/2})^{-1/2}.$$

Therefore, $\lambda_i \geq 0$ for $i = 1, \ldots, q$. Thus $g(t)$ is a concave function in t for any choice of $\boldsymbol{a} \in [0,1]^n$, which is the sufficient and necessary condition for $\log\det(\boldsymbol{F}'\boldsymbol{A}\boldsymbol{F} + \rho\boldsymbol{R}_i^{-1})$ to be a concave function of $\boldsymbol{a}$. □

Proof of the deletion function (5.1)

Proof. Denote $\boldsymbol{F}_{-i}$ as the model matrix for $\boldsymbol{X}_{-i}$, which is the design matrix without the ith design point, and $\boldsymbol{W}_{0,-i}$, $\boldsymbol{W}_{1,-i}$, and $\boldsymbol{W}_{2,-i}$ the weight matrices accordingly. According to the properties of matrix determinants, we can show the following.

$$\begin{aligned}
\det\left(\boldsymbol{F}_{-i}'\boldsymbol{W}_{0,-i}\boldsymbol{F}_{-i}\right) &= \det\left(\sum_{j\neq i}\pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x}_j)\boldsymbol{f}(\boldsymbol{x}_j)'\right) \\
&= \det\left(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F} - \pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'\right) \\
&= \det(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F})\left[1 - \pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x}_i)'(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F})^{-1}\boldsymbol{f}(\boldsymbol{x}_i)\right] \\
&= \det(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F})\left[1 - \pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_0(\boldsymbol{x}_i)\right].
\end{aligned}$$

$$
\begin{aligned}
&\det\left(\boldsymbol{F}_{-i}'\boldsymbol{W}_{1,-i}\boldsymbol{F}_{-i}+\rho\boldsymbol{R}^{-1}\right)\\
=&\det\left(\sum_{j\neq i}\pi(\boldsymbol{x}_i,\boldsymbol{\eta})\boldsymbol{f}(\boldsymbol{x}_j)\boldsymbol{f}(\boldsymbol{x}_j)'+\rho\boldsymbol{R}^{-1}\right)\\
=&\det\left(\boldsymbol{F}'\boldsymbol{W}_1\boldsymbol{F}+\rho\boldsymbol{R}^{-1}-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'\right)\\
=&\det\left(\boldsymbol{F}'\boldsymbol{W}_1\boldsymbol{F}+\rho\boldsymbol{R}^{-1}\right)\left[1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})\boldsymbol{f}(\boldsymbol{x}_i)'(\boldsymbol{F}'\boldsymbol{W}_1\boldsymbol{F}+\rho\boldsymbol{R}^{-1})^{-1}\boldsymbol{f}(\boldsymbol{x}_i)\right]\\
=&\det\left(\boldsymbol{F}'\boldsymbol{W}_1\boldsymbol{F}+\rho\boldsymbol{R}^{-1}\right)\left[1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})v_1(\boldsymbol{x}_i)\right].
\end{aligned}
$$

Similarly,

$$
\det\left(\boldsymbol{F}_{-i}'\boldsymbol{W}_{2,-i}\boldsymbol{F}_{-i}+\rho\boldsymbol{R}_2^{-1}\right)=\det\left(\boldsymbol{F}'\boldsymbol{W}_2\boldsymbol{F}+\rho\boldsymbol{R}^{-1}\right)\left[1-(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_2(\boldsymbol{x}_i)\right].
$$

The deletion function (5.1) is then obtained. □

Shortcut formulas for $\boldsymbol{M}_{i,-j}$.

Proof. Denote $\boldsymbol{M}_{i,-j}$ for $i=0,1,2$ as the updated $\boldsymbol{M}_i$ when the jth design point is removed. The following shortcut formulas are used in constructing the initial design.

$$
\boldsymbol{M}_{i,-j}=\boldsymbol{M}_i+\left[\frac{\pi(\boldsymbol{x}_j,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_j,\boldsymbol{\eta}))}{1-\pi(\boldsymbol{x}_j,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_j,\boldsymbol{\eta}))v_0(\boldsymbol{x}_j)}\right]\boldsymbol{M}_i\boldsymbol{f}(\boldsymbol{x}_j)\boldsymbol{f}(\boldsymbol{x}_j)'\boldsymbol{M}_i,\qquad \text{for } i=0,1,2.
$$

□

Proof of $\Delta(\boldsymbol{x},\boldsymbol{x}_i)$ in (5.2).

Proof. Denote $\boldsymbol{F}^*$ as the updated model matrix for updated design $\boldsymbol{X}^*$, and $\boldsymbol{W}_i^*$ for $i=0,1,2$ as the updated weight matrices accordingly. Let

$$
\boldsymbol{G}_0=[\sqrt{\pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta})}\boldsymbol{f}(\boldsymbol{x}),i\sqrt{\pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})}\boldsymbol{f}(\boldsymbol{x}_i)],
$$

where $i=\sqrt{-1}$.

$$
\begin{aligned}
&\det(\boldsymbol{F}^{*'}\boldsymbol{W}_0^*\boldsymbol{F}^*)=\det\left(\sum_{j\neq i}\pi(\boldsymbol{x}_j,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_j,\boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x}_j)\boldsymbol{f}(\boldsymbol{x}_j)'\right.\\
&\left.-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x}_i)\boldsymbol{f}(\boldsymbol{x}_i)'+\pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))\boldsymbol{f}(\boldsymbol{x})\boldsymbol{f}(\boldsymbol{x})'\right)\\
&=\det(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F}+\boldsymbol{G}_0\boldsymbol{G}_0')\\
&=\det(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F})\det\left(\boldsymbol{I}_2+\boldsymbol{G}_0'\boldsymbol{M}_0\boldsymbol{G}_0\right).
\end{aligned}
$$

It can be computed that

$$
\det\left(\boldsymbol{I}_2+\boldsymbol{G}_0'\boldsymbol{M}_0\boldsymbol{G}_0\right)=\Delta_0(\boldsymbol{x},\boldsymbol{x}_i),
$$

where $\Delta_0(\boldsymbol{x},\boldsymbol{x}_i)$ is

$$
\begin{aligned}
\Delta_0(\boldsymbol{x},\boldsymbol{x}_i)=&\left[1+\pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))v_0(\boldsymbol{x})\right]\left[1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_0(\boldsymbol{x}_i)\right]\\
&+\pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))\pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_0(\boldsymbol{x},\boldsymbol{x}_i)^2.
\end{aligned}
$$

Similarly, define

$$\begin{aligned}
\boldsymbol{G}_1 &= [\sqrt{\pi(\boldsymbol{x},\eta)}\boldsymbol{f}(\boldsymbol{x}), i\sqrt{\pi(\boldsymbol{x}_i,\eta)}\boldsymbol{f}(\boldsymbol{x}_i)] \quad \text{and} \\
\boldsymbol{G}_2 &= [\sqrt{(1-\pi(\boldsymbol{x},\boldsymbol{\eta})}\boldsymbol{f}(\boldsymbol{x}), i\sqrt{(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})}\boldsymbol{f}(\boldsymbol{x}_i)].
\end{aligned}$$

Following a similar derivation,

$$\begin{aligned}
\det(\boldsymbol{F}^{*'}\boldsymbol{W}_1^*\boldsymbol{F}^* + \rho\boldsymbol{R}) &= \det(\boldsymbol{F}'\boldsymbol{W}_1\boldsymbol{F} + \rho\boldsymbol{R})\Delta_1(\boldsymbol{x},\boldsymbol{x}_i), \\
\det(\boldsymbol{F}^{*'}\boldsymbol{W}_2^*\boldsymbol{F}^* + \rho\boldsymbol{R}) &= \det(\boldsymbol{F}'\boldsymbol{W}_2\boldsymbol{F} + \rho\boldsymbol{R})\Delta_2(\boldsymbol{x},\boldsymbol{x}_i),
\end{aligned}$$

where $\Delta_1(\boldsymbol{x},\boldsymbol{x}_i)$ and $\Delta_2(\boldsymbol{x},\boldsymbol{x}_i)$ are

$$\begin{aligned}
\Delta_1(\boldsymbol{x},\boldsymbol{x}_i) &= [1+\pi(\boldsymbol{x},\boldsymbol{\eta})v_1(\boldsymbol{x})]\,[1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})v_1(\boldsymbol{x}_i)] + \pi(\boldsymbol{x},\boldsymbol{\eta})\pi(\boldsymbol{x}_i,\boldsymbol{\eta})v_1(\boldsymbol{x},\boldsymbol{x}_i)^2, \\
\Delta_2(\boldsymbol{x},\boldsymbol{x}_i) &= [1+(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))v_2(\boldsymbol{x})]\,[1-(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_2(\boldsymbol{x}_i)] \\
&\quad + (1-\pi(\boldsymbol{x},\boldsymbol{\eta}))(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_2(\boldsymbol{x},\boldsymbol{x}_i)^2.
\end{aligned}$$

Thus $\Delta(\boldsymbol{x},\boldsymbol{x}_i)$ is computed as in (5.2). □

Proof of update formulas $\boldsymbol{M}_i^*$ for $i = 0, 1, 2$

Proof. Use the same notation of $\boldsymbol{G}_i$ for $i = 0, 1, 2$ as in the previous proof. Define the functions

$$\begin{aligned}
\boldsymbol{S}_i(\boldsymbol{x}) &= \boldsymbol{M}_i\boldsymbol{f}(\boldsymbol{x})\boldsymbol{f}(\boldsymbol{x})'\boldsymbol{M}_i, \quad \text{for } i = 0,1,2, \\
\boldsymbol{S}_i(\boldsymbol{x}_1,\boldsymbol{x}_2) &= \boldsymbol{M}_i\boldsymbol{f}(\boldsymbol{x}_1)\boldsymbol{f}(\boldsymbol{x}_2)'\boldsymbol{M}_i, \quad \text{for } i = 0,1,2.
\end{aligned}$$

It is straightforward to derive

$$\begin{aligned}
\boldsymbol{M}_0^* &= \left(\boldsymbol{F}'\boldsymbol{W}_0\boldsymbol{F} + \boldsymbol{G}_0\boldsymbol{G}_0'\right)^{-1} \\
&= \boldsymbol{M}_0 - \boldsymbol{M}_0\boldsymbol{G}_0\left(\boldsymbol{I}_2 + \boldsymbol{G}_0'\boldsymbol{M}_0\boldsymbol{G}_0\right)^{-1}\boldsymbol{G}'\boldsymbol{M}_0.
\end{aligned}$$

For simpler notation, denote $a(\boldsymbol{x}) = \pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))$ and $a(\boldsymbol{x}_i) = \pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))$.

$$\begin{aligned}
&\left(\boldsymbol{I}_2 + \boldsymbol{G}_0'\boldsymbol{M}_0\boldsymbol{G}_0\right)^{-1} \\
=&\begin{pmatrix} 1 + a(\boldsymbol{x})v_0(\boldsymbol{x}), & i\sqrt{a(\boldsymbol{x})a(\boldsymbol{x}_i)}v_0(\boldsymbol{x},\boldsymbol{x}_i) \\ i\sqrt{a(\boldsymbol{x})a(\boldsymbol{x}_i)}v_0(\boldsymbol{x},\boldsymbol{x}_i), & 1 - a(\boldsymbol{x}_i)v_0(\boldsymbol{x}_i) \end{pmatrix}^{-1} \\
=&\frac{1}{\Delta_0(\boldsymbol{x},\boldsymbol{x}_i)}\begin{pmatrix} 1 - a(\boldsymbol{x}_i)v_0(\boldsymbol{x}_i), & -i\sqrt{a(\boldsymbol{x})a(\boldsymbol{x}_i)}v_0(\boldsymbol{x},\boldsymbol{x}_i) \\ -i\sqrt{a(\boldsymbol{x})a(\boldsymbol{x}_i)}v_0(\boldsymbol{x},\boldsymbol{x}_i), & 1 + a(\boldsymbol{x})v_0(\boldsymbol{x}) \end{pmatrix}.
\end{aligned}$$

$$
\begin{aligned}
\boldsymbol{M}_0^* &= \boldsymbol{M}_0 - \frac{1}{\Delta_0(\boldsymbol{x},\boldsymbol{x}_i)}\boldsymbol{M}_0\left[\sqrt{a(\boldsymbol{x})}v_0(\boldsymbol{x}), i\sqrt{a(\boldsymbol{x}_i)}v_0(\boldsymbol{x}_i)\right] \\
&\times \begin{pmatrix} 1 - a(\boldsymbol{x}_i)v_0(\boldsymbol{x}_i), & -i\sqrt{a(\boldsymbol{x})a(\boldsymbol{x}_i)}v_0(\boldsymbol{x},\boldsymbol{x}_i) \\ -i\sqrt{a(\boldsymbol{x})a(\boldsymbol{x}_i)}v_0(\boldsymbol{x},\boldsymbol{x}_i), & 1 + a(\boldsymbol{x})v_0(\boldsymbol{x}) \end{pmatrix} \times \begin{bmatrix} \sqrt{a(\boldsymbol{x})}\boldsymbol{f}(\boldsymbol{x})' \\ i\sqrt{a_i(\boldsymbol{x}_i)}\boldsymbol{f}(\boldsymbol{x}_i)' \end{bmatrix} \boldsymbol{M}_0. \\
&= \boldsymbol{M}_0 - \frac{1}{\Delta_0(\boldsymbol{x},\boldsymbol{x}_i)}\left\{\pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))\left[1 - \pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_0(\boldsymbol{x}_i)\right]\boldsymbol{S}_0(\boldsymbol{x})\right. \\
&-\pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\left[1 + \pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))v_0(\boldsymbol{x})\right]\boldsymbol{S}_0(\boldsymbol{x}_i) \\
&\left. + \pi(\boldsymbol{x}_i,\boldsymbol{\eta})(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\pi(\boldsymbol{x},\boldsymbol{\eta})(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))v_0(\boldsymbol{x},\boldsymbol{x}_i)\left[\boldsymbol{S}_0(\boldsymbol{x},\boldsymbol{x}_i) + \boldsymbol{S}_0(\boldsymbol{x}_i,\boldsymbol{x})\right]\right\}
\end{aligned}
$$

Update formulas for $\boldsymbol{M}_1^*$ and $\boldsymbol{M}_2^*$ can be derived similarly as follows.

$$
\begin{aligned}
\boldsymbol{M}_1^* = \boldsymbol{M}_1 - \frac{1}{\Delta_1(\boldsymbol{x},\boldsymbol{x}_i)}&\left\{\pi(\boldsymbol{x},\boldsymbol{\eta})\left[1 - \pi(\boldsymbol{x}_i,\boldsymbol{\eta})v_1(\boldsymbol{x}_i)\right]\boldsymbol{S}_1(\boldsymbol{x}) - \pi(\boldsymbol{x}_i,\boldsymbol{\eta})\left[1 + \pi(\boldsymbol{x},\boldsymbol{\eta})v_1(\boldsymbol{x})\right]\boldsymbol{S}_1(\boldsymbol{x}_i)\right. \\
&\left. + \pi(\boldsymbol{x}_i,\boldsymbol{\eta})\pi(\boldsymbol{x},\boldsymbol{\eta})v_1(\boldsymbol{x},\boldsymbol{x}_i)\left[\boldsymbol{S}_1(\boldsymbol{x},\boldsymbol{x}_i) + \boldsymbol{S}_1(\boldsymbol{x}_i,\boldsymbol{x})\right]\right\}, \\
\boldsymbol{M}_2^* = \boldsymbol{M}_2 - \frac{1}{\Delta_2(\boldsymbol{x},\boldsymbol{x}_i)}&\left\{(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))\left[1 - (1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))v_2(\boldsymbol{x}_i)\right]\boldsymbol{S}_2(\boldsymbol{x})\right. \\
&-(1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))\left[1 + (1-\pi(\boldsymbol{x},\boldsymbol{\eta}))v_2(\boldsymbol{x})\right]\boldsymbol{S}_2(\boldsymbol{x}_i) \\
&\left. + (1-\pi(\boldsymbol{x}_i,\boldsymbol{\eta}))(1-\pi(\boldsymbol{x},\boldsymbol{\eta}))v_2(\boldsymbol{x},\boldsymbol{x}_i)\left[\boldsymbol{S}_2(\boldsymbol{x},\boldsymbol{x}_i) + \boldsymbol{S}_2(\boldsymbol{x}_i,\boldsymbol{x})\right]\right\}.
\end{aligned}
$$

□

S2 Table

Table S1: Local Bayesian D-optimal Designs for $\rho = 0$ and 0.3 and other three alternative designs. The values in columns 7-11 are frequencies.

Point	x_1	x_2	x_3	x_4	x_5	D_{QQ} $\rho = 0$	D_{QQ} $\rho = 0.3$	D_G	D_L	D_n
1	-1	-1	-1	-1	-1	1	2	1	1	2
2	1	-1	-1	-1	-1	1	1	2	1	1
3	-1	1	-1	-1	-1	1	1	2	1	1
4	1	1	-1	-1	-1	2	1	2	1	2
5	-1	-1	1	-1	-1	1	0	2	1	1
6	1	-1	1	-1	-1	1	1	0	1	1
7	-1	1	1	-1	-1	2	2	1	1	2
8	1	1	1	-1	-1	1	2	1	1	1
9	-1	-1	-1	0	-1	2	2	1	1	1
10	1	-1	-1	0	-1	0	0	1	1	1
11	-1	1	-1	0	-1	1	1	2	1	2
12	1	1	-1	0	-1	1	2	1	1	1
13	-1	-1	1	0	-1	1	1	1	1	2
14	1	-1	1	0	-1	2	2	1	1	1
15	-1	1	1	0	-1	1	1	0	1	0
16	1	1	1	0	-1	1	1	1	1	2
17	-1	-1	-1	1	-1	1	0	1	1	2
18	1	-1	-1	1	-1	2	2	1	1	1
19	-1	1	-1	1	-1	2	2	1	1	1
20	1	1	-1	1	-1	1	1	1	1	1
21	-1	-1	1	1	-1	2	2	1	1	1
22	1	-1	1	1	-1	0	1	1	1	1
23	-1	1	1	1	-1	0	1	1	1	2
24	1	1	1	1	-1	2	1	1	1	1
25	-1	-1	-1	-1	0	1	0	1	1	0
26	1	-1	-1	-1	0	0	0	1	1	1
27	-1	1	-1	-1	0	0	0	0	1	0
28	1	1	-1	-1	0	0	1	1	1	0
29	-1	-1	1	-1	0	0	1	1	1	1
30	1	-1	1	-1	0	0	0	0	1	0
31	-1	1	1	-1	0	0	0	0	1	0
32	1	1	1	-1	0	1	0	1	1	0
33	-1	-1	-1	0	0	0	0	1	1	0
34	1	-1	-1	0	0	1	1	1	1	1
35	-1	1	-1	0	0	0	0	0	1	0
36	1	1	-1	0	0	1	0	1	1	0
37	-1	-1	1	0	0	1	1	1	1	0
38	1	-1	1	0	0	0	0	1	1	0
39	-1	1	1	0	0	0	0	0	1	0
40	1	1	1	0	0	0	0	1	1	0
41	-1	-1	-1	1	0	0	2	1	0	0
42	1	-1	-1	1	0	0	0	1	1	0
43	-1	1	-1	1	0	0	0	0	1	0
44	1	1	-1	1	0	1	0	1	0	0
45	-1	-1	1	1	0	0	0	1	1	0
46	1	-1	1	1	0	1	1	1	0	0
47	-1	1	1	1	0	1	0	1	0	0
48	1	1	1	1	0	0	1	1	1	1
49	-1	-1	-1	-1	1	1	1	1	1	1
50	1	-1	-1	-1	1	2	2	1	1	2
51	-1	1	-1	-1	1	1	1	0	1	1
52	1	1	-1	-1	1	1	1	1	1	1
53	-1	-1	1	-1	1	2	1	1	1	2
54	1	-1	1	-1	1	0	0	0	1	0
55	-1	1	1	-1	1	1	1	1	1	1
56	1	1	1	-1	1	1	2	1	1	2
57	-1	-1	-1	0	1	1	1	1	1	2
58	1	-1	-1	0	1	1	1	1	1	0
59	-1	1	-1	0	1	2	2	1	1	1
60	1	1	-1	0	1	1	1	1	1	2
61	-1	-1	1	0	1	2	2	1	0	1
62	1	-1	1	0	1	1	1	1	1	2
63	-1	1	1	0	1	0	0	1	1	1
64	1	1	1	0	1	2	2	1	0	1
65	-1	-1	-1	1	1	2	1	1	1	2
66	1	-1	-1	1	1	1	1	1	1	1
67	-1	1	-1	1	1	1	1	1	1	1
68	1	1	-1	1	1	1	2	1	1	2
69	-1	-1	1	1	1	1	1	1	1	1
70	1	-1	1	1	1	1	1	0	1	1
71	-1	1	1	1	1	2	2	1	1	2
72	1	1	1	1	1	1	0	1	1	1