# Supplement: Cost Considerations for Efficient Group Testing Studies

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This supplement contains two sections: all proofs of the theorems and lemmas are in Section S1, and some results about the $D$-optimal group testing designs are in Section S2.

## S1. Proofs of theorems and lemmas

In this section, we provide all technical proofs for this work. Lemmas 1 and 2 are respectively proved in Sections S1.1 and S1.2. The proof of Theorem 1 is similar to the proof of its traditional version, see for example, Atkinson, Donev and Tobias (2007), and has therefore been omitted. Theorem 2 is proved in Section S1.3. The proof of Lemma 3 is similar to Lemma 2 and has also been omitted.

## S1.1 Proof of Lemma 1

It is clear that a design with at least three points is valid. We show that a design with fewer than three points is not valid. This result is shown by contradiction. Without loss of generality, suppose there exists a design $\xi = \{(x_i, w_i)\}_{i=1}^2$ such that $p_0 = e_1^{\mathrm{T}}\theta$ is estimable under $\xi$, where $x_L \le x_1 < x_2 \le x_U$, $w_1, w_2 \ge 0$, $w_1 + w_2 = 1$. Let $e_1 = (1, 0, 0)^{\mathrm{T}}$. Therefore, $e_1$ belongs to the range of $M(\xi)$, where

$$\begin{aligned} M(\xi) &= \sum_{i=1}^{2} w_i \lambda(x_i) f(x_i) f(x_i)^{\mathrm{T}} \\ &= (f(x_1), f(x_2)) \cdot \mathrm{diag}(w_1\lambda(x_1), w_2\lambda(x_2)) \cdot (f(x_1), f(x_2))^{\mathrm{T}}. \end{aligned}$$

Hence, $e_1$ belongs to the range of $(f(x_1), f(x_2))$, or equivalently, the determinant of $(f(x_1)\ f(x_2)\ e_1) = 0$. However,

$$|f(x_1)\ f(x_2)\ e_1| = \begin{vmatrix} x_1(p_1+p_2-1)(1-p_0)^{x_1-1} & x_2(p_1+p_2-1)(1-p_0)^{x_2-1} & 1 \\ 1-(1-p_0)^{x_1} & 1-(1-p_0)^{x_2} & 0 \\ -(1-p_0)^{x_1} & -(1-p_0)^{x_2} & 0 \end{vmatrix}$$

$$= (1-p_0)^{x_1} - (1-p_0)^{x_2} > 0$$

for arbitrary $x_1 < x_2$ and $p_0 \in (0, 1)$. This contradiction shows that $p_0$ is only estimable under a design with at least three points.

## S1.2 Proof of Lemma 2

Let $\xi$ be a design supported on $\{x_1, x_2, x_3\} \subset [x_L, x_U]$. Note that in Lemma 1 we show that a valid design must have at least three support points and therefore has a nonsingular information matrix. Our problem now is to find the vector of the positive weights $\{w_i^s\}_{i=1}^3$ at these three given points that minimizes $(M(\xi)^{-1})_{11}$. Here $M(\xi)$ can be written as

$$M(\xi) = F \cdot \text{diag}(w_i \lambda(x_3))_{i=1}^3 \cdot F^{\text{T}},$$

where $F$ is nonsingular and $\text{diag}(w_i \lambda(x_3))_{i=1}^3$ is positive-definite. Let $e_1 = (1, 0, 0)^{\text{T}}$. Then we have

$$\begin{aligned}\left(M(\xi)^{-1}\right)_{11} &= e_1^{\text{T}} \cdot (F^{-1})^{\text{T}} \cdot \text{diag}(w_i^{-1} \lambda(x_i)^{-1})_{i=1}^3 \cdot F^{-1} \cdot e_1 \\ &= (v_1, v_2, v_3) \cdot \text{diag}(w_i^{-1} \lambda(x_i)^{-1})_{i=1}^3 \cdot (v_1, v_2, v_3)^{\text{T}} \qquad \text{(S1)} \\ &= \sum_{i=1}^{3} u_i^2 / w_i.\end{aligned}$$

Since $u_i^2 > 0$ for $i = 1, 2, 3$, we apply the method of Lagrange multipliers directly to minimize the value in (S1) subject to the constraints on the weights, and then the desired result holds.

## S1.3 Proof of Theorem 2

We only show the case with cost parameter $q > 0$. When $q = 0$, this theorem degenerates to Theorem 3 in Huang et al. (2017). We prove this theorem by three steps: (i) a $D_s$-optimal design $\xi_s$ must have exactly three group sizes (denoted by $x_1^s < x_2^s < x_3^s$); (ii) the $D_s$-optimal design is unique; (iii) $x_1^s = x_L$.

(i) We show that if $\xi_s$ is a $D_s$-optimal design, the function $\phi_s(x, \xi_s)$ cannot have four or more distinct roots in $[x_L, x_U]$. Therefore, together with Theorem 1(c) and Lemma 1, $\xi_s$ has exactly three support points. This result is shown by contradiction.

Suppose that there exists a $D_s$-optimal design $\xi_s$ such that $\phi_s(x, \xi_s)$ has at least four distinct roots in $[x_L, x_U]$. We denote the minimum among these roots as $x_{\min}$ and the maximum as $x_{\max}$. By Theorem 1(b,c), there exists a small $\epsilon_1 > 0$ such that the function $\phi_s(x, \xi_s) + \epsilon$ has at least $4 \times 2 - 2 = 6$ roots in interval $(x_{\min}, x_{\max})$ for arbitrary $\epsilon \in (0, \epsilon_1)$.

On the other hand, by equation (3.2), we have that

$$
\begin{aligned}
&\lambda(x)^{-1} \left(\phi_s(x, \xi_s) + \epsilon\right) \\
&\quad = f(x)^{\mathrm{T}} M(\xi_s)^{-1} f(x) - f_s(x)^{\mathrm{T}} M_s(\xi_s)^{-1} f_s(x) + (\epsilon - 1)\lambda(x)^{-1} \\
&\quad = (a_0 + a_1 x) + (a_2 + a_3 x)(1 - p_0)^x + (a_4 + a_5 x + a_6 x^2)(1 - p_0)^{2x}
\end{aligned}
$$

and it is continuous on $\mathbb{R}$, where $a_0, a_2, a_3, a_4, a_5 \in \mathbb{R}$,

$$a_1 = (\epsilon - 1)p_1(1 - p_1)q_0 < 0 \quad \text{for } \epsilon \in (0, \min(\epsilon_1, 1)), \text{ and}$$

$$a_6 = \left(M(\xi_s)^{-1}\right)_{11} \times (p_1 + p_2 - 1)^2/(1 - p_0)^2 > 0.$$

Because of the fact that $\sum_{i=0}^{h} r_i(x)e^{v_i x}$ has at most $\sum_{i=0}^{h} s_i + h$ real roots, where $r_i(x)$ is a real polynomial of degree $s_i$ and $v_i \in \mathbb{R}$ (Karlin and Studden, 1966, page 10), $\lambda(x)^{-1}\left(\phi_s(x, \xi_s) + \epsilon\right)$ has at most $1 + 1 + 2 + 2 = 6$ real roots.

Since $\lambda(x) > 0$ for $x > 0$, a positive root of $\phi_s(x, \xi_s) + \epsilon$ is also a root of $\lambda(x)^{-1}\left(\phi_s(x, \xi_s) + \epsilon\right)$. Therefore, the two paragraphs above indicate that for $\epsilon \in (0, \min(\epsilon_1, 1))$, $\lambda(x)^{-1}\left(\phi_s(x, \xi_s) + \epsilon\right)$ has exactly six roots in $(x_{\min}, x_{\max})$ and no root outside. However, since

$$\lambda(x)^{-1}\left(\phi_s(x_{\max}, \xi_s) + \epsilon\right) = \lambda(x)^{-1}\epsilon > 0 \quad \text{and}$$

$$\lim_{x \to \infty} \lambda(x)^{-1}\left(\phi_s(x, \xi_s) + \epsilon\right)/x = a_1 < 0,$$

it yields that $\lambda(x)^{-1}\left(\phi_s(x, \xi_s) + \epsilon\right)$ has a root in $[x_{\max}, \infty)$, and so a contradiction occurs. This shows that a $D_s$-optimal design has exactly three distinct group sizes, and thus their optimal weights follow the results at Lemma 2.

(ii) The result is shown by contradiction. Suppose that $\xi_s \neq \xi_s'$ are both $D_s$-optimal designs. Since $\xi_s$ and $\xi_s'$ have three support points and

Lemma 2, $\xi_s \neq \xi_s'$ implies that $\xi^* = \frac{1}{2}\xi_s + \frac{1}{2}\xi_s'$ has at least four distinct support points. By Theorem 1, $\xi^*$ is also a $D_s$-optimal design but has at least four distinct support points, which contradicts the result in step (i). Therefore, the $D_s$-optimal design must be unique.

(iii) The result is shown by contradiction. Suppose that the $D_s$-optimal design $\xi_s$ has support points $x_1^s < x_2^s < x_3^s$ with $x_1^s > x_L$. Let $\epsilon_2 = \phi_s(x_L, \xi^*) < 0$ ($\epsilon_2 \neq 0$ by (i)), and set $\epsilon \in (0, \min(1, \epsilon_1, -\epsilon_2))$. By arguments similar to step (i), $\lambda(x)^{-1}(\phi_s(x, \xi_s) + \epsilon)$ has at least $3 \times 2 - 2 = 4$ roots in $(x_1^*, x_3^*)$, has a root in $(x_3^*, \infty)$, and has at most six real roots. However, since

$$\lambda(x)^{-1}(\phi_s(x_1^s, \xi_s) + \epsilon) = \lambda(x)^{-1}\epsilon > 0,$$

$$\lambda(x)^{-1}(\phi_s(x_L, \xi_s) + \epsilon) = \lambda(x)^{-1}(\epsilon_2 + \epsilon) < 0, \quad \text{and}$$

$$\lim_{x \to -\infty} \lambda(x)^{-1}(\phi_s(x, \xi_s) + \epsilon) / (x^2(1 - p_0)^2 x) = a_6 > 0,$$

it yields that $\lambda(x)^{-1}(\phi_s(x, \xi_s) + \epsilon)$ has two roots in $(-\infty, x_1^s)$. Hence, we have that $\lambda(x)^{-1}(\phi_s(x, \xi_s) + \epsilon)$ has at least seven real roots and so a contradiction occurs. This shows that $x_1^s$ must be $x_L$.

## S2. $D$-optimal designs

In this section we present the $D$-optimal budget-constraint group testing designs under the setting that $p_1$ and $p_2$ are unknown constants. Similar to the definition of $D_s$-optimal designs with equation (2.5), a $D$-optimal design maximizes the criterion function

$$\Phi_D\{M(\xi)\} = \log(|M(\xi)|).$$

The following theorem characterizes the $D$-optimal designs. The proof is similar to Theorem 2 and has been omitted.

**Theorem S1.** *The $D$-optimal design $\xi^*$ is unique. It is equally supported on the three group sizes $x_L = x_1^* < x_2^* < x_3^* \leq x_U$, where $x_2^*$ and $x_3^*$ maximizes $\lambda(x_2)\lambda(x_3)\left|(f(x_L), f(x_2), f(x_3))\right|^2$.*

Theorem S1 can be used to numerically obtain the $D$-optimal design through a two-dimension optimization. In Figure S1 we compare the group sizes of the $D_s$-optimal designs in Example 1 with those of the corresponding $D$-optimal designs. We can see that the intermediate sizes are close, where $x_2^s$ is slightly smaller than $x_2^*$, but $x_3^s$ is somewhat larger than $x_3^*$.

## References

Atkinson, A. C., Donev, A. N. and Tobias, R.D. (2007). *Optimum experimental designs, with SAS*. Oxford University Press, Oxford.

Huang, S.-H., Huang, M.-N. L., Shedden, K. and Wong, W. K. (2017). Optimal group testing designs for estimating prevalence with uncertain testing errors. *J. Roy. Statist. Soc. Ser. B*, **79**, 1547-1563.

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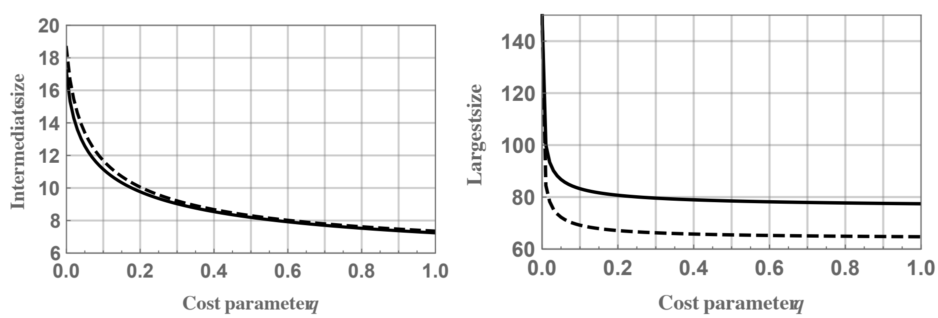


(a) $x_2^s$ (solid) and $x_2^*$ (dashed) vs. $q$ (b) $x_3^s$ (solid) and $x_3^*$ (dashed) vs. $q$

Figure S1: Group sizes of the $D_s$-optimal design ($\xi_s$) and the $D$-optimal design ($\xi^*$) for Example 1, where $\xi_s$ is supported on $\{x_1^s, x_2^s, x_3^s\}$ and $\xi^*$ is on $\{x_1^*, x_2^*, x_3^*\}$, where the smallest sizes $1 = x_1^s = x_1^*$. The intermediate sizes $x_2^s$ and $x_2^*$ are shown in (a), the largest sizes $x_3^s$ and $x_3^*$ are in (b).