Constrained D-optimal Design for Paid Research Study

Yifei Huang[1], Liping Tong[2], Jie Yang[1]

[1] *University of Illinois at Chicago*, [2] *Advocate Aurora Health*

Supplementary Material

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S1 General lift-one algorithm (without constraints)

For readers' reference, in this section, we provide the lift-one algorithm for general parametric models. The lift-one algorithms for specific models can be found in Yang et al. (2016) for GLMs with binary responses, Yang and Mandal (2015) for general GLMs, Yang et al. (2017) for cumulative link models, and Bu et al. (2020) for multinomial logistic models.

Algorithm 3. Original lift-one algorithm under a general setup

1° *Start with an arbitrary allocation* $\mathbf{w}_a = (w_1, \ldots, w_m)^T \in S_0$ *satisfying* $f(\mathbf{w}_a) > 0$ *and* $0 \le w_i < 1$, $i = 1, \ldots, m$.

2° *Set up a random order of* i *going through* $\{1, 2, \ldots, m\}$. *For each* i, *do steps* $3^\circ \sim 5^\circ$.

3° *Denote*

$$\mathbf{w}_i(z) = \left(\frac{1-z}{1-w_i}w_1, \ldots, \frac{1-z}{1-w_i}w_{i-1}, z, \frac{1-z}{1-w_i}w_{i+1}, \ldots, \frac{1-z}{1-w_i}w_m\right)^T$$

and $f_i(z) = f(\mathbf{w}_i(z))$, $z \in [0, 1]$.

4° *Use an analytic solution or the quasi-Newton algorithm to find* z_* *maximizing* $f_i(z)$ *with* $z \in [0, 1]$. *Define* $\mathbf{w}_*^{(i)} = \mathbf{w}_i(z_*)$. *Note that* $f(\mathbf{w}_*^{(i)}) = f_i(z_*)$.

5° *If* $f(\mathbf{w}_*^{(i)}) > f(\mathbf{w}_a)$, *replace* $\mathbf{w}_a$ *with* $\mathbf{w}_*^{(i)}$, *and* $f(\mathbf{w}_a)$ *with* $f(\mathbf{w}_*^{(i)})$.

6° *Repeat* $2^\circ \sim 5^\circ$ *until convergence, that is,* $f(\mathbf{w}_*^{(i)}) \le f(\mathbf{w}_a)$ *for each* i.

7° *Report* $\mathbf{w}_a$ *as the D-optimal allocation.*

In practice, we may set up the stopping rule as $\frac{\max_{1\le i\le m} f(\mathbf{w}_*^{(i)})}{\min_{1\le i\le m} f(\mathbf{w}_*^{(i)})} \le 1+\epsilon$ for Step 6°, where ϵ is a small positive number such as 10^{-8}. Then Algorithm 3 guarantees a strict increase, which is at least $f(\mathbf{w}_a)\cdot\epsilon$ in each round of iterations from Step 2° to Step 5°. Since S_0 is compact, the maximum of $f(\mathbf{w})$ on S_0 is finite. Algorithm 3 will stop in less than $\frac{\max_{\mathbf{w}\in S_0} f(\mathbf{w})-f(\mathbf{w}_a)}{f(\mathbf{w}_a)\epsilon}$ rounds of iterations. The same strategy can be used for Algorithm 1 as well.

S2 Commonly used GLM models

In Table 5, we list commonly used GLM models, the corresponding link functions, and ν functions.

Table 5: Examples of $\nu(\eta_i)$

Distribution of Y_{ij}	Link function $g(\mu_i)$	$\nu(\eta_i)$
Normal(μ_i, σ^2)	identity: μ_i	σ^{-2} with known $\sigma^2 > 0$
Bernoulli(μ_i)	logit: $\log\left(\frac{\mu_i}{1-\mu_i}\right)$	$\frac{e^{\eta_i}}{(1+e^{\eta_i})^2}$
Bernoulli(μ_i)	probit: $\Phi^{-1}(\mu_i)$	$\frac{\phi^2(\eta_i)}{\Phi(\eta_i)[1-\Phi(\eta_i)]}$
Bernoulli(μ_i)	c-log-log: $\log(-\log(1-\mu_i))$	$\frac{\exp\{2\eta_i\}}{\exp\{e^{\eta_i}\}-1}$
Bernoulli(μ_i)	log-log: $\log(-\log(\mu_i))$	$\frac{\exp\{2\eta_i\}}{\exp\{e^{\eta_i}\}-1}$
Bernoulli(μ_i)	cauchit: $\tan\left(\pi\left(\mu_i-\frac{1}{2}\right)\right)$	$\frac{(1+\eta_i^2)^{-2}}{\pi^2/4-\arctan^2(\eta_i)}$
Poisson(μ_i)	log: $\log(\mu_i)$	$\exp\{\eta_i\}$
Gamma(k, μ_i/k)	reciprocal: μ_i^{-1}	$k\eta_i^{-2}$ with known $k > 0$
Inverse Gaussian(μ_i, λ)	inverse squared: μ_i^{-2}	$\lambda\eta_i^{-3/2}/4$ with known $\lambda > 0$

S3 Two examples of finding r_{i1} and r_{i2} in Algorithm 1

Following the general procedure described in Subsection 3.2 for finding r_{i1} and r_{i2} in Step 3° of Algorithm 1, we provide the following two examples.

Example 9. If $S = \{(w_1, \ldots, w_m)^T \in S_0 \mid nw_i \leq N_i, i = 1, \ldots, m\}$ as in Example 1, then $\mathbf{w}_i(z) \in S$ if and only if

$$\begin{cases} 0 \leq z \leq 1 \\ nz \leq N_i \\ n\frac{1-z}{1-w_i} w_j \leq N_j,\ j \neq i \end{cases}$$

which is equivalent to

$$\begin{cases} 0 \leq z \leq 1 \\ z \leq N_i/n \\ z \geq 1 - \frac{N_j}{n} \cdot \frac{1-w_i}{w_j},\ j \neq i \text{ and } w_j > 0 \end{cases}$$

Therefore, r_{i1} and r_{i2} in Step 3° of Algorithm 1 are

$$\begin{cases} r_{i1} = & \max\left(\{0\} \cup \{1 - N_j/n \cdot (1-w_i)/w_j \mid j \neq i, w_j > 0\}\right) \\ r_{i2} = & \min\{1, N_i/n\} \end{cases} \tag{S3.1}$$

It can be verified that if $\mathbf{w} \in S$, then $0 \leq r_{i1} \leq r_{i2} \leq 1$. □

Example 10. If $S = \{(w_1, \ldots, w_m)^T \in S_0 \mid n\sum_{i=1}^{4} w_i \leq 392, n\sum_{i=5}^{8} w_i \leq 410\}$ as in Example 2, then r_{i1} and r_{i2} can be obtained as follows:

Case one: If $i \in \{1,2,3,4\}$, then $\mathbf{w}_i(z) \in S$ if and only if

$$\begin{cases} 0 \le z \le 1 \\ z + \sum_{j=1, j\neq i}^{4} \frac{w_j(1-z)}{1-w_i} \le 392/n \\ \sum_{j=5}^{8} \frac{w_j(1-z)}{1-w_i} \le 410/n \end{cases}$$

which is equivalent to

$$\begin{cases} 0 \le z \le 1 \\ z \le \frac{392(1-w_i) - n\sum_{j=1, j\neq i}^{4} w_j}{n(1-\sum_{j=1}^{4} w_j)} \\ z \ge 1 - \frac{410(1-w_i)}{n\sum_{j=5}^{8} w_j} \end{cases}$$

Therefore,

$$\begin{cases} r_{i1} = \max\{0, 1 - \frac{410(1-w_i)}{n\sum_{j=5}^{8} w_j}\} \\ r_{i2} = \min\{1, \frac{392(1-w_i) - n\sum_{j=1, j\neq i}^{4} w_j}{n(1-\sum_{j=1}^{4} w_j)}\} \end{cases}$$

Case two: If $i \in \{5,6,7,8\}$, then $\mathbf{w}_i(z) \in S$ if and only if

$$\begin{cases} 0 \le z \le 1 \\ \sum_{j=1}^{4} \frac{w_j(1-z)}{1-w_i} \le 392/n \\ z + \sum_{j=5, j\neq i}^{8} \frac{w_j(1-z)}{1-w_i} \le 410/n \end{cases}$$

Similarly, we obtain

$$\begin{cases} r_{i1} = \max\{0, 1 - \frac{392(1-w_i)}{n\sum_{j=1}^{4} w_j}\} \\ r_{i2} = \min\{1, \frac{410(1-w_i) - n\sum_{j=5, j\neq i}^{8} w_j}{n(1-\sum_{j=5}^{8} w_j)}\} \end{cases}$$

□

S4 Another example of robustness under GLM models

Example 11. To further test the robustness to model misspecifications in Example 6, we assume the true parameters to be $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_{21}, \beta_{22})^T = (0, 0.1, 0.5, 2)^T$, which is different from the one in Example 6. In this case, we have different D-optimal allocations for logit, probit, log-log, and complementary log-log links. Actually, using logit link, we obtain $\mathbf{w}_{\text{logit}} = (0.189, 0.184, 0.050, 0.189, 0.181, 0.207)^T$. If the true link is probit with D-optimal allocation $\mathbf{w}_{\text{probit}} = (0.193, 0.185, 0.050, 0.193, 0.181, 0.198)^T$, then the relative efficiency of $\mathbf{w}_{\text{logit}}$ is 99.98%. Since the $\mathbf{W}$ matrix is the same for log-log and complementary log-log links, the corresponding D-optimal allocations are both $\mathbf{w}_{\log} = (0.189, 0.198, 0.050, 0.193, 0.198, 0.172)^T$. The relative efficiency of $\mathbf{w}_{\text{logit}}$ with respect to $\mathbf{w}_{\log}$ is 99.68%. In other words, our D-optimal allocations are very robust with respect to link function misspecifications.

We also provide in Table 6 the average (sd) of RMSEs of the estimated coefficients from 100 independent simulations under Model (4.7). The RMSE results in Table 6 match the efficiency results. The logit link (the true link in the simulations) leads to the lowest average RMSE, while the other links have a little higher average RMSE.

Table 6: Average (sd) of RMSE of Estimated Parameters Based on Allocations Assuming Different Links over 100 Simulations from Model (4.7)

Link Function	Average (sd) of RMSE				
	β_0	all except β_0	β_1	β_{21}	β_{22}
Logit	0.231(0.166)	1.123(0.609)	0.269(0.198)	0.268(0.177)	0.423(0.370)
Probit	0.222(0.154)	1.142(0.620)	0.258(0.212)	0.276(0.228)	0.452(0.340)
cloglog/loglog	0.214(0.181)	1.306(1.438)	0.231(0.189)	0.261(0.190)	0.779(2.249)

S5 Another example of trauma clinical study

In this section, we provide an example where at least one constraint is attained at the D-optimal allocations.

Example 12. For the trauma clinical study described in Example 2, for illustration purposes, we consider the sampling problem with modified constraints as follows

$$n(w_1 + w_2 + w_3 + w_4) \leq 592, \quad n(w_5 + w_6 + w_7 + w_8) \leq 210$$

with $n = 600$. In other words, we reduce the number of available severe cases to 210. We derive allocations for different samplers as for Example 8, which are listed in Table 7. Note that the constraint $n(w_5+w_6+w_7+w_8) \leq$

210 is attained in both locally D-optimal and EW D-optimal allocations. It should also be noted that among the $B = 1,000$ bootstrapped samples only 807 fitted parameter vectors by SAS, in this case, are feasible. The quantiles of relative efficiencies of sampler allocations with respect to 807 locally D-optimal allocations are listed in Table 8, which shows again that the EW D-optimal sampler is highly efficient with respect to the locally D-optimal allocations and much more efficient than the proportionally stratified and uniformly stratified samplers. □

Table 7: Allocations (Proportions) for Stratified Samplers in Example 12

Severity	Mild				Severe			
Dose	1	2	3	4	1	2	3	4
Proportional	116 (0.193)	105 (0.175)	115 (0.192)	108 (0.180)	41 (0.068)	37 (0.062)	40 (0.067)	38 (0.063)
Uniform	98 (0.163)	98 (0.163)	97 (0.162)	97 (0.162)	55 (0.092)	50 (0.083)	54 (0.090)	51 (0.085)
Locally D-opt ($\hat{\boldsymbol{\theta}}$)	234 (0.390)	4 (0.007)	3 (0.005)	149 (0.249)	126 (0.210)	0 (0)	3 (0.005)	81 (0.134)
EW D-opt	253 (0.421)	0 (0)	0 (0)	137 (0.229)	77 (0.128)	8 (0.013)	0 (0)	125 (0.209)

Table 8: Quantiles of Relative Efficiencies in Example 12

Sampler	Minimum	1st Quartile	Median	3rd Quartile	Maximum
SRSWOR	51.80%	75.04%	75.80%	76.47%	78.98%
Proportional	52.36%	75.25%	75.62%	76.05%	77.42%
Uniform	57.19%	82.35%	82.71%	83.09%	84.29%
EW D-opt	69.05%	100%	100%	100%	100%

S6 Proofs

Proof of Lemma 1: If $w_i = 1$ for some i, then $w_j = 0$ for all $j \neq i$ and $f(\mathbf{w}) = \left|\sum_{j=1}^m w_j \mathbf{F}_j\right| = |\mathbf{F}_i| = 0$, which leads to a contradiction. □

Proof of Theorem 1: Let $\mathbf{F}_i = (a_{ist})_{s,t=1,\ldots,p}$, $i = 1, \ldots, m$. Then $\sum_{i=1}^m w_i \mathbf{F}_i = (\sum_{i=1}^m a_{ist} w_i)_{s,t=1,\ldots,p}$. According to the definition of matrix determinant (see, for example, Section 4.4.1 in Seber (2008)),

$$f(\mathbf{w}) = \left|\sum_{i=1}^m w_i \mathbf{F}_i\right| = \sum_{\pi} \text{sgn}(\pi) \cdot \prod_{s=1}^p \left(\sum_{i=1}^m a_{is\ \pi(s)} w_i\right)$$

is a homogeneous polynomial of $w_1, \ldots, w_m$, where π goes through all permutations of $\{1, \ldots, p\}$, and $\text{sgn}(\pi) = -1$ or 1 depending on whether π is odd or even. Since $f(\mathbf{w}) > 0$ for some $\mathbf{w} \in S$, then $f(\mathbf{w})$ is of order-p, not a zero function.

Since $f(\mathbf{w}) = |\sum_{i=1}^m w_i \mathbf{F}_i|$ is a polynomial function of $w_1, \ldots, w_m$, then it must be continuous on S. According to the Weierstrass theorem (see, for example, Theorem 3.1 in Sundaram et al. (1996)), there must exist a $\mathbf{w}_* \in S$ such that $f(\mathbf{w})$ attains its maximum at $\mathbf{w}_*$. □

Lemma 6. *If $M_1, M_2 \in \mathbb{R}^{p\times p}$ are both positive semi-definite, then for any $\alpha \in (0,1)$,*

$$\log|\alpha M_1 + (1-\alpha)M_2| \geq \alpha \log|M_1| + (1-\alpha)\log|M_2|$$

where the equality holds only if $M_1 = M_2$ or $|M_1| = |M_2| = 0$.

Proof of Lemma 6: When M_1 and M_2 are both positive definite, according to Theorem 1.1.14 in Fedorov (1972), the inequality is always valid, and the equality holds only if $M_1 = M_2$. If one of M_1 and M_2 is degenerate, then the right side of the equation $\alpha\log|M_1| + (1-\alpha)\log|M_2| = -\infty$. Since $\log|\alpha M_1 + (1-\alpha)M_2| \geq -\infty$ is always true, the inequality is still valid when M_1 and M_2 are positive semi-definite matrices. If only one of M_1 and M_2 is degenerate, then $\alpha M_1 + (1-\alpha)M_2$ is still positive definite and only inequality holds. □

Lemma 6 is an extended version of, for example, Theorem 1.1.14 in Fedorov (1972). It is needed in the proof of Lemma 2, which provides necessary results relevant to Step 7° of Algorithm 1.

Proof of Lemma 2: According to the constrained lift-one algorithm, $\mathbf{w}_a = (w_1, \ldots, w_m)^T \in S$, $f(\mathbf{w}_a) > 0$, and $\mathbf{w}_i(z) \in S$ for $z \in [r_{i1}, r_{i2}]$.

To avoid trivial cases, we assume $r_{i1} < r_{i2}$. For any $[z_1, z_2] \subseteq [r_{i1}, r_{i2}]$ and $\alpha \in (0, 1)$, it can be verified that $\mathbf{w}_i(\alpha z_1 + (1-\alpha)z_2) = \alpha \mathbf{w}_i(z_1) + (1-\alpha)\mathbf{w}_i(z_2)$. Denote $\mathbf{w}_i(z_1) = (w_{11}, \ldots, w_{1m})^T \in S$ and $\mathbf{w}_i(z_2) = (w_{21}, \ldots, w_{2m})^T \in S$. According to Lemma 6,

$$
\begin{aligned}
\log f_i(\alpha z_1 + (1-\alpha)z_2) &= \log f(\mathbf{w}_i(\alpha z_1 + (1-\alpha)z_2)) \\
&= \log f(\alpha \mathbf{w}_i(z_1) + (1-\alpha)\mathbf{w}_i(z_2)) \\
&= \log \left| \sum_{j=1}^m [\alpha w_{1j} + (1-\alpha) w_{2j}] \mathbf{F}_j \right| \\
&= \log \left| \alpha \cdot \sum_{j=1}^m w_{1j}\mathbf{F}_j + (1-\alpha) \cdot \sum_{j=1}^m w_{2j}\mathbf{F}_j \right| \\
&\geq \alpha \cdot \log \left| \sum_{j=1}^m w_{1j}\mathbf{F}_j \right| + (1-\alpha) \cdot \log \left| \sum_{j=1}^m w_{2j}\mathbf{F}_j \right| \\
&= \alpha \log f(\mathbf{w}_i(z_1)) + (1-\alpha) \log f(\mathbf{w}_i(z_2)) \\
&= \alpha \log f_i(z_1) + (1-\alpha) \log f_i(z_2)
\end{aligned}
$$

That is, $\log f_i(z)$ is a concave function on $[r_{i1}, r_{i2}]$.

If z_* maximizes $f_i(z)$ with $z \in [r_{i1}, r_{i2}]$, then $f_i(z_*) \geq f_i(w_i) = f(\mathbf{w}_a) > 0$. As a direct conclusion of Theorem 1, $f_i(z)$ is polynomial of z and thus differentiable. Since $\log f_i(z)$ is concave, then $\partial \log f_i(z)/\partial z = f_i'(z)/f_i(z)$ is decreasing. The rest of the theorem is straightforward since $f_i(z) > 0$ for all z between w_i and z_*. □

Proof of Theorem 2: First of all, $f(\mathbf{w}_*) \geq f(\mathbf{w}) > 0$. Suppose $\mathbf{w}_*$ is not

D-optimal in S. Then there exists a $\mathbf{w}_o = (w_1^o, \ldots, w_m^o)^T \in S$, such that, $f(\mathbf{w}_o) > f(\mathbf{w}_*) > 0$.

Denote $\mathbf{F}(\mathbf{w}) = \sum_{i=1}^m w_i \mathbf{F}_i$ for $\mathbf{w} = (w_1, \ldots, w_m)^T$. Then $\mathbf{F}(\mathbf{w})$ is a linear functional of $\mathbf{w}$, which implies $\mathbf{F}(x\mathbf{w}_o + (1-x)\mathbf{w}_*) = x\mathbf{F}(\mathbf{w}_o) + (1-x)\mathbf{F}(\mathbf{w}_*)$. Note that $f(\mathbf{w}) = |\mathbf{F}(\mathbf{w})|$. Since $f(\mathbf{w}_o) > f(\mathbf{w}_*) > 0$, then $\mathbf{F}(\mathbf{w}_o) \neq \mathbf{F}(\mathbf{w}_*)$ and $|\mathbf{F}(\mathbf{w}_o)| > |\mathbf{F}(\mathbf{w}_*)| > 0$. According to Lemma 6, $\log|\mathbf{F}(x\mathbf{w}_o + (1-x)\mathbf{w}_*)| = \log|x\mathbf{F}(\mathbf{w}_o) + (1-x)\mathbf{F}(\mathbf{w}_*)| > x\log|\mathbf{F}(\mathbf{w}_o)| + (1-x)\log|\mathbf{F}(\mathbf{w}_*)|$ for any $x \in (0,1)$.

We further denote $\mathbf{F}_x = \mathbf{F}(x\mathbf{w}_o + (1-x)\mathbf{w}_*)$ for $x \in [0,1]$. We claim that $\mathbf{F}_{x_1} \neq \mathbf{F}_{x_2}$ as long as $x_1 \neq x_2$. Actually, if $x_1 \neq x_2$, then $\mathbf{F}_{x_1} = \mathbf{F}_{x_2}$ implies $\mathbf{F}(\mathbf{w}_o) = \mathbf{F}(\mathbf{w}_*)$, which is not true in this case.

Now we define $f_*(x) = f(x\mathbf{w}_o + (1-x)\mathbf{w}_*) = |\mathbf{F}(x\mathbf{w}_o + (1-x)\mathbf{w}_*)| = |\mathbf{F}_x|$, $x \in [0,1]$. Then $\log f_*(x) = \log|\mathbf{F}(x\mathbf{w}_o + (1-x)\mathbf{w}_*)| > x\log|\mathbf{F}(\mathbf{w}_o)| + (1-x)\log|\mathbf{F}(\mathbf{w}_*)| > -\infty$ for each $x \in (0,1)$. Thus $f_*(x) > 0$ for each $x \in [0,1]$, which implies that the corresponding Fisher information matrix $\mathbf{F}_x$ is positive definite.

We claim that $\log f_*(x)$ is a strictly concave function on $x \in [0,1]$. Actually, for any $0 \leq x_1 < x_2 \leq 1$ and any $\alpha \in (0,1)$, according to

Lemma 6,

$$
\begin{aligned}
& \log f_*(\alpha x_1 + (1-\alpha)x_2) \\
= \;& \log f\left(\alpha[x_1\mathbf{w}_o + (1-x_1)\mathbf{w}_*] + (1-\alpha)[x_2\mathbf{w}_o + (1-x_2)\mathbf{w}_*]\right) \\
= \;& \log\left|\mathbf{F}\left(\alpha[x_1\mathbf{w}_o + (1-x_1)\mathbf{w}_*] + (1-\alpha)[x_2\mathbf{w}_o + (1-x_2)\mathbf{w}_*]\right)\right| \\
= \;& \log\left|\alpha\mathbf{F}\left(x_1\mathbf{w}_o + (1-x_1)\mathbf{w}_*\right) + (1-\alpha)\mathbf{F}\left(x_2\mathbf{w}_o + (1-x_2)\mathbf{w}_*\right)\right| \\
= \;& \log|\alpha\mathbf{F}_{x_1} + (1-\alpha)\mathbf{F}_{x_2}| \\
> \;& \alpha\log|\mathbf{F}_{x_1}| + (1-\alpha)\log|\mathbf{F}_{x_2}| \\
= \;& \alpha\log f_*(x_1) + (1-\alpha)f_*(x_2)
\end{aligned}
$$

As a direct conclusion, the first derivative of $\log f_*(x)$ is strictly decreasing as $x \in [0,1]$ increases. According to the mean value theorem (see, for example, Theorem 5.10 in Rudin (1976)), there exists a $c \in (0,1)$ such that

$$
\begin{aligned}
\left.\frac{\partial \log f_*(x)}{\partial x}\right|_{x=0} \;\geq\; \left.\frac{\partial \log f_*(x)}{\partial x}\right|_{x=c} &= \frac{\log f_*(1) - \log f_*(0)}{1-0} \\
&= \log f(\mathbf{w}_o) - \log f(\mathbf{w}_*) > 0
\end{aligned}
$$

Let $\varphi(\mathbf{w}) = \log f(\mathbf{w})$. Then the gradient of $\varphi(\mathbf{w})$ is $\nabla\varphi(\mathbf{w}) = f(\mathbf{w})^{-1}\nabla f(\mathbf{w})$. According to the definition of $f_*(x)$, the directional derivative of $f(\mathbf{w})$ at $\mathbf{w}_*$ along $\mathbf{w}_o - \mathbf{w}_*$ is

$$
\nabla f(\mathbf{w}_*)^T(\mathbf{w}_o - \mathbf{w}_*) = f(\mathbf{w}_*)\cdot\nabla\varphi(\mathbf{w}_*)^T(\mathbf{w}_o - \mathbf{w}_*) = f(\mathbf{w}_*)\cdot\left.\frac{\log f_*(x)}{\partial x}\right|_{x=0} > 0 \tag{S6.2}
$$

For $i = 1, \ldots, m$, let $\bar{\mathbf{w}}_i = (0, \ldots, 0, 1, 0, \ldots, 0)^T \in \mathbb{R}^m$ whose ith coordinate is 1. In the constrained lift-one algorithm at $\mathbf{w}_*$, we have $\mathbf{w}_i(z) = (1-\alpha)\mathbf{w}_* + \alpha\bar{\mathbf{w}}_i = \mathbf{w}_* + \alpha(\bar{\mathbf{w}}_i - \mathbf{w}_*)$ with $\alpha = \frac{z - w_i^*}{1 - w_i^*}$. Note that $w_i^* < 1$ and $\mathbf{w}_i(w_i^*) = \mathbf{w}_*$. It can be verified that the directional derivative of $f(\mathbf{w})$ at $\mathbf{w}_*$ along $\bar{\mathbf{w}}_i - \mathbf{w}_*$ is

$$\nabla f(\mathbf{w}_*)^T(\bar{\mathbf{w}}_i - \mathbf{w}_*) = (1 - w_i^*) f_i'(w_i^*) \tag{S6.3}$$

Actually,

$$\begin{aligned}
\nabla f(\mathbf{w}_*)^T(\bar{\mathbf{w}}_i - \mathbf{w}_*) &= f(\mathbf{w}_*) \cdot \nabla\varphi(\mathbf{w}_*)^T(\bar{\mathbf{w}}_i - \mathbf{w}_*) \\
&= f(\mathbf{w}_*) \cdot \lim_{\alpha\to 0} \frac{\varphi\left(\mathbf{w}_* + \alpha(\bar{\mathbf{w}}_i - \mathbf{w}_*)\right) - \varphi(\mathbf{w}_*)}{\alpha} \\
\left(\text{replace } \alpha \text{ with } \tfrac{z - w_i^*}{1 - w_i^*}\right) &= f(\mathbf{w}_*)(1 - w_i^*) \cdot \lim_{z\to w_i^*} \frac{\varphi\left(\mathbf{w}_i(z)\right) - \varphi(\mathbf{w}_i(w_i^*))}{z - w_i^*} \\
&= f(\mathbf{w}_*)(1 - w_i^*) \cdot \lim_{z\to w_i^*} \frac{\log f\left(\mathbf{w}_i(z)\right) - \log f(\mathbf{w}_i(w_i^*))}{z - w_i^*} \\
&= f(\mathbf{w}_*)(1 - w_i^*) \cdot \lim_{z\to w_i^*} \frac{\log f_i(z) - \log f_i(w_i^*)}{z - w_i^*} \\
&= f(\mathbf{w}_*)(1 - w_i^*) \cdot \left.\frac{\partial \log f_i(z)}{\partial z}\right|_{z = w_i^*} \\
&= f(\mathbf{w}_*)(1 - w_i^*) \cdot \frac{f_i'(w_i^*)}{f_i(w_i^*)} \\
&= (1 - w_i^*) f_i'(w_i^*)
\end{aligned}$$

Since $\sum_{i=1}^m w_i^o = 1$, then $\mathbf{w}_o - \mathbf{w}_* = \sum_{i=1}^m w_i^o(\bar{\mathbf{w}}_i - \mathbf{w}_*)$. Since $f_i'(w_i^*) \leq 0$ for each i, then

$$\nabla f(\mathbf{w}_*)^T(\mathbf{w}_o - \mathbf{w}_*) = \sum_{i=1}^m w_i^o \nabla f(\mathbf{w}_*)^T(\bar{\mathbf{w}}_i - \mathbf{w}_*) = \sum_{i=1}^m w_i^o (1 - w_i^*) f_i'(w_i^*) \leq 0$$

which leads to a contradiction with (S6.2). □

Proof of Corollary 1: First of all, $f(\mathbf{w}_*) > 0$. Denote $\mathbf{w}_* = (w_1^*, \ldots, w_m^*)^T \in S_0$. Then $0 \leq w_i^* < 1$ for each i according to Lemma 1. Since $w_i^* < r_{i2}$ for each i, we have $f_i'(w_i^*) \leq 0$ according to Lemma 2. Then $\mathbf{w}_*$ must be D-optimal in S as a direct conclusion of Theorem 2. □

Proof of Theorem 3: There are two cases for $\mathbf{w}_*$ reaching Step 10°.

Case one: $\mathbf{w}_*$ is a converged allocation in Step 6° and satisfies the conditions in Step 7°, that is, $f_i'(w_i^*) \leq 0$ for each i. According to Corollary 1, $\mathbf{w}_*$ must be D-optimal in S.

Case two: $\mathbf{w}_*$ is a converged allocation in Step 6°, which satisfies the condition in Step 8° but violates some condition in Step 7°. That is, $f_i'(w_i^*) > 0$ for some i but $\max_{\mathbf{w} \in S} g(\mathbf{w}) \leq 0$, where $g(\mathbf{w}) = \sum_{i=1}^m w_i(1 - w_i^*) f_i'(w_i^*)$. Since $\text{rank}(\mathbf{F}_i) < p$ for each i and $f(\mathbf{w}_*) > 0$, according to Lemma 1, $w_i^* < 1$ for each i. Suppose $\mathbf{w}_*$ is not D-optimal in S. Then there exists a $\mathbf{w}_o = (w_1^o, \ldots, w_m^o)^T \in S$, such that, $f(\mathbf{w}_o) > f(\mathbf{w}_*) > 0$. According to the proof of Theorem 2,

$$0 < \nabla f(\mathbf{w}_*)^T (\mathbf{w}_o - \mathbf{w}_*) = \sum_{i=1}^m w_i^o (1 - w_i^*) f_i'(w_i^*) = g(\mathbf{w}_o)$$

which contradicts the condition $\max_{\mathbf{w} \in S} g(\mathbf{w}) \leq 0$ in Step 8°. Therefore, $\mathbf{w}_*$ must be D-optimal in S. □

Proof of Theorem 5: (i) If $\sum_{i=1}^m c_i = 1$, then $S = \{(c_1, \ldots, c_m)^T\}$ which implies that $\mathbf{w}_o = (c_1, \ldots, c_m)^T$ is the only solution.

(ii) Suppose $\sum_{i=1}^m c_i > 1$. Without any loss of generality, we assume that $a_1 \geq a_2 \geq \cdots \geq a_m$. There exists a unique $k \in \{1, \ldots, m-1\}$ such that $\sum_{l=1}^k c_l \leq 1 < \sum_{l=1}^{k+1} c_l$. It can be verified that $\mathbf{w}_o = (c_1, \ldots, c_k, 1 - \sum_{l=1}^k c_l, 0, \ldots, 0)^T$ maximizes $g(\mathbf{w}) = \sum_{i=1}^m a_i w_i$. The rest part is straightforward. □

Proof of Lemma 3: According to the proof of Theorem 1,

$$h(\alpha) = f((1-\alpha)\mathbf{w}_* + \alpha\mathbf{w}_o) = \sum_\pi \mathrm{sgn}(\pi) \cdot \prod_{s=1}^p \left(\sum_{i=1}^m a_{is\ \pi(s)} (w_i^* + \alpha(w_i^o - w_i^*)) \right)$$

is an order-p polynomial of α. The rest of the lemma is straightforward. □

Proof of Theorem 6: First of all, we claim that $\mathbf{F}(\mathbf{w}_o) \neq \mathbf{F}(\mathbf{w}_*)$, where $\mathbf{F}(\mathbf{w}) = \sum_{i=1}^m w_i \mathbf{F}_i$ is the Fisher information matrix corresponding to the allocation $\mathbf{w} = (w_1, \ldots, w_m)^T$. Actually, if $\mathbf{F}(\mathbf{w}_o) = \mathbf{F}(\mathbf{w}_*)$, then $h(\alpha) = f((1-\alpha)\mathbf{w}_* + \alpha\mathbf{w}_o) = |\mathbf{F}((1-\alpha)\mathbf{w}_* + \alpha\mathbf{w}_o)| = |(1-\alpha)\mathbf{F}(\mathbf{w}_*) + \alpha\mathbf{F}(\mathbf{w}_o)| \equiv |\mathbf{F}(\mathbf{w}_*)|$. It implies $h'(0) = 0$. On the other hand, we denote $\varphi(\mathbf{w}) =$

$\log f(\mathbf{w})$, then $\nabla\varphi(\mathbf{w}) = f(\mathbf{w})^{-1}\nabla f(\mathbf{w})$ and

$$\begin{aligned}
g(\mathbf{w}_o) &= \nabla f(\mathbf{w}_*)^T(\mathbf{w}_o - \mathbf{w}_*) \\
&= f(\mathbf{w}_*) \cdot \nabla\varphi(\mathbf{w}_*)^T(\mathbf{w}_o - \mathbf{w}_*) \\
&= f(\mathbf{w}_*) \cdot \lim_{\alpha\to 0} \frac{\varphi(\mathbf{w}_* + \alpha(\mathbf{w}_o - \mathbf{w}_*)) - \varphi(\mathbf{w}_*)}{\alpha} \\
&= f(\mathbf{w}_*) \cdot \lim_{\alpha\to 0} \frac{\varphi((1-\alpha)\mathbf{w}_* + \alpha\mathbf{w}_o) - \varphi(\mathbf{w}_*)}{\alpha} \\
&= f(\mathbf{w}_*) \cdot \lim_{\alpha\to 0} \frac{\log h(\alpha) - \log h(0)}{\alpha} \\
&= f(\mathbf{w}_*) \cdot \frac{h'(0)}{h(0)} \\
&= h'(0)
\end{aligned}$$

Note that $h(0) = f(\mathbf{w}_*) > 0$. Then $g(\mathbf{w}_o) > 0$ implies $h'(0) > 0$, which leads to a contradiction. We must have $\mathbf{F}(\mathbf{w}_o) \neq \mathbf{F}(\mathbf{w}_*)$.

(i) Note that $h(\alpha) = f((1-\alpha)\mathbf{w}_* + \alpha\mathbf{w}_o)$ is the same as the function $f_*(x)$ defined in the proof of Theorem 2. Since $\mathbf{F}(\mathbf{w}_o) \neq \mathbf{F}(\mathbf{w}_*)$ and $|\mathbf{F}(\mathbf{w}_*)| > 0$, we still have $h(\alpha) = f_*(\alpha) > 0$ for any $\alpha \in (0,1)$. Combining $h(0) = f(\mathbf{w}_*) > 0$, we have $h(\alpha) > 0$ for any $\alpha \in [0,1)$. Note that $h(1) = f(\mathbf{w}_o)$ could be zero.

(ii) $h'(0) > 0$ since $h'(0) = g(\mathbf{w}_o) > 0$.

Since $\mathbf{F}(\mathbf{w}_o) \neq \mathbf{F}(\mathbf{w}_*)$, we still have $\mathbf{F}_{x_1} \neq \mathbf{F}_{x_2}$ given $x_1 \neq x_2$ as in the proof of Theorem 2. Then $\log h(\alpha)$ is strictly concave for $\alpha \in [0,1)$ and $\frac{h'(\alpha)}{h(\alpha)}$ is strictly decreasing as α increases in $[0,1)$.

(iii) If $h(1) > 0$ and $h'(1) \geq 0$, then $\frac{h'(\alpha)}{h(\alpha)}$ is strictly decreasing as α increases in $[0, 1]$. Since $\frac{h'(1)}{h(1)} \geq 0$, then $\frac{h'(\alpha)}{h(\alpha)} > \frac{h'(1)}{h(1)} \geq 0$ implies $h'(\alpha) > 0$ for all $\alpha \in (0, 1)$. Therefore, $h(\alpha)$ attains its maximum at $\alpha_* = 1$ only.

(iv) If $h(1) > 0$ and $h'(1) < 0$, then $\frac{h'(1)}{h(1)} < 0$. Since $\frac{h'(\alpha)}{h(\alpha)}$ is strictly decreasing on $\alpha \in [0, 1]$, then there is one and only one $\alpha_* \in (0, 1)$ such that $\frac{h'(\alpha_*)}{h(\alpha_*)} = 0$. That is, $h'(\alpha) > 0$ if $0 \leq \alpha < \alpha_*$; $= 0$ if $\alpha = \alpha_*$; and < 0 if $\alpha_* < \alpha \leq 1$. Therefore, $h(\alpha)$ attains its maximum at $\alpha_* \in (0, 1)$ only.

If $h(1) = f(\mathbf{w}_o) = 0$, we must have some $\alpha_- \in (0, 1)$, such that $h'(\alpha_-) < 0$ since $h(0) > h(1)$. Since $\frac{h'(\alpha)}{h(\alpha)}$ is strictly decreasing on $\alpha \in [0, 1)$, then there is one and only one $\alpha_* \in (0, \alpha_-)$ such that $\frac{h'(\alpha_*)}{h(\alpha_*)} = 0$. That is, $h'(\alpha) > 0$ if $0 \leq \alpha < \alpha_*$; $= 0$ if $\alpha = \alpha_*$; and < 0 if $\alpha_* < \alpha < 1$. Therefore, $h(\alpha)$ attains its maximum at $\alpha_* \in (0, 1)$ only.

Since in general $h(1) = f(\mathbf{w}_o) \geq 0$, cases (iii) and (iv) actually cover all scenarios. Therefore, α_* exists and is unique all the time. □

Proof of Lemma 5: First of all, $\mathbf{w}_*$ exists and is unique. Actually, $\mathbf{w}_*$ exists since $S = \{\mathbf{w} \in S_0 \mid 0 \leq w_i \leq c_i, i = 1, \ldots, m\}$ is bounded and closed.

Secondly, $\mathbf{w}_*$ is unique and $f(\mathbf{w}_*) > 0$. Actually, we denote $S_+ = \{\mathbf{w} \in S \mid f(\mathbf{w}) > 0\}$, which is not empty since $\sum_{i=1}^m c_i \geq 1$. Given $\mathbf{w}_{(i)} = (w_1^{(i)}, \ldots, w_m^{(i)})^T \in S_+$, $i = 1, 2$, by letting $M_i = \text{diag}\{w_1^{(i)}, \ldots, w_m^{(i)}\}$ in

Lemma 6, it can be verified that $\log f(\alpha \mathbf{w}_{(1)} + (1-\alpha)\mathbf{w}_{(2)}) > \alpha \log f(\mathbf{w}_{(1)}) + (1-\alpha)\log f(\mathbf{w}_{(2)})$ for all $\alpha \in (0,1)$ if $\mathbf{w}_{(1)} \neq \mathbf{w}_{(2)}$. In other words, $\log f(\mathbf{w})$ is strictly concave on S_+, which leads to the uniqueness of $\mathbf{w}_*$.

Case (i): If without the constraints $w_i \leq c_i$, $\mathbf{w}_* = (1/m, \ldots, 1/m)^T$ maximizes $f(\mathbf{w})$ due to the relationship between geometric average and arithmetic average. If $\min_{1\leq i\leq m} c_i \geq 1/m$, then such a $\mathbf{w}_*$ belongs to S and thus is also the solution with constraints.

Case (ii): Without any loss of generality, we assume $c_1 \leq \cdots \leq c_m$. Then $c_i = c_{(i)}$, $i = 1, \ldots, m$. Similarly, we let $c_{m+1} = 1$. Note that $c_1 = \min_{1\leq i\leq m} c_i < 1/m$ and $c_m = \max_{1\leq i\leq m} c_i \leq 1$.

First we show that there exist $k \in \{1, \ldots, m-1\}$ and $u \in [c_k, c_{k+1})$ that $\mathbf{w}_* := (c_1, \ldots, c_k, u, \ldots, u)^T \in S$, that is, $\sum_{i=1}^k c_i + (m-k)u = 1$. Actually, if we define

$$h(x) = \begin{cases} mx & \text{if } 0 \leq x < c_1 \\ \sum_{i=1}^l c_i + (m-l)x & \text{if } c_l \leq x < c_{l+1}, l = 1, \ldots, m-1 \\ \sum_{i=1}^m c_i & \text{if } x \geq c_m \end{cases}$$

then $h(x)$ is continuous on $[0,1]$ and is strictly increasing on $[0, c_m]$. Since $h(0) = 0$ and $h(c_m) = \sum_{i=1}^m c_i > 1$, then there exists a unique $u \in (0, c_m) = (0, \max_{1\leq i\leq m} c_i)$ and a corresponding $1 \leq k \leq m-1$ such that $h(u) = \sum_{i=1}^k c_i + (m-k)u = 1$.

Secondly, we show that $\mathbf{w}_* = (c_1, \ldots, c_k, u, \cdots, u)^T$ is a converged allocation in Step 6° of Algorithm 1. Actually, for $1 \leq i \leq k$, $w_i = c_i$, $r_{i1} = r_{i2} = c_i$ for Step 3° of Algorithm 1, which leads to $z_* = c_i$. Note that in this case, $f_i'(z) = c_i^{-1} \prod_{l=1}^k c_l u^{m-k}(1-c_i)^{1-m}(1-z)^{m-2}(1-mz)$ and thus $f_1'(z_*) = f_1'(c_1) > 0$. For $k+1 \leq i \leq m$, $w_i = u < c_i$, $r_{i1} = u$ and $r_{i2} = c_i$, $f_i'(z) = \prod_{i=1}^k c_i u^{m-k-1}(1-u)^{1-m}(1-z)^{m-2}(1-mz) < 0$ for all $z \in [u, c_i]$, which leads to $z_* = u$ in this case.

Thirdly, we show that $\max_{\mathbf{w} \in S} g(\mathbf{w}) = 0$ as defined in Step 8° in Algorithm 1. It can be verified that in this case, for $\mathbf{w} = (w_1, \ldots, w_m)^T \in S$

$$g(\mathbf{w}) = \prod_{l=1}^k c_l \cdot u^{m-k} \left(\sum_{i=1}^k c_i^{-1} w_i + u^{-1} \sum_{i=k+1}^m w_i - m \right)$$

Since $c_1^{-1} \geq c_2^{-1} \geq \cdots \geq c_k^{-1} \geq u^{-1} > 0$, it can be verified that $\mathbf{w}_*$ also maximizes $g(\mathbf{w})$ and $g(\mathbf{w}_*) = 0$.

By applying Theorem 3 to GLMs with $m = p$, it can be verified that $\mathbf{w}_*$ maximizes $f(\mathbf{w})$ with $\mathbf{w} \in S$.

Case (iii): If $\sum_{i=1}^m c_i = 1$, then $S = \{(c_1, \ldots, c_m)^T\}$ and $\mathbf{w}_* = (c_1, \ldots, c_m)^T$ is the only feasible solution. □

Proof of Theorem 7: For GLM (4.4), if $m = p$, then $f(\mathbf{w}) = |\mathbf{X}^T \mathbf{W} \mathbf{X}| = |\mathbf{X}|^2 \prod_{i=1}^m \nu_i \cdot \prod_{i=1}^m w_i$. According to Lemma 5, the constrained uniform allocation $\mathbf{w}_*$ maximizes $\prod_{i=1}^m w_i$, $\mathbf{w} \in S$. That is, $\mathbf{w}_*$ is D-optimal on S.

Similarly, since $f_{\mathrm{EW}}(\mathbf{w}) = |\mathbf{X}^T E(\mathbf{W}) \mathbf{X}| = |\mathbf{X}|^2 \prod_{i=1}^m E(\nu_i) \cdot \prod_{i=1}^m w_i$, $\mathbf{w}_*$

is EW D-optimal on S as well. $\square$

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