Designer’s Choice for Paid Research Study

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Abstract

We consider constrained sampling problems in paid research studies or clinical trials. When qualified volunteers are more than the budget allowed, we recommend a D-optimal sampling strategy based on the optimal design theory and develop a constrained lift-one algorithm to find the optimal allocation. Unlike the literature which mainly dealt with linear models, our solution solves the constrained sampling problem under fairly general statistical models, including generalized linear models and multinomial logistic models, and with more general constraints. We justify theoretically the optimality of our sampling strategy and show by simulation studies and real world examples the advantages over simple random sampling and proportionally stratified sampling strategies.

\textit{Key words and phrases}: Constrained sampling, D-optimal design, Generalized linear model, Lift-one algorithm, Multinomial logistic model

1 Introduction

We consider a constrained sampling problem frequently arising in paid research studies or clinical trials, especially when recruiting volunteers via internet or emails, which could gather attention widely and quickly. For example, some investigators plan to conduct a research study to evaluate the effect of a new treatment on anxiety. Besides the treatment cost, the investigators also need to prepare certain compensation for participants’ time. Due to limited funding, the investigators could only support up to \( n = 200 \) participants while there are \( N = 500 \) eligible volunteers. The question is how they select 200 participants out of 500 to evaluate the treatment effect most accurately.

There are three possible situations: \textit{Case (i)}, the investigators know nothing about the volunteers except contact information, or the covariate information provided by the volunteers does not seem relevant to the treatment effect; \textit{Case (ii)}, the investigators collect some covariates provided by the volunteers in their applications, for example, gender and age, which may play some but unknown role in the treatment effect; and \textit{Case (iii)}, the investigators knew from a previous study that a certain regression model is appropriate for the treatment effect under investigation and they knew some information about the regression coefficients of the collected covariates.
For Case (i), to sample \( n \) subjects out of \( N \), the simple random sampling without replacement (SRSWOR, see, for example, Chapter 2 of Lohr (2019)) is commonly used, which randomly chooses an index set \( 1 \leq i_1 < i_2 < \cdots < i_n \leq N \) such that each index set of \( n \) distinct subjects has the equal chance \( n!(N - n)!/N! \) to be chosen.

For Case (ii), suppose there are \( d \) covariates and \( m \) distinct combinations of covariates under consideration. For example, \( d = 2 \) covariates, gender (male or female) and age \((18\sim25, 26\sim64, 65 \text{ and above})\), lead to \( m = 6 \) possible categories (combinations of covariates) of eligible volunteers, known as strata in sampling theory (see, for example, Chapter 3 in Lohr (2019)). Suppose the frequencies of volunteers in the \( m \) categories are \( N_1, \ldots, N_m \), respectively. The question is how we determine \( n_i \leq N_i \) such that \( n = \sum_{i=1}^{m} n_i \), known as the allocation of subjects to the categories or strata. Once an allocation \((n_1, \ldots, n_m)\) is determined, \( n_i \) subjects will be chosen randomly from the \( i \)th category or stratum for each \( i \), known as stratified sampling. A commonly used stratified sampler chooses \( n_i \propto N_i \), known as the proportionally stratified sampler, which can estimate the population mean with a smaller variance than SRSWOR (Section 3.4.1 in Lohr (2019)). However, the goal of the sampling problem in this paper is not the mean of response but the treatment effect or regression coefficients of an underlying model. From an optimal design point of view (Fedorov, 1972; Silvey, 1980; Pukelsheim, 1993; Atkinson et al., 2007; Fedorov and Leonov, 2014), we want to find \( n_i \)'s such that the regression coefficients can be estimated most accurately. When no prior knowledge about the regression model is available, uniform allocation, which assigns roughly the same number of subjects to each category, is commonly used. For our constrained sampling problem with \( n_i \leq N_i \), we recommend (constrained) uniformly stratified sampler, which chooses \( n_i = \min\{k, N_i\} \) or \( \min\{k, N_i\} + 1 \) with \( k \) satisfying \( \sum_{i=1}^{m} \min\{k, N_i\} \leq n < \sum_{i=1}^{m} \min\{k + 1, N_i\} \).

For Case (iii), a certain regression model is expected for subsequent data analysis, and the investigators have some information about the regression coefficients. Since the responses of paid research studies are often categorical, the optimal allocation (Section 3.4.2 in Lohr (2019)) associated with variances of responses does not fit our needs. We propose optimal stratified samplers based on the optimal design theory, called the designer’s choice, which minimizes the variances of the estimated regression coefficients instead of the estimated population mean. According to different optimality criteria used (Fedorov, 1972; Atkinson et al., 2007; Stufken and Yang, 2012; Fedorov and Leonov, 2014), we call the corresponding sampler D-optimal sampler, A-optimal sampler, etc. In this paper, we focus on D-criterion, which is the most frequently used (Zocchi and Atkinson, 1999; Atkinson et al., 2007; Yang et al., 2017).

Unlike the classical optimal design theory or constrained optimal design theory (see Section 2 for more literature review), the design problem discussed here is under more general constraints including but not limited to \( n_i \leq N_i, n_i + n_j \leq N_{ij}, \) etc. In this case, we show that classical algorithms, such as lift-one algorithms (Yang et al., 2016; Yang and Mandal, 2015; Yang et al., 2017; Bu et al., 2020), may not work in general (see Section 3.1).

In this paper, we develop a new algorithm, called the constrained lift-one algorithm, to find optimal allocations under fairly general constraints and statistical models. We provide theoretical justifications for the optimality of the recommended allocations (see Section 3). Our simulation studies with generalized linear models (see Section 4) and a
real data example with multinomial logistic models (see Section 5) show that uniformly
stratified sampler usually works better than SRSWOR and proportionally stratified sam-
pler, and our designer’s choice, (locally) D-optimal and EW D-optimal samplers can
significantly improve the efficiency further when some information about the regression
coefficients is available.

2 Constrained D-optimal Allocation

In general, we consider an experiment with \( m \geq 2 \) pre-determined experimental settings
or level combinations \( x_i = (x_{i1}, \ldots, x_{id})^T \in \mathbb{R}^d \) of \( d \geq 1 \) covariates. Suppose we allocate
\( n_i \geq 0 \) subjects to the \( i \)th experimental setting \( x_i \), and the responses are independent
and follow a parametric model \( M(x_i; \theta) \) with unknown parameters \( \theta \in \Theta \subseteq \mathbb{R}^p, p \geq 2 \).
Under regularity conditions, the Fisher information matrix of the sample can be written
as \( F = \sum_{i=1}^m n_i F_i \in \mathbb{R}^{p \times p} \), where \( F_i \) corresponds to the Fisher information at \( x_i \), and is a
positive semi-definite matrix (see, for example, Section 1.5 in Fedorov and Leonov (2014)
and references therein).

In design theory, \( n = (n_1, \ldots, n_m)^T \) is called an exact allocation of \( n = \sum_{i=1}^m n_i \) experi-
mental units, while \( w = (w_1, \ldots, w_m)^T = (n_1/n, \ldots, n_m/n)^T \) is called an approximate
allocation, which is easier to be dealt with theoretically. The constrained D-optimal design
problem considered in this paper is to find the approximate allocation \( w \), which maxi-
mizes \( |F| \) on a collection of feasible approximate allocations \( S \subset S_0 := \{(w_1, \ldots, w_m)^T \in \mathbb{R}^m \mid w_i \geq 0, i = 1, \ldots, m; \sum_{i=1}^m w_i = 1 \} \). We assume that \( S \) is either a closed convex
set itself or a finite (overlapped or disjoint) union of closed convex sets. Note that \( S \) is not restricted to a closed convex set, it could be a non-convex set as long as it is a finite
union of closed convex sets. If \( S = \bigcup_{k=1}^K S_k \), where \( S_k \)'s are all closed convex subsets of
\( S_0 \), no matter overlapped or disjoint, we can always find an optimal allocation for each
\( S_k \) and then pick up the best one among the optimal allocations. Therefore, in theory,
we only need to solve the case when \( S \) itself is closed and convex.

Example 2.1. Consider a paid research study with \( N = 500 \) eligible volunteers. Suppose
\( d = 2 \) covariates, gender \((x_{i1} = 0 \text{ for female and } 1 \text{ for male})\) and age group \((x_{i2} = 0 \text{ for } 18 \sim 25, 1 \text{ for } 26 \sim 64, \text{ and } 2 \text{ for } 65 \text{ or above})\), are important factors. There are \( m = 6 \) cat-
ergories with \( x_i = (x_{i1}, x_{i2})^T \) corresponds to \((0, 0), (0, 1), (0, 2), (1, 0), (1, 1), (1, 2)\), respec-
tively. Suppose the numbers of volunteers \( N_i \) in the \( i \)th category are \( 50, 40, 10, 200, 150, 50 \),
respectively. The budget can only support up to \( n = 200 \) participants who will be under
the same treatment. Their responses that will be recorded are binary, 0 for no effect
and 1 for effective. The goal is to study how the effective rate changes along with gen-
der and age group. In this case, the collection of feasible approximate allocations is
\( S = \{(w_1, \ldots, w_6)^T \in S_0 \mid nw_i \leq N_i, i = 1, \ldots, 6 \} \), which is closed and convex. \( \square \)

Example 2.2. Chuang-Stein and Agresti (1997, Table V) provided a dataset of \( N = 802 \) trauma patients, stratified according to the trauma severity at the time of study
entry with 392 mild and 410 moderate/severe patients enrolled. The study involved four
treatment groups determined by dose level, \( x_{i2} = 1 \) (Placebo), 2 (Low dose), 3 (Medium
dose), and 4 (High dose). Combining with severity grade \((x_{i1} = 0 \text{ for mild or } 1 \text{ for moderate/severe})\),

\[ w = (w_1, \ldots, w_m)^T \in S_0 \mid nw_i \leq N_i, i = 1, \ldots, 6 \]
for moderate/severe), there are \( m = 8 \) distinct experimental settings with \((x_{i1}, x_{i2}) = (0, 1), (0, 2), (0, 3), (0, 4), (1, 1), (1, 2), (1, 3), (1, 4), \) respectively. The responses belong to five ordered categories, Death (1), Vegetative state (2), Major disability (3), Minor disability (4) and Good recovery (5), known as the Glasgow Outcome Scale (Jennett and Bond, 1975). Suppose due to limited budget, only \( n = 600 \) participants could be supported, the collection of feasible approximate allocations is \( S = \{(w_1, \ldots, w_8)^T \in S_0 \mid n(w_1 + w_2 + w_3 + w_4) \leq 392, n(w_5 + w_6 + w_7 + w_8) \leq 410\} \), which is closed and convex.

In the statistical literature, optimal designs under constraints were considered mainly for linear models with \( F_i = h(x_i)h(x_i)^T \), where \( h(x) = (h_1(x), \ldots, h_p(x))^T \) are known predictor functions (see Elfving (1952); Lee (1988); Cook and Fedorov (1995); Fedorov and Leonov (2014) and references therein). Among them, Wynn (1977a,b, 1982) connected finite population sampling with optimal designs under constraints \( n w_i \leq N_i \) as in Example 2.1; and Welch (1982), Fedorov (1989), Pronzato (2004, 2006) developed algorithms searching for “optimum submeasures” or “optimum bounded designs”. In this paper, \( F_i \) could be much more complicated and depend on unknown parameters \( \theta \), such as \( \nu(h(x_i)^T \theta)h(x_i)h(x_i)^T \) for generalized linear models (see Section 4) or \( X_i^T U_i X_i \) for multinomial logistic models (see Corollary 3.1 in Bu et al. (2020) and Section 5).

In this paper, we adopt the D-criterion, which maximizes the objective function \( f(w) = |\sum_{i=1}^{m} w_i F_i|, \ w \in S \). To avoid trivial cases, throughout this paper, we assume that \( f(w) > 0 \) for some \( w \in S \). For statistical models under our consideration, such as typical generalized linear models (see Section 4) and multinomial logistic models (see Section 5), \( \text{rank}(F_i) < p \) for each \( x_i \in X \), the collection of all feasible design points, known as the design space. Although positive definite \( F_i \) exists for some special multinomial logistic models, it is uncommon and out of the scope of this paper.

**Lemma 2.1.** Suppose \( \text{rank}(F_i) < p \) for each \( i \). If \( f(w) > 0 \), then \( 0 \leq w_i < 1 \) for each \( i \).

**Theorem 2.1.** Suppose \( S \subseteq S_0 \) is closed and \( f(w) > 0 \) for some \( w \in S \). Then \( f(w) \) is an order-\( p \) homogeneous polynomial of \( w_1, \ldots, w_m \), and a D-optimal allocation \( w_* \) that maximizes \( f(w) \) on \( S \) must exist.

Lemma 2.1 and Theorem 2.1 confirm the existence of the constrained D-optimal allocation. Their proofs, as well as proofs of all other lemmas and theorems, are relegated to Section S5 in the Supplementary Material.

For nonlinear models (Fedorov and Leonov, 2014), generalized linear models (Yang and Mandal, 2015), or multinomial logistic models (Bu et al., 2020), \( F \) depends on the unknown parameters \( \theta \). We need an assumed \( \theta \) to obtain a D-optimal allocation, known as a locally D-optimal allocation (Chernoff, 1953). When the investigators only have a rough idea about the parameters, with an assumed prior distribution on \( \Theta \), the parameter space, Bayesian D-optimality (Chaloner and Verdinelli, 1995) maximizes \( E(\log |F|) \) and provides a more robust allocation. To overcome its computational intensity, an alternative solution, the EW D-optimality (Atkinson et al., 2007; Yang et al., 2016), which maximizes \( \log |E(F)| \) or \( |E(F)| \), was recommended by Yang et al. (2016, 2017) and Bu et al. (2020) for various models. In this paper, we focus on locally D-optimality and EW D-optimality.
3 Constrained Lift-one Algorithm

For an unconstrained optimal design problem, many numerical algorithms have been proposed using directional derivatives (Wynn, 1970; Fedorov, 1972; Atkinson et al., 2014; Fedorov and Leonov, 2014). Among them, the lift-one algorithm (Yang et al., 2016; Yang and Mandal, 2015; Yang et al., 2017; Bu et al., 2020) breaks the problem into univariate optimizations, utilizes analytic solutions whenever possible, reduces unnecessary weights to exact zeros, and works the same well for both locally D-optimality and EW D-optimality. For readers’ reference, we provide the lift-one algorithm for general parametric models in Section S1 of the Supplementary Material.

Nevertheless, the original lift-one algorithm does not fit our needs for constrained optimal allocation. We provide a counterexample in Section 3.1, where the converged allocation by the lift-one algorithm is not D-optimal under constraints.

3.1 Counterexample for the lift-one algorithm

In this section, we provide an example such that the converged allocation of the lift-one algorithm is not D-optimal under constraints.

Example 3.1. Consider an experiment with the logistic regression model

\[ g(\mu_i) = \log(\mu_i / (1 - \mu_i)) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} \]

with \( \mu_i = E(Y_i \mid x_i) \) and \( x_i = (x_{i1}, x_{i2})^T \in \{(-1, -1), (-1, +1), (+1, -1)\} \). In this case, \( f(w) = w_1 w_2 w_3 \) up to a constant \( C > 0 \) (see Section 4 for more details).

When there is no constraint, \( w \in S_0 \) and \( f(w) = w_1 w_2 (1 - w_1 - w_2) \). The partial derivatives are \( \partial f / \partial w_1 = w_2 (1 - w_2 - 2w_1) \) and \( \partial f / \partial w_2 = w_1 (1 - w_1 - 2w_2) \). It can be verified that \( f(w) \) attains its global maximum at \( w_*^{(1)} = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})^T \in S_0 \), which is the (globally) D-optimal design without any constraint (see Figure 1 for a 2D display).

Suppose we consider a constrained D-optimal design problem with the collection of feasible allocations \( S = \{(w_1, w_2, w_3)^T \in S_0 \mid \frac{1}{3} w_1 - \frac{1}{3} w_2 - \frac{1}{3} w_3 \leq 0, w_1 \geq \frac{3}{11}\} \), which is closed and convex. Actually, it can be verified that \( S \) is a triangle with vertices \( w_* = (\frac{3}{11}, \frac{2}{11}, \frac{6}{11})^T, w_o = (\frac{3}{11}, \frac{6}{11}, 0)^T \) and \( w_a = (\frac{3}{7}, \frac{4}{7}, 0)^T \) (that is, the shaded region in Figure 1). We let the lift-one algorithm (see Algorithm 3 in the Supplementary Material) start with \( w_0 = (\frac{3}{11}, \frac{2}{11}, \frac{6}{11})^T \in S \) (that is, \( w_* \) in Figure 1). Following Step 3° of Algorithm 3 with the range of \( z \) adjusted according to \( S \) (see also Step 3° of Algorithm 1 in Section 3), \( f_1(z) = \frac{25}{27} z (1-z)^2 \) with \( z \in [r_{11}, r_{12}] = \{\frac{3}{11}\}, f_2(z) = \frac{2}{9} z (1-z)^2 \) with \( z \in [r_{21}, r_{22}] = \{\frac{3}{7}\}, \) and \( f_3(z) = \frac{6}{25} z (1-z)^2 \) with \( z \in [r_{31}, r_{32}] = \{\frac{6}{11}\} \). In other words, due to constraints, the lift-one algorithm stops and returns \( w_0 \) (or \( w_* \) in Figure 1) as the converged allocation. However, since the unconstrained solution \( w_*^{(1)} \) is still in \( S \), \( w_* \) is not D-optimal in \( S \). □

3.2 New algorithm for constrained D-optimal allocations

To find D-optimal allocations under constraints, we develop a new algorithm, called constrained lift-one algorithm, for finding D-optimal allocations in a closed and convex \( S \) for paid research studies under fairly general statistical models.
Algorithm 1. Constrained lift-one algorithm under a general setup

1° Start with an arbitrary allocation $\mathbf{w}_0 = (w_1, \ldots, w_m)^T \in S$ satisfying $f(\mathbf{w}_0) > 0$.

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

3° For $z \in [0, 1]$, let $\mathbf{w}_i(z) = \left(\frac{1-z}{1-w_1}w_1, \ldots, \frac{1-z}{1-w_i}w_{i-1}, z, \frac{1-z}{1-w_i}w_{i+1}, \ldots, \frac{1-z}{1-w_m}w_m\right)^T$ and $f_i(z) = f(\mathbf{w}_i(z))$. Determine $0 \leq r_{i1} \leq r_{i2} \leq 1$, such that, $\mathbf{w}_i(z) \in S$ if and only if $z \in [r_{i1}, r_{i2}]$.

4° Use an analytic solution or the quasi-Newton algorithm to find $z_*$ maximizing $f_i(z)$ with $z \in [r_{i1}, r_{i2}]$. Define $\mathbf{w}_i^{(i)} = \mathbf{w}_i(z_*)$. Note that $f(\mathbf{w}_i^{(i)}) = f_i(z_*)$.

5° If $f(\mathbf{w}_i^{(i)}) > f(\mathbf{w}_0)$, replace $\mathbf{w}_0$ with $\mathbf{w}_i^{(i)}$, and $f(\mathbf{w}_0)$ with $f(\mathbf{w}_i^{(i)})$.

6° Repeat 2° to 5° until convergence, that is, $f(\mathbf{w}_i^{(i)}) \leq f(\mathbf{w}_0)$ for each $i$. Denote $\mathbf{w}_* = (w_1^*, \ldots, w_m^*)^T$ as the converged allocation.

7° Calculate $f_i^*(w_i^*)$ for all $i$. If $f_i^*(w_i^*) \leq 0$ for all $i$, then go to 10°. Otherwise, go to 8°.

8° Find $\mathbf{w}_o = \arg\max_{\mathbf{w} \in S} g(\mathbf{w})$, where $g(\mathbf{w}) = \sum_{i=1}^{m} w_i (1-w_i^*) f_i^*(w_i^*)$ is a linear function of $\mathbf{w} = (w_1, \ldots, w_m)^T$. If $g(\mathbf{w}_o) \leq 0$, then go to 10°. Otherwise, go to 9°.

9° Use an analytic solution or the quasi-Newton algorithm to find $\alpha_*$ maximizing $h(\alpha) = f((1-\alpha)\mathbf{w}_* + \alpha \mathbf{w}_o)$ with $\alpha \in [0, 1]$. Let $\mathbf{w}_0 = (1-\alpha_*)\mathbf{w}_* + \alpha_* \mathbf{w}_o$ and go back to 2°.

10° Report $\mathbf{w}_*$ as the D-optimal allocation.

Compared with the original lift-one algorithm (see Algorithm 3 in the Supplementary Material), the steps 1° to 6° are essentially the same except for the intervals $[r_{i1}, r_{i2}]$ in
Step $3^\circ$ due to constraints. Our major contributions are the new steps $7^\circ \sim 9^\circ$. Since the lift-one algorithm utilizes the directional derivatives, its optimization directions are restricted to the directions between the current allocation and the vertices of the unconstrained set $S_0$. It works for unconstrained problems but not for constrained problem, since the optimal solutions may not be covered by these directions under constraints. The new steps $7^\circ \sim 9^\circ$ come into play when the D-optimal allocation is not covered by the lift-one directions. Step $7^\circ$ and $8^\circ$ check whether the current solution is D-optimal. If not, we need Step $9^\circ$ to find a new starting point and search better solutions via other directions. We will justify in Section 3.3 the D-optimality of the converged allocation reported by Algorithm 1. In sections 3.4 and 3.5, we will provide more technical details for steps $8^\circ$ and $9^\circ$.

Example 3.2. If $S = S_0$, then $[r_{i_1}, r_{i_2}]$ in Step $3^\circ$ of Algorithm 1 is $[0, 1]$ for each $i$. $\square$

Example 3.3. If $S = \{(w_1, \ldots, w_m)^T \in S_0 \mid nw_i \leq N_i, i = 1, \ldots, m\}$ as in Example 2.1, then $r_{i_1}$ and $r_{i_2}$ in Step $4^\circ$ of Algorithm 1 are

$$
\begin{align*}
&\{ r_{i_1} = \max \{(0) \cup \{1 - \min\{N_i/n\}(1 - w_i)/w_j \mid w_j > 0, j \neq i\} \} \\
&\{ r_{i_2} = \min\{1, N_i/n\} \}
\end{align*}
$$

It can be verified that if $w \in S$, then $0 \leq r_{i_1} \leq r_{i_2} \leq 1$. $\square$

Example 3.1 (continued) To check the conditions in Step $7^\circ$ of Algorithm 1, the derivative functions at $w_* = \left(\frac{3}{11}, \frac{2}{7}, \frac{6}{11}\right)^T$ are $f'_1(z) = \frac{3}{16}(1 - z)(1 - 3z)$, $f'_2(z) = \frac{3}{2}(1 - z)(1 - 3z)$, and $f'_3(z) = \frac{6}{25}(1-z)(1-3z)$. Then $f'_1(w'_1) = \frac{3}{121} > 0$ and $f'_2(w'_2) = \frac{10}{121} > 0$ violate the conditions in Step $7^\circ$, which implies that $w_*$ may not be D-optimal. We then go ahead to check the condition in Step $8^\circ$. In this case, $g(w) = \sum_{i=1}^m w_i(1 - w'_i)f'_i(w'_i) = \frac{24}{1331}w_1 + \frac{90}{1331}w_2 - \frac{42}{1331}w_3$. It can be verified that (see Theorem 3.4 in Section 3.4) $S = \{(\frac{3}{11}, \frac{2}{7}, \frac{6}{11}), 0\} \in S$ maximizes $g(w)$, $w \in S$. Actually, $S$, in this case, is the convex hull of its vertex set $\{w_*, w_o, w_a\}$. Note that $g(w_o) = \frac{72}{1331} > 0$ violates the condition in Step $8^\circ$. For Step $9^\circ$, we define $h(\alpha) = f((1 - \alpha)w_* + \alpha w_o) = \frac{36}{1331}(1 - \alpha)(1 + 3\alpha)$, then $h'(\alpha) = \frac{72}{1331}(1 - 3\alpha)$ and $\alpha_* = \arg\max_{\alpha \in [0, 1]} h(\alpha) = \frac{1}{3}$. Let $w^{(1)}_0 = (1 - \alpha_*)w_* + \alpha_* w_o = \left(\frac{3}{11}, \frac{4}{7}, \frac{4}{11}\right)^T$ and go back to Step $2^\circ$ of Algorithm 1. For $i = 1$, $f'_1(z) = \frac{3}{16}(1 - z)(1 - 3z)$, the algorithm returns $z_* = \frac{1}{3}$ and $w^{(1)}_i = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})^T$. Replace $w_0$ with $w^{(1)}_i = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})^T$, which is known to be D-optimal in $S_0$. It can be verified that $w_* = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})^T$ is a converged allocation in Step $6^\circ$ which also satisfies $f'_i(w'_i) \leq 0$ for each $i$. That is, $w^{(1)}_i$ will be reported by Algorithm 1. $\square$

Given an approximate allocation $w = (w_1, \ldots, w_m)^T \in S$, if all additional constraints for $S$ take the form of $\sum_{i=1}^m a_i w_i \leq c$ with $a_i \geq 0$ and $c > 0$ such as in Examples 2.1 and 2.2, we develop the following round-off algorithm to obtain an exact allocation $n = (n_1, \ldots, n_m)^T$ satisfying $n_i/n \in S$ and $\sum_{i=1}^m n_i = n$.

Algorithm 2. Constrained round-off algorithm for obtaining an exact allocation

$1^\circ$ First let $n_i = \lfloor nw_i \rfloor$, that is, the largest integer no more than $nw_i$, $i = 1, \ldots, m$, and $k = n - \sum_{i=1}^m n_i$. Denote $I = \{i \in \{1, \ldots, m\} \mid w_i > 0, (n_1, \ldots, n_{i-1}, n_i + 1, n_{i+1}, \ldots, n_m)/n \in S\}$.
2° While $k > 0$, do

2.1 For $i \in I$, calculate $d_i = f(n_1, \ldots, n_{i-1}, n_i + 1, n_{i+1}, \ldots, n_m)$.
2.2 Denote $i_* = \arg \max_{i \in I} d_i$.
2.3 Let $n_{i_*} \leftarrow n_{i_*} + 1$ and $k \leftarrow k - 1$.
2.4 If $(n_1, \ldots, n_{i_*-1}, n_{i_*} + 1, n_{i_*+1}, \ldots, n_m) / n \notin S$, then $I \leftarrow I \setminus \{i_*\}$.

3° Output $\mathbf{n} = (n_1, \ldots, n_m)^T$.

The allocation obtained by Algorithm 1 with $f(\mathbf{w}) = |\sum_{i=1}^m w_i \mathbf{F}_i|$ is known as a locally D-optimal allocation since it may require assumed values of $\theta$. With a specified prior distribution $h(\theta)$ on the parameter space $\Theta$, we may replace $f(\mathbf{w})$ with $f_{EW}(\mathbf{w}) = |\sum_{i=1}^m w_i E(\mathbf{F}_i)|$ and the obtained allocation by Algorithm 1 is called an EW D-optimal allocation (see Section 2).

### 3.3 D-optimality of Algorithm 1

In this section, we justify the D-optimality of the allocations found by Algorithm 1. Throughout this section, we assume that $S \subseteq S_0$ is closed and convex.

**Lemma 3.1.** 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 $|M_1| = |M_2| = 0$.

Lemma 3.1 is an extended version of, for example, Theorem 1.1.14 in Fedorov (1972). The next theorem provides necessary results relevant to Step 7° of Algorithm 1.

**Theorem 3.1.** Suppose $f(\mathbf{w}_0) > 0$ for $\mathbf{w}_0 = (w_1, \ldots, w_m)^T \in S$. Let $f_i(z) = f(\mathbf{w}_i(z))$ as defined in Algorithm 1. Then $\log f_i(z)$ is a concave function on $[r_{i1}, r_{i2}]$. Furthermore, suppose $z_*$ maximizes $f_i(z)$ with $z \in [r_{i1}, r_{i2}]$. Then (1) if $z_* = r_{i1} < r_{i2}$, then $f_i'(z_*) \leq 0$; (2) if $z_* = r_{i2} > r_{i1}$, then $f_i'(z_*) \geq 0$; and (3) if $z_*$ is in $(r_{i1}, r_{i2})$, then $f_i'(z_*) = 0$.

**Theorem 3.2.** Suppose $f(\mathbf{w}) > 0$ for some $\mathbf{w} \in S$. Let $\mathbf{w}_* = (w_1^*, \ldots, w_m^*)^T \in S$ be a converged allocation in Step 6° of Algorithm 1. If $w_i^* < r_{i2}$ for each $i$, then $\mathbf{w}_*$ must be D-optimal in $S$.

With the aid of Theorem 3.1, Theorem 3.2 and the following corollary justify the D-optimality of the converged allocation $\mathbf{w}_*$ if it qualifies the conditions in Step 7° of Algorithm 1.

**Corollary 3.1.** Suppose $\text{rank}(\mathbf{F}_i) < p$ for each $i$ and $f(\mathbf{w}) > 0$ for some $\mathbf{w} \in S$. Let $\mathbf{w}_* \in S$ be a converged allocation in Step 6° of Algorithm 1. (i) If $S = S_0$, then $\mathbf{w}_*$ must be D-optimal in $S_0$; (ii) if $f_i'(w_i^*) \leq 0$ for each $i$, then $\mathbf{w}_*$ must be D-optimal in $S$.

Corollary 3.1 (i) also implies that the converged allocation of the original lift-one algorithm (Algorithm 3 in the Supplementary Material) must be D-optimal in $S_0$.

The following theorem is the major one of this section, which justifies the D-optimality of the allocation found by Algorithm 1.

**Theorem 3.3.** Suppose $\text{rank}(\mathbf{F}_i) < p$ for each $i$ and $f(\mathbf{w}) > 0$ for some $\mathbf{w} \in S$. Let $\mathbf{w}_*$ be the reported allocation in Step 10° of Algorithm 1. Then $\mathbf{w}_*$ is D-optimal in $S$.  

8
3.4 Maximization of $g(w)$ in Step 8° of Algorithm 1

In this section, we provide the solutions for the maximization of $g(w) = \sum_{i=1}^{m} w_i (1 - w_i^*) f_i'(w_i^*), \ w = (w_1, \ldots, w_m)^T \in S$, where $S$ is a closed convex subset of $S_0$. Let $a_i = (1 - w_i^*) f_i'(w_i^*)$ and $a = (a_1, \ldots, a_m)^T$. Then $g(w) = a^T w$ is a linear function of $w \in S$.

For many applications, including all the examples considered in this paper, the convex subset $S$ is determined by several linear equations or constraints as follows:

$$\text{Max} \quad a^T w$$
$$\text{subject to} \quad Gw \preceq h, \ Aw = b$$

where $G \in \mathbb{R}^{r \times m}$, $h \in \mathbb{R}^r$, $A \in \mathbb{R}^{s \times m}$, $b \in \mathbb{R}^s$ are known matrices or vectors, and $\preceq$ is componentwise “≤”. It is known as a linear program (LP) problem (see, for example, Section 4.3 in Boyd and Vandenberghe (2004)) and can be efficiently solved by using, for example, R function `lpSolve`.

For general cases, $S$ is a closed convex subset of $S_0$. Since $S_0 \subset \mathbb{R}^m$ is bounded, then $S$ is bounded and thus compact. According to Theorem 5.6 in Lay (1982), $S$ is the convex hull of its profile $E$, which consists of all extreme points of $S$. Since $g(w)$ is a linear function on $S$, according to Theorem 5.7 in Lay (1982), there exists a $w_o \in E$ such that

$$w_o = \arg\max_{w \in E} g(w) = \arg\max_{w \in S} g(w)$$

In other words, we only need to search $w_o$ among the profile $E$ of $S$, which is only a subset of the boundary of $S$. Following the proof of Theorem 5.7 in Lay (1982), we obtain the following convenient results for special cases:

**Theorem 3.4.** If there exists a $V = \{w_1, \ldots, w_k\} \subset S$, such that, $S$ can be rewritten as $\{b_1 w_1 + \cdots + b_k w_k \mid b_1 \geq 0, \ldots, b_k \geq 0, \sum_{i=1}^{k} b_i = 1\}$, then $w_o = \arg\max_{w \in V} g(w)$ maximizes $g(w)$.

In other words, if $S$ is the convex hull of a finite set $V$ (such an $S$ is called a polytope or convex polytope in the literature; see, for example, Definition 2.24 in Lay (1982)), we only need to search $w_o$ among the finite set $V$. Note that the $V$, known as the vertex set, may not be unique and may not be the profile of $S$.

**Example 3.4.** If $S = S_0$, then $V = \{\bar{w}_1, \ldots, \bar{w}_m\}$ is a vertex set of $S$, where $\bar{w}_i = (0, \ldots, 0, 1, 0, \ldots, 0)^T \in \mathbb{R}^m$ whose $i$th coordinate is 1.

Given $a_i = (1 - w_i^*) f_i'(w_i^*)$, $i = 1, \ldots, m$, we call $r_1, \ldots, r_m$ the ranks of them, if $\{r_1, \ldots, r_m\} = \{1, \ldots, m\}$ and $a_{r_1} \geq a_{r_2} \geq \cdots \geq a_{r_m}$. For $S$ taking the form as in Example 2.1, we have an analytic solution for $w_o$:

**Theorem 3.5.** Suppose $S = \{w \in S_0 \mid w_i \leq c_i, i = 1, \ldots, m\}$ with $0 < c_i \leq 1$, $i = 1, \ldots, m$ and $\sum_{i=1}^{m} c_i \geq 1$. Then a $w_o = (w_1^o, \ldots, w_m^o)^T$ maximizing $g(w) = \sum_{i=1}^{m} a_i w_i$ can be obtained as follows: (i) if $\sum_{i=1}^{m} c_i = 1$, $w_o = (c_1, \ldots, c_m)^T$; (ii) if $\sum_{i=1}^{m} c_i > 1$, then $w_i^o = c_i$ if $i \in \{r_1, \ldots, r_k\}$; 1-$\sum_{i=1}^{k} c_{r_i}$ if $i = r_{k+1}$; and 0 otherwise, where $r_1, \ldots, r_m$ are the ranks of $a_1, \ldots, a_m$ and $k \in \{1, \ldots, m - 1\}$ satisfying $\sum_{i=1}^{k} c_{r_i} \leq 1 < \sum_{i=1}^{k+1} c_{r_i}$.

**Example 3.1 (continued)** In this case, $S = \{(w_1, w_2, w_3) \in S_0 \mid \frac{4}{9} w_1 - \frac{1}{3} w_2 - \frac{1}{9} w_3 \leq 0, w_1 \geq \frac{2}{3}\}$ and its vertex set $V = \{w_*, w_o, w_o\}$ (see Figure 1). □
3.5 Maximization of $h(\alpha)$ in Step 9° of Algorithm 1

Suppose $w_o = (w_1, \ldots, w_m)^T \in S$ is a converged allocation in Step 6° of Algorithm 1, and $w_o = (w_1, \ldots, w_m)^T \in S$ is obtained in Step 8° with $g(w_o) > 0$. We provide the following results to find $\alpha_*$ maximizing $h(\alpha) = f((1 - \alpha)w_* + \alpha w_o)$ in Step 9°.

**Lemma 3.2.** The function $h(\alpha)$ in Step 9° of Algorithm 1 can be written as

$$h(\alpha) = c_0 + c_1 \alpha + \cdots + c_{p-1} \alpha^{p-1} + c_p \alpha^p$$

where $c_0 = f(w_*)$, $(c_1, \ldots, c_p)^T = B_p^{-1}(h(\frac{1}{p}) - c_0, \ldots, h(\frac{p-1}{p}) - c_0, h(1) - c_0)^T$, and $B_p$ is a $p \times p$ matrix with its $(s, t)$th entry $(\frac{s}{p})^t$.

According to Lemma 3.2, we may determine the coefficients of $h(\alpha)$ by calculating $h(\frac{1}{p}), \ldots, h(\frac{p-1}{p})$ (note that $h(1) = f(w_o)$), and then calculate $h'(\alpha)$ by

$$h'(\alpha) = c_1 + 2c_2 \alpha + \cdots + (p - 1)c_{p-1} \alpha^{p-2} + pc_p \alpha^{p-1}$$

**Theorem 3.6.** Suppose $f(w_*) > 0$, $g(w_o) = \sum_{i=1}^m w_i^o (1 - w_i^*) f_i(w_i^*) > 0$, $h(\alpha) = f((1 - \alpha)w_* + \alpha w_o)$, and $\alpha_* = \arg\max_{\alpha \in [0,1]} h(\alpha)$ as defined in Step 9° of Algorithm 1. Then (i) $h(\alpha) > 0$ for all $\alpha \in [0,1]$; (ii) $h'(0) > 0$; (iii) if $h(1) > 0$ and $h'(1) \geq 0$, then $\alpha_* = 1$; (iv) if $h(1) > 0$ and $h'(1) < 0$, or $h(1) = 0$, then there exists a unique $\alpha_0 \in (0,1)$ such that $h'(\alpha_0) = 0$, which implies $\alpha_* = \alpha_0$.

Based on Theorem 3.6 and Equation (4), if $h'(1) < 0$, one may use, for example, the R function `uniroot`, to find $\alpha_* \in (0,1)$ numerically. To avoid numerical errors, we need to double check $\alpha_* \neq 1$ when $f(w_o) < f(w_*)$.

4 D-optimal Samplers for Generalized Linear Models

In this section, we utilize locally and EW D-optimal samplers for univariate responses, such as in Example 2.1. Recall that we assign $n_i$ participants to the $i$th category. We let $Y_{ij}$ stand for the univariate response of the $j$th participant of the $i$th category. Generalized linear models (McCullagh and Nelder, 1989; Dobson and Barnett, 2018)

$$E(Y_{ij} \mid x_i) = \mu_i \text{ and } g(\mu_i) = \eta_i = h(x_i)^T \theta$$

have been widely used, where $i = 1, \ldots, m$, $j = 1, \ldots, n_i$, $g$ is a given function known as the link function, $h(x_i) = (h_1(x_i), \ldots, h_p(x_i))^T$ are $p$ predictors specified by the model, and $\theta = (\theta_1, \ldots, \theta_p)^T$ are the regression coefficients. Commonly used generalized linear models (GLM) cover normal response (that is, linear models), binary response (Bernoulli, such as Example 2.1), count response (Poisson), and real positive response (Gamma, Inverse Gaussian), etc (see Table 5 in the Supplementary Material for a list).

Assuming that $Y_{ij}$’s are independent, the Fisher information matrix (see, for example, Yang and Mandal (2015))

$$F(w) = n \sum_{i=1}^m w_iF_i = n \sum_{i=1}^m w_i\nu_i h(x_i)h(x_i)^T = nX^TWX$$
where \( \mathbf{w} = (w_1, \ldots, w_m)^T \), \( w_i = n_i/n \), \( \mathbf{X} = (h(x_1), \ldots, h(x_m))^T \) is an \( m \times p \) matrix, \( \mathbf{W} = \text{diag}\{w_1\nu_1, \ldots, w_m\nu_m\} \), and \( \nu_i = \nu(\eta_i) = (\partial\mu_i/\partial\eta_i)^2/\text{Var}(Y_{ij}), \ i = 1, \ldots, m \). We provide examples of \( \nu(\eta_i) \) for commonly used GLMs in Table 5 of the Supplementary Material. For GLMs, \( f(\mathbf{w}) = |\mathbf{X}^T\mathbf{W}\mathbf{X}| \) and \( f_{EW}(\mathbf{w}) = |\mathbf{X}^TE(\mathbf{W})\mathbf{X}| \) (see Section 2).

According to Lemma 4.1 in Yang and Mandal (2015), \( f_i(z) = az(1-z)^{p-1} + b(1-z)^p \), where \( b = f_i(0), a = [f(\mathbf{w}) - b(1-w_i)^p]/[w_i(1-w_i)^{p-1}] \) if \( w_i > 0 \); and \( b = f(\mathbf{w}), a = f_i(1/2)2^p - b \) otherwise. In both cases, \( a \geq 0, b \geq 0 \), and \( a + b > 0 \). To implement Step 7 of Algorithm 1, we need the first-order derivative of \( f_i(z) \)

\[
f_i'(z) = [a - bp + (b - a)pz](1-z)^{p-2}
\]  

(6)

Here \( m \geq p \geq 2 \). Similar to Lemma 4.2 in Yang and Mandal (2015), we provide the following lemma for maximizing \( f_i(z) \) with constraints:

**Lemma 4.1.** Denote \( l(x) = ax(1-x)^{p-1} + b(1-x)^p \) with \( a \geq 0, b \geq 0 \) and \( a + b > 0 \). Let \( \delta = (a-bp)/[(a-b)p] \) when \( a \neq b \). Then

\[
x_\ast = \begin{cases} 
\delta, & \text{if } a > bp \text{ and } r_1 \leq \delta \leq r_2; \\
2, & \text{if } a > bp \text{ and } \delta > r_2; \\
1, & \text{otherwise}.
\end{cases}
\]

(7)

maximizes \( l(x) \) with constraints \( 0 \leq r_1 \leq x \leq r_2 \leq 1 \).

**Example 2.1 (continued)** In this case, \( N = 500 \) eligible volunteers are available for \( m = 6 \) categories with frequencies \( (N_1, N_2, \ldots, N_6) = (50, 40, 10, 200, 150, 50) \). For illustration purpose, we consider a logistic regression model (GLM with Bernoulli(\( \mu_i \)) and logit link):

\[
\logit(P(Y_{ij} = 1 \mid x_{i1}, x_{i2})) = \beta_0 + \beta_1 x_{i1} + \beta_{21}1_{(x_{i2}=1)} + \beta_{22}1_{(x_{i2}=2)}
\]

(8)

where \( i = 1, \ldots, 6, \ j = 1, \ldots, n_i \), \( \logit(\mu) = \log(\mu/(1-\mu)) \). Model (8) is known as a main-effects model where both gender and age group are treated as factors.

To sample \( n = 200 \) from \( m = 6 \) categories or strata, the proportionally stratified allocation is \( \mathbf{w}_p = (0.10, 0.08, 0.02, 0.40, 0.30, 0.10)^T \) or \( \mathbf{n}_p = (20, 16, 4, 80, 60, 20)^T \), while the uniformly stratified allocation is \( \mathbf{w}_u = (0.19, 0.19, 0.05, 0.19, 0.19, 0.19)^T \) or \( \mathbf{n}_u = (38, 38, 10, 38, 38, 38)^T \). By implementing Algorithm 1 and Algorithm 2 in \( \mathbb{R} \) with assumed \( \mathbf{\beta} = (\beta_0, \beta_1, \beta_{21}, \beta_{22})^T = (0, 3, 3, 3)^T \), we obtain the (locally) D-optimal allocation \( \mathbf{w}_o = (0.25, 0.20, 0.05, 0.50, 0, 0)^T \) or \( \mathbf{n}_o = (50, 40, 10, 100, 0, 0)^T \). Compared with \( \mathbf{w}_o \), the relative efficiency of \( \mathbf{w}_p \) is \( (|\mathbf{F}(\mathbf{w}_p)|/|\mathbf{F}(\mathbf{w}_o)|)^{1/p} = 53.93\% \) with the number of parameters \( p = 4 \), and the relative efficiency of \( \mathbf{w}_u \) is \( (|\mathbf{F}(\mathbf{w}_u)|/|\mathbf{F}(\mathbf{w}_o)|)^{1/p} = 78.99\% \). Both are much less efficient.

We also look into the robustness of our optimal allocations to model misspecification. Assuming that the true link of our simulation study is probit link, complementary log-log link, or log-log link (see Table 5 in the Supplementary Material), we compare the efficiencies of our results to the true D-optimal allocations. Notice that the log-log link shares the same \( \mathbf{W} \) matrix as the complementary log-log link. Since \( \mathbf{\beta} = (0, 3, 3, 3) \) satisfies the conditions of Theorem 3.2 in Yang and Mandal (2015), the D-optimal designs are saturated and different links lead to the same D-optimal allocation. Therefore,
our D-optimal allocation remains 100% relative efficiencies with respect to link misspecifications. In Section S3 of the Supplementary Material, we provide an example with different assumed parameter values, which still have 99% relative efficiencies with link misspecifications.

To compare the accuracy of the estimated regression coefficients based on different samplers, we use the root mean squared error (RMSE, \( \sum_{i \in I} (\hat{\beta}_i - \beta_i)^2/|I| \)) given an index set \( I \). For illustration purposes, we assume that the true parameters are \((\beta_0, \beta_1, \beta_21, \beta_22) = (0, 3, 3, 3)\) and run 100 simulations based on Model (8). In each simulation, we simulate \( N = 500 \) observations and use SRSWOR, proportionally stratified sampler, uniformly stratified sampler, and D-optimal sampler, respectively, to sample \( n = 200 \) observations out of \( N = 500 \). We then fit Model (8) using the \( n = 200 \) observations to get the estimated parameters \((\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_21, \hat{\beta}_22)\). The average and standard deviation (sd) of RMSEs across 100 simulations are listed in Table 1. According to the RMSE with index set \( I = \{1, 21, 22\} \) (that is, the column “all except \( \beta_0 \)” in Table 1), SRSWOR is least accurate, proportional stratified sampler is a little better, uniformly stratified sampler is much better, and locally D-optimal sampler is the best, which is much closer to the full data estimates. For readers’ reference, we also list the RMSEs for individual \( \beta_i \)'s.

If we know something but not exactly \( \theta = (0, 3, 3, 3)^T \), we recommend EW D-optimal samplers instead. For illustration purpose, we consider three types of prior distributions: (i) uniform prior \( \theta \sim \text{Unif}(-2, 2) \times \text{Unif}(-1, 5) \times \text{Unif}(-1, 5) \times \text{Unif}(-1, 5) \); (ii) normal prior \( h(\theta) = \phi \left( \frac{\beta_0}{0.5} \right) \times \phi \left( \frac{\beta_1-2}{0.5} \right) \times \phi \left( \frac{\beta_21-2}{0.5} \right) \times \phi \left( \frac{\beta_22-2}{0.5} \right) \); (iii) Gamma prior \( \theta \sim N(0, 1) \times \text{Gamma}(1, 2) \times \text{Gamma}(1, 2) \times \text{Gamma}(1, 2) \). The relevant expectations \( E[\nu(h^T(x_i)\theta)] \) can be numerically computed using, for example, R function \texttt{hcubature} in package \texttt{cubature}. Compared with the locally D-optimal allocation \( w_o \), which samples only from four categories, EW allocations are not so extreme, such as \( w_{oEW} = (0.240, 0.200, 0.050, 0.211, 0.101, 0.198) \) with uniform prior, \( w_{nEW} = (0.200, 0.200, 0.050, 0.214, 0.096, 0.200) \) with normal prior, and \( w_{gEW} = (0.240, 0.200, 0.050, 0.214, 0.096, 0.200) \) with gamma prior. Compared with \( w_o \), their relative efficiencies are 85.90%, 94.96%, and 86.32%, respectively, which are still much better than SRSWOR, proportionally stratified and uniformly stratified samplers. In terms of RMSE (see Table 1), the conclusions are consistent.

Table 1: Average (sd) of RMSE over 100 Simulations under Model (8)

| Sampler                | \( \hat{\beta}_0 \) (sd) | all except \( \hat{\beta}_0 \) (sd) | \( \hat{\beta}_1 \) (sd) | \( \hat{\beta}_21 \) (sd) | \( \hat{\beta}_22 \) (sd) |
|------------------------|---------------------------|-----------------------------------|---------------------------|---------------------------|---------------------------|
| Full Data              | 0.195(0.145)              | 6.317(4.070)                      | 0.363(0.289)              | 2.751(5.468)              | 9.098(7.018)              |
| SRSWOR                 | 0.314(0.216)              | 9.984(3.226)                      | 0.917(2.543)              | 8.098(7.885)              | 12.976(5.245)             |
| Proportionally Stratified | 0.412(0.304)            | 9.496(3.682)                      | 1.016(2.545)              | 7.311(7.942)              | 12.469(5.682)             |
| Uniformly Stratified   | 0.235(0.193)              | 7.967(4.659)                      | 3.855(6.673)              | 3.353(6.254)              | 9.657(7.297)              |
| Locally D-opt          | 0.202(0.150)              | 7.103(4.098)                      | 0.485(0.438)              | 3.890(6.507)              | 9.883(6.821)              |
| Unif EW D-opt          | 0.201(0.145)              | 7.556(4.653)                      | 1.538(3.942)              | 3.920(6.561)              | 9.273(7.151)              |
| Normal EW D-opt        | 0.202(0.147)              | 7.252(4.407)                      | 1.347(3.664)              | 3.982(6.687)              | 9.302(7.150)              |
| Gamma EW D-opt         | 0.205(0.153)              | 7.718(4.476)                      | 1.535(4.008)              | 3.955(6.652)              | 9.585(7.080)              |

Known as the uniform allocation, \( w = (1/m, \ldots, 1/m)^T \) has a special role in optimal
design theory, which is recommended for linear models or as a robust design (see, for example, Yang et al. (2012)). In this paper, we introduce constrained uniform allocations such as \( w_u \) in Example 2.1. They are D-optimal for saturated cases (that is, \( m = p \)).

**Lemma 4.2.** Suppose \( w_\ast = (w_1\ast, \ldots, w_m\ast)^T \) maximizes \( f(w) = \prod_{i=1}^m w_i \) under the constraints \( 0 \leq w_i \leq c_i, \ i = 1, \ldots, m \) and \( \sum_{i=1}^m w_i = 1 \), where \( 0 < c_i \leq 1, \ i = 1, \ldots, m \) and \( \sum_{i=1}^m c_i \geq 1 \). Then (i) if \( \min_{1 \leq i \leq m} c_i \geq 1/m \), then \( w_\ast = (1/m, \ldots, 1/m)^T \); (ii) if \( 0 \leq \min_{1 \leq i \leq m} c_i < 1/m \) and \( \sum_{i=1}^m c_i > 1 \), then there exists \( 1 \leq k \leq m-1 \) and \( c(k) \leq u < c(k+1) \), such that, \( w_i \ast = c_i \) if \( c_i \leq u \), and \( w_i \ast = u \) if \( c_i > u \), where \( 0 < c(1) \leq c(2) \leq \cdots \leq c(m) \leq 1 \) are order statistics of \( c_1, \ldots, c_m \); (iii) if \( \sum_{i=1}^m c_i = 1 \), then \( w_i \ast = c_i, \ i = 1, \ldots, m \).

We call the \( w_\ast \) described in Lemma 4.2 a **constrained uniform allocation** and the corresponding sampler a (constrained) **uniformly stratified sampler**.

**Theorem 4.1.** For GLM (5) with \( m = p \), if \( S = \{ w \in S_0 \mid w_i \leq c_i, i = 1, \ldots, m \} \) with \( 0 < c_i \leq 1, \ i = 1, \ldots, m \) and \( \sum_{i=1}^m c_i \geq 1 \), then the constrained uniform allocation described in Lemma 4.2 is both D-optimal and EW D-optimal.

**Example 4.1.** If we consider another logistic regression model

\[
\logit(P(Y_{ij} = 1 \mid x_{i1}, x_{i2})) = \beta_0 + \beta_1 x_{i1} + \beta_2 (x_{i1} = 1) + \beta_3 (x_{i2} = 1) + \beta_4 (x_{i2} = 2)
\]

for Example 2.1, which adds two order-2 interactions to Model (8). Then \( m = p = 6 \). According to Theorem 4.1, the constrained uniform allocation \( w_u = (0.19, 0.19, 0.05, 0.19, 0.19, 0.05)^T \) is both D-optimal and EW D-optimal. In this case, the uniformly stratified sampler is same as the D-optimal and EW D-optimal samplers.

To compare the SRSWOR, proportionally stratified, uniformly stratified/locally D-optimal/EW D-optimal samplers, for illustration purposes, we assume that the true parameters are \( (\beta_0, \beta_1, \beta_2, 0.9, 0.2) = (0, -0.1, -0.5, -2, -0.5, -1) \). We run 100 simulations using Model (9). In this scenario, to sample \( n = 200 \) from \( m = 6 \) categories, the proportionally stratified allocation \( w_p \) and the uniformly stratified allocation \( w_u \) are the same as in Example 2.1. In this case, the D-optimal allocation \( w_\ast = w_u \). The relative efficiency of \( w_p \) and \( w_u \) compared with \( w_\ast \) are 73.30% and 100%, respectively. In terms of robustness to model misspecifications, the relative efficiencies with true links as probit, log-log and complementary log-log are again 100% due to Theorem 4.1. The average and standard deviation of the 100 RMSEs are reported in Table 2. Again, the D-optimal sampler (same as the uniformly stratified sampler in this scenario) significantly reduces the RMSEs based on SRSWOR or proportionally stratified sampler.

### Table 2: Average (sd) of RMSE over 100 Simulations under Model (9)

| Sampler                      | \( \beta_0 \)     | all except \( \beta_0 \) | \( \beta_1 \)     | \( \beta_2 \)     | \( \beta_3 \)     | \( \beta_4 \)     | \( \beta_5 \)     | \( \beta_6 \)     |
|------------------------------|-------------------|---------------------------|-------------------|-------------------|-------------------|-------------------|-------------------|-------------------|
| Full Data                    | 0.240(0.200)      | 7.753(3.125)              | 0.250(0.230)      | 0.350(0.263)      | 1.622(0.406)      | 0.405(0.319)      | 5.004(3.434)      |                   |
| SRSWOR                       | 0.340(0.268)      | 6.230(3.348)              | 0.386(0.290)      | 0.552(0.398)      | 0.905(0.826)      | 0.613(0.508)      | 7.184(6.845)      |                   |
| Proportionally Stratified    | 0.379(0.316)      | 6.347(3.267)              | 0.459(0.369)      | 0.593(0.512)      | 0.406(0.877)      | 0.742(0.568)      | 6.757(6.904)      |                   |
| Uniformly/D-opt/EW D-opt     | 0.267(0.203)      | 4.186(3.944)              | 0.425(0.304)      | 0.367(0.272)      | 1.497(0.936)      | 0.602(0.497)      | 5.435(6.887)      |                   |
5 D-optimal Samplers for Multinomial Logit Models

In this section, we utilize D-optimal samplers for categorical responses as in Example 2.2. More specifically, for the $i$th experimental setting $x_i = (x_{i1}, \ldots, x_{id})^T$, $n_i$ categorical responses are collected i.i.d. from a discrete distribution with $J \geq 2$ categories, $i = 1, \ldots, m$. The summary statistics follow a multinomial response $Y_i = (Y_{i1}, \ldots, Y_{ij})^T \sim \text{Multinomial}(n_i; \pi_{i1}, \ldots, \pi_{iJ})$, where $Y_{ij}$ is the number of responses of the $j$th category, $\pi_{ij}$ is the probability that the response falls into the $j$th category at $x_i$. Assuming $\pi_{ij} > 0$ for all $i = 1, \ldots, m$ and $j = 1, \ldots, J$, multinomial logit models have been widely used in the literature (see Bu et al. (2020) and references therein), including commonly used baseline-category, cumulative, adjacent-categories, and continuation-ratio logit models.

Example 2.2 (continued) In this case, the response has $J = 5$ categories, and there are $m = 8$ distinct experimental settings determined by $d = 2$ factors, severity ($x_{i1} \in \{0, 1\}$) and dose ($x_{i2} \in \{1, 2, 3, 4\}$). For illustration purposes, we first fit the original data using the four different multinomial logit models with main-effects, each with proportional odds (po) or nonproportional odds (npo) assumptions (Bu et al., 2020). According to the Akaike information criterion (AIC), we choose the cumulative logit model with npo for this study:

$$
\log \left( \frac{\pi_{i1} \cdots \pi_{ij}}{\pi_{i,j+1} \cdots \pi_{i5}} \right) = \beta_{j1} + \beta_{j2}x_{i1} + \beta_{j3}x_{i2}
$$

with $i = 1, \ldots, 8$ and $j = 1, 2, 3, 4$. The fitted parameters $\hat{\theta} = (\hat{\beta}_{11}, \hat{\beta}_{21}, \hat{\beta}_{31}, \hat{\beta}_{41}, \hat{\beta}_{12}, \hat{\beta}_{22}, \hat{\beta}_{42}, \hat{\beta}_{13}, \hat{\beta}_{23}, \hat{\beta}_{33}, \hat{\beta}_{43})^T = (-4.047, -2.225, -0.302, 1.386, 4.214, 3.519, 2.420, 1.284, -0.131, -0.376, -0.237, -0.120)^T$ is used for finding the locally D-optimal allocation $\mathbf{w}_o$ and $\mathbf{n}_o$ for choosing $n = 600$ participants. Since we do not have true parameter values for real data, in order to design EW D-optimal sampler, following Example 5.2 in Bu et al. (2020), we extract $B = 1,000$ bootstrapped samples from the original data and fit the cumulative npo model with bootstrapped samples to obtain randomized parameter vectors $\hat{\theta}_{(1)}, \ldots, \hat{\theta}_{(B)}$ serving as an empirical distribution of $\theta$. Among the fitted parameters by SAS PROC LOGISTIC command, 956 parameter vectors are feasible, that is, in the parameter space $\Theta = \{\theta \in \mathbb{R}^{12} | \beta_{j1} + \beta_{j2}x_{i1} + \beta_{j3}x_{i2} < \beta_{j+1,1} + \beta_{j+1,2}x_{i1} + \beta_{j+1,3}x_{i2}, j = 1, 2, 3; i = 1, \ldots, 8\}$ of cumulative logit model (see Section 5.1 in Bu et al. (2020)). We denote them by $\theta_i$, $i = 1, \ldots, 956$. Then we replace $\mathbf{F}_i$ with $\hat{E}(\mathbf{F}_i) = \sum_{i=1}^{956} \mathbf{F}_i(\theta_i)/956$ to obtain the EW D-optimal allocation $\mathbf{w}_{\text{EW}}$ and $\mathbf{n}_{\text{EW}}$, which maximizes $| \sum_{i=1}^{8} w_i \hat{E}(\mathbf{F}_i) |$. The corresponding allocations are listed in Table 3. In Table 4, we list the quantiles of relative efficiencies of SRSWOR (realized allocations after sampling), proportionally stratified, uniformly stratified, and EW D-optimal allocations with respect to the locally D-optimal allocations based on $\hat{\theta}_1, \ldots, \hat{\theta}_{956}$, respectively. From Table 4, we conclude that in this case, the EW D-optimal sampler is highly efficient compared with the locally D-optimal sampler, and both of them are much more efficient than SRSWOR, proportionally or uniformly stratified sampler.

According to Table 4, the two additional constraints in Example 2.2, $n(w_1 + w_2 + w_3 + w_4) \leq 392$ and $n(w_5 + w_6 + w_7 + w_8) \leq 410$, are not attained for locally D-optimal and EW D-optimal allocations. In other words, the constrained D-optimal allocations are the same as unconstrained ones in this case. In Example S4.1 of the Supplementary
Material, we provide another example of the sampling problems with the trauma clinical study where the constraints make a difference.

Table 3: Allocations (Proportions) for Stratified Samplers in Example 2.2

| Severity | Dose | 1   | 2   | 3   | 4   | 1   | 2   | 3   | 4   |
|----------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| Proportional | 78   | 70  | 75  | 72  | 79  | 72  | 80  | 74  |
|           | (0.130) | (0.117) | (0.125) | (0.120) | (0.132) | (0.120) | (0.133) | (0.123) |
| Uniform | 75   | 75  | 75  | 75  | 75  | 75  | 75  | 75  |
|           | (0.125) | (0.125) | (0.125) | (0.125) | (0.125) | (0.125) | (0.125) | (0.125) |
| Locally D-opt ($\theta$) | 155  | 0   | 0   | 100 | 168 | 0   | 0   | 177 |
|           | (0.258) | (0) | (0) | (0.167) | (0.280) | (0) | (0) | (0.295) |
| EW D-opt | 147  | 0   | 0   | 109 | 168 | 0   | 0   | 176 |
|           | (0.245) | (0) | (0) | (0.182) | (0.280) | (0) | (0) | (0.293) |

Table 4: Quantiles of Relative Efficiencies in Example 2.2

| Sampler | Minimum | 1st Quartile | Median | 3rd Quartile | Maximum |
|---------|---------|--------------|--------|--------------|---------|
| SRSWOR  | 76.23%  | 80.16%       | 80.65% | 81.15%       | 84.11%  |
| Proportional | 77.32%  | 80.33%       | 80.66% | 80.97%       | 83.39%  |
| Uniform | 77.23%  | 80.05%       | 80.40% | 80.71%       | 83.13%  |
| EW D-opt | 98.91%  | 99.80%       | 99.90% | 99.96%       | 100%    |

6 Conclusion

To sample $n$ subjects out of $N > n$ candidates for paid research studies or clinical trials, if the goal is to estimate the treatment effects or regression coefficients as accurately as possible, we do not recommend the simple random sampler or (proportionally) stratified sampler which are commonly used in sampling practice. Typically we have some covariates, such as gender and age, collected with candidates and known to have some influence on treatment effects. If we do not have any idea about the regression coefficients associated with the covariates, we recommend (constrained) uniformly stratified sampler (see Lemma 4.2); if we have some information about the regression coefficients, such as signs or ranges, we recommend EW D-optimal sampler; if we have a good idea about the regression coefficients such as estimates from a prior study, we recommend (locally) D-optimal sampler. We call these recommended samplers, Designer’s choices, since their constructions and justifications are based on optimal design theory. Our simulation studies show that the recommended samplers can be much more efficient than classical samplers for paid research studies or clinical trials.
Supplementary Materials

S.1 General lift-one algorithm (without constraints): The lift-one algorithm for general parametric models without constraints; S.2 Commonly used GLM models: A table that lists commonly used GLM models, the corresponding link functions and \( \nu \) functions; S.3 Another example of robustness under GLM models: An example that shows the robustness of our method for model misspecification with GLMs, where the assumed parameter values avoid the special cases similar to Theorem 3.2 in Yang and Mandal (2015); S.4 Another example of trauma clinical study: An example that the D-optimal allocations attain one of the constraints; S.5 Proofs: Proofs for lemmas and theorems in this paper.

Acknowledgements

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Yang, J., L. Tong, and A. Mandal (2017). D-optimal designs with ordered categorical data. *Statistica Sinica* 27, 1879–1902.

Zocchi, S. and A. Atkinson (1999). Optimum experimental designs for multinomial logistic models. *Biometrics* 55, 437–444.
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 \( w_0 = (w_1, \ldots, w_m)^T \in S_0 \) satisfying \( f(w_0) > 0 \).

2° Set up a random order of \( i \) going through \( \{1, 2, \ldots, m\} \). For each \( i \), do steps 3° ~ 5°.

3° Denote

\[
w_i(z) = \left( \frac{1-z}{1-w_i}, \frac{1-z}{1-w_i} w_{i-1}, z, \frac{1-z}{1-w_i} w_{i+1}, \ldots, \frac{1-z}{1-w_i} w_m \right)^T
\]

and \( f_i(z) = f(w_i(z)), z \in [0, 1] \).

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

5° If \( f(w^{(i)}_\star) > f(w_0) \), replace \( w_0 \) with \( w^{(i)}_\star \), and \( f(w_0) \) with \( f(w^{(i)}_\star) \).

6° Repeat 2° ~ 5° until convergence, that is, \( f(w^{(i)}_\star) \leq f(w_0) \) for each \( i \).

7° Report \( w_0 \) as the D-optimal allocation.
S2 Commonly used GLM models

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

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

S3 Another example of robustness under GLM models

Example S3.1. To further test the robustness to model misspecifications in Example 2.1 with Model (8), we set the true parameters as $\beta = (\beta_0, \beta_1, \beta_{21}, \beta_{22})^T = (0, 0.1, 0.5, 2)^T$. In this case, we have different D-optimal allocations for logit, probit, log-log, and complementary log-log links. Actually, with logit link, we obtain $w_{\text{logit}} = (0.189, 0.184, 0.050, 0.189, 0.181, 0.207)^T$. Compared with the true D-optimal allocation with probit link $w_{\text{probit}} = (0.193, 0.185, 0.050, 0.193, 0.181, 0.198)^T$, the relative efficiency of $w_{\text{logit}}$ is 99.98%. Since the $W$ matrix is the same for log-log and complementary log-log links, the corresponding D-optimal allocations are both $w_{\text{log}} = (0.189, 0.198, 0.050, 0.193, 0.198, 0.172)^T$. The relative efficiency of $w_{\text{logit}}$ with respect to $w_{\text{log}}$ is 99.68%. In other words, our D-optimal allocations are very robust with respect to link function misspecifications.

S4 Another example of trauma clinical study

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

Example S4.1. For the trauma clinical study described in Example 2.2, for illustration purpose, 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 2.2, which are listed in Table 6.
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 7, 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 6: Allocations (Proportions) for Stratified Samplers in Example S4.1

| Severity | Dose | Mild | Severe |
|----------|------|------|--------|
|          |      | 1    | 2      | 3    | 4    | 1    | 2    | 3    | 4    |
| Proportional |      | 116  | 105    | 115  | 108  | 41   | 37   | 40   | 38   |
| Uniform   |      | 98   | 98     | 97   | 97   | 55   | 50   | 54   | 51   |
| Locally D-opt (\( \theta \)) |      | 234  | 4      | 3    | 149  | 126  | 0    | 3    | 81   |
| EW D-opt  |      | 253  | 0      | 0    | 137  | 77   | 8    | 0    | 125  |

### Table 7: Quantiles of Relative Efficiencies in Example S4.1

| 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\%  |

### S5 Proofs

**Proof of Lemma 2.1:** Actually, if \( w_i = 1 \) for some \( i \), then \( w_j = 0 \) for all \( j \neq i \) and \( f(w) = \left| \sum_{j=1}^{m} w_j F_j \right| = |F_i| = 0 \), which leads to a contradiction. □

**Proof of Theorem 2.1:** Let \( F_i = (a_{ist})_{s,t=1,...,p} \), \( i = 1, \ldots, m \). Then \( \sum_{i=1}^{m} w_i F_i = (\sum_{i=1}^{m} a_{ist} w_i)_{s,t=1,...,p} \). According to the definition of matrix determinant (see, for example, Section 4.4.1 in Seber (2008)),

\[
f(w) = \left| \sum_{i=1}^{m} w_i F_i \right| = \sum_{\pi} \text{sgn}(\pi) \cdot \prod_{s=1}^{p} \left( \sum_{i=1}^{m} a_{is} \pi(s) w_i \right)
\]
is a homogeneous polynomial of \( w_1, \ldots, w_m \), where \( \pi \) goes through all permutations of \( \{1, \ldots, p\} \), and \( \text{sgn}(\pi) = -1 \) or 1 depending on whether \( \pi \) is odd or even. Since \( f(w) > 0 \) for some \( w \in S \), then \( f(w) \) is of order-\( p \), not a zero function.

Since \( f(w) = |\sum_{i=1}^{m} w_i F_i| \) 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 \( w_\ast \in S \) such that \( f(w) \) attains its maximum at \( w_\ast \).

**Proof of Lemma 3.1:** 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.

**Proof of Theorem 3.1:** According to the constrained lift-one algorithm, \( w_0 = (w_1, \ldots, w_m)^T \in S \), \( f(w_0) > 0 \), and \( w_i(z) \in S \) 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 \( w_i(\alpha z_1 + (1 - \alpha)z_2) = \alpha w_i(z_1) + (1 - \alpha)w_i(z_2) \). Denote \( w_i(z_1) = (w_{i1}, \ldots, w_{i1})^T \in S \) and \( w_i(z_2) = (w_{i2}, \ldots, w_{i2})^T \in S \). According to Lemma 3.1,

\[
\log f_i(\alpha z_1 + (1 - \alpha)z_2) = \log f(\alpha w_i(z_1) + (1 - \alpha)w_i(z_2)) \\
= \log \left| \sum_{j=1}^{m} [\alpha w_{ij} + (1 - \alpha)w_{ij}] F_j \right| \\
\geq \alpha \log \left| \sum_{j=1}^{m} w_{ij} F_j \right| + \log \left| \sum_{j=1}^{m} w_{ij} F_j \right| \\
= \alpha \log f_i(z_1) + (1 - \alpha) \log f_i(z_2)
\]

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 \( f_i(z_*) = f_i(w_i) = f(w_0) > 0 \). As a direct conclusion of Theorem 2.1, \( f_i(z) \) is a polynomial of \( z \) and thus differentiable. Since \( \log f_i(z) \) is concave, then \( \frac{\partial \log f_i(z)}{\partial z} = f_i'(z)/f_i(z) \) 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 3.2:** First of all, \( f(w_\ast) \geq f(w) > 0 \). Suppose \( w_\ast \) is not D-optimal in \( S \). Then there exists a \( w_\circ = (w_{\circ 1}, \ldots, w_{\circ m})^T \in S \), such that, \( f(w_\circ) > f(w_\ast) > 0 \).

Denote \( F(w) = \sum_{i=1}^{p} w_i F_i \) for \( w = (w_1, \ldots, w_m)^T \). Then \( F(w) \) is a linear functional of \( w \), which implies \( F(x w_\circ + (1 - x) w_\ast) = x F(w_\circ) + (1 - x) F(w_\ast) \). Note that \( f(w) = |F(w)| \). Since \( f(w_\circ) > f(w_\ast) > 0 \), then \( F(w_\circ) \neq F(w_\ast) \) and \( |F(w_\circ)| > |F(w_\ast)| > 0 \). According to Lemma 3.1, \( \log |F(x w_\circ + (1 - x) w_\ast)| = \log |x F(w_\circ) + (1 - x) F(w_\ast)| > x \log |F(w_\circ)| + (1 - x) \log |F(w_\ast)| \) for any \( x \in (0, 1) \).
We further denote \( F_x = F(xw_0 + (1-x)w_*) \) for \( x \in [0,1] \). We claim that \( F_{x_1} \neq F_{x_2} \) as long as \( x_1 \neq x_2 \). Actually, if \( x_1 \neq x_2 \), then \( F_{x_1} = F_{x_2} \) implies \( F(w_o) = F(w_*) \), which is not true in this case.

Now we define \( f_\alpha(x) = f(xw_o + (1-x)w_*) = |F(xw_o + (1-x)w_*)| = |F_x|, \) \( x \in [0,1] \). Then \( \log f_\alpha(x) = \log |F(xw_o + (1-x)w_*)| > x \log |F(w_o)| + (1-x) \log |F(w_*)| > -\infty \) for each \( x \in (0,1) \). Thus \( f_\alpha(x) > 0 \) for each \( x \in [0,1] \), which implies that the corresponding Fisher information matrix \( F_x \) is positive definite.

We claim that \( \log f_\alpha(x) \) 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 3.1,

\[
\log f_\alpha(x_1 + (1-\alpha)x_2) = \log f_\alpha(x_1w_o + (1-x_1)w_*) + (1-\alpha)[x_2w_o + (1-x_2)w_*] \\
= \log |F(x_1w_o + (1-x_1)w_*)| + (1-\alpha)[F_1w_o + (1-x_2)w_*]) \\
= \log |\alpha F_1w_o + (1-x_1)w_*| + (1-\alpha)F_2w_o + (1-x_2)w_*) \\
= \log |\alpha F_{x_1} + (1-\alpha)F_{x_2}| \\
> \alpha \log |F_{x_1}| + (1-\alpha) \log |F_{x_2}| \\
= \alpha \log f_\alpha(x_1) + (1-\alpha)f_\alpha(x_2)
\]

As a direct conclusion, the first derivative of \( \log f_\alpha(x) \) 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

\[
\left. \frac{\partial \log f_\alpha(x)}{\partial x} \right|_{x=0} \geq \left. \frac{\partial \log f_\alpha(x)}{\partial x} \right|_{x=c} = \frac{\log f_\alpha(1) - \log f_\alpha(0)}{1-0} = \log f_\alpha(w_o) - \log f_\alpha(w_*) > 0
\]

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

\[
\nabla f(w_*)^T(w_o - w_*) = f(w_*) \cdot \nabla \varphi(w_*)^T(w_o - w_*) = f(w_*) \cdot \frac{\log f_\alpha(x)}{\partial x} \bigg|_{x=0} > 0 \quad (S5.1)
\]

For \( i = 1, \ldots, m \), let \( w_i = (0, \ldots, 0, 1, 0, \ldots, 0)^T \in \mathbb{R}^m \) whose \( i \)th coordinate is 1. In the constrained lift-one algorithm at \( w_* \), we have \( w_i(z) = (1-\alpha)w_* + \alpha w_i = w_* + \alpha(w_i - w_*) \) with \( \alpha = \frac{z - w_i^*}{1-w_i^*} \). Note that \( w_i^* < r_i2 \leq 1 \) and \( w_i(w_i^*) = w_* \). It can be verified that the directional derivative of \( f(w) \) at \( w_* \) along \( w_i - w_* \) is

\[
\nabla f(w_*)^T(w_i - w_*) = (1 - w_i^*)f_i'(w_i^*) \quad (S5.2)
\]
Actually,

\[
\nabla f(w_*)^T(\bar{w}_i - w_*) = f(w_*) \cdot \nabla \varphi(w_*)^T(\bar{w}_i - w_*)
\]

\[
= f(w_*) \cdot \lim_{\alpha \to 0} \varphi'(w_* + \alpha(\bar{w}_i - w_*)) - \varphi(w_*)
\]

(replace \( \alpha \) with \( \frac{z - w_*}{1 - w_*} \))

\[
= f(w_*)(1 - w_i^*) \cdot \lim_{z \to w_*} \frac{\varphi(w_i(z)) - \varphi(w_i(w_*))}{z - w_*}
\]

\[
= f(w_*)(1 - w_i^*) \cdot \log f_i(z) - \log f_i(w_i^*)
\]

\[
= f(w_*)(1 - w_i^*) \cdot \frac{\partial \log f_i(z)}{\partial z} \bigg|_{z = w_*}
\]

\[
= f(w_*)(1 - w_i^*) \cdot \frac{f_i'(w_i^*)}{f_i(w_i^*)}
\]

\[
= (1 - w_i^*)f_i'(w_i^*)
\]

Since \( w_i^* < r_i2 \) for each \( i \), then \( f_i'(w_i^*) \leq 0 \) for each \( i \) according to Theorem 3.1.

Since \( \sum_{i=1}^m w_i^* = 1 \), then \( w_o - w_* = \sum_{i=1}^m w_i^*(\bar{w}_i - w_*) \). Then

\[
\nabla f(w_*)^T(w_o - w_*) = \sum_{i=1}^m w_i^* \nabla f(w_*)^T(\bar{w}_i - w_*) = \sum_{i=1}^m w_i^*(1 - w_i^*)f_i'(w_i^*) \leq 0
\]

which leads to a contradiction with (S5.1). \( \square \)

**Proof of Corollary 3.1:**

(i) First of all, \( f(w_*) > 0 \). Denote \( w_* = (w_1^*, \ldots, w_m^*)^T \in S_0 \).

Then \( 0 \leq w_i^* < 1 \) for each \( i \) according to Lemma 2.1. Since there is no additional restriction on \( w \), then \([r_{i1}, r_{i2}] = [0, 1] \) and \( w_i^* < 1 \) for each \( i \). According to Theorem 3.2, \( w_* \) must be D-optimal in \( S_0 \).

(ii) Note that \( f(w_*) > 0 \) and \( 0 \leq w_i^* < 1 \) for each \( i \) according to Lemma 2.1. Following a similar proof as for Theorem 3.2, we obtain

\[
\nabla f(w_*)^T(w - w_*) = \sum_{i=1}^m w_i \nabla f(w_*)^T(\bar{w}_i - w_*) = \sum_{i=1}^m w_i(1 - w_i^*)f_i'(w_i^*) \leq 0
\]

for any \( w = (w_1, \ldots, w_m)^T \in S \). Then \( w_* \) must be D-optimal in \( S \). \( \square \)

**Proof of Theorem 3.3:** There are two cases for \( w_* \) reaching Step 10°.

**Case one:** \( w_* \) 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 3.1, \( w_* \) must be D-optimal in \( S \).

**Case two:** \( w_* \) 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 \( \max_{w \in S} g(w) \leq 0 \), where \( g(w) = \sum_{i=1}^m w_i(1 - w_i^*)f_i'(w_i^*) \). Since \( \text{rank}(F_i) < p \) for each \( i \) and \( f(w_*) > 0 \), according to Lemma 2.1, \( w_i^* < 1 \) for each \( i \). Suppose \( w_* \) is not D-optimal
According to the proof of Theorem 3.2, 

\[ 0 < \nabla f(w_*)^T (w_o - w_*) = \sum_{i=1}^{m} w_i^o (1 - w_i^*) f_i'(w_i^*) = g(w_o) \]

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

**Proof of Theorem 3.5:** (i) If \( \sum_{i=1}^{m} c_i = 1 \), then \( S = \{(c_1, \ldots, c_m)^T \} \) which implies that \( w_o = (c_1, \ldots, c_m)^T \) 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 \( \sum_{i=k}^{m} c_i \leq 1 < \sum_{i=k+1}^{m} c_i \). It can be verified that \( w_o = (c_1, \ldots, c_k, 1 - \sum_{i=k+1}^{m} c_i, 0, \ldots, 0)^T \) maximizes \( g(w) = \sum_{i=1}^{m} c_i w_i \). The rest part is straightforward.

**Proof of Lemma 3.2:** According to the proof of Theorem 2.1, 

\[ h(\alpha) = f((1 - \alpha)w_* + \alpha w_o) = \sum_{\pi} \sgn(\pi) \cdot \prod_{s=1}^{p} \left( \sum_{i=1}^{m} a_{i \pi(s)} (w_i^* + \alpha (w_i^o - w_i^*)) \right) \]

is an order-\( p \) polynomial of \( \alpha \). The rest of the lemma is straightforward. \( \square \)

**Proof of Theorem 3.6:** First of all, we claim that \( F(w_o) \neq F(w_*) \), where \( F(w) = \sum_{i=1}^{m} w_i F_i \) is the Fisher information matrix corresponding to the allocation \( w = (w_1, \ldots, w_m) \). Actually, if \( F(w_o) = F(w_*) \), then \( h(\alpha) = f((1 - \alpha)w_* + \alpha w_o) = |F((1 - \alpha)w_* + \alpha w_o)| = |(1 - \alpha)F(w_*) + \alpha F(w_o)| = |F(w_*)| \). It implies \( h'(0) = 0 \). On the other hand, we denote \( \varphi(w) = \log f(w) \), then \( \nabla \varphi(w) = f(w)^{-1} \nabla f(w) \) and 

\[
\begin{align*}
g(w_o) &= \nabla f(w_*)^T (w_o - w_*) \\
&= f(w_*) \cdot \nabla \varphi(w_*)^T (w_o - w_*) \\
&= f(w_*) \cdot \lim_{\alpha \to 0} \frac{\varphi(w_* + \alpha (w_o - w_*)) - \varphi(w_*)}{\alpha} \\
&= f(w_*) \cdot \lim_{\alpha \to 0} \frac{\varphi((1 - \alpha)w_* + \alpha w_o) - \varphi(w_*)}{\alpha} \\
&= f(w_*) \cdot \lim_{\alpha \to 0} \frac{\log h(\alpha) - \log h(0)}{\alpha} \\
&= f(w_*) \cdot \frac{h'(0)}{h(0)} \\
&= h'(0)
\end{align*}
\]

Note that \( h(0) = f(w_*) > 0 \). Then \( g(w_o) > 0 \) implies \( h'(0) > 0 \), which leads to a contradiction. We must have \( F(w_o) \neq F(w_*) \).

(i) Note that \( h(\alpha) = f((1 - \alpha)w_* + \alpha w_o) \) is the same as the function \( f_*(x) \) defined in the proof of Theorem 3.2. Since \( F(w_o) \neq F(w_*) \) and \( |F(w_*)| > 0 \), we still have \( h(\alpha) = f_*(\alpha) > 0 \) for any \( \alpha \in (0, 1) \). Combining \( h(0) = f(w_*) > 0 \), we have \( h(\alpha) > 0 \) for any \( \alpha \in [0, 1) \). Note that \( h(1) = f(w_o) \) could be zero.
(ii) \( h'(0) > 0 \) since \( h'(0) = g(w_o) > 0 \).

Since \( \mathbf{F}(w_o) \neq \mathbf{F}(w_*) \), we still have \( \mathbf{F}_{x_1} \neq \mathbf{F}_{x_2} \) given \( x_1 \neq x_2 \) as in the proof of Theorem 3.2. Then \( \log h(\alpha) \) is strictly concave for \( \alpha \in [0, 1) \) and \( \frac{h'(\alpha)}{h(\alpha)} \) is strictly decreasing as \( \alpha \) increases in \([0, 1)\).

(iii) If \( h(1) > 0 \) and \( h'(1) \geq 0 \), then \( \frac{h'(\alpha)}{h(\alpha)} \) is strictly decreasing as \( \alpha \) increases in \([0, 1)\).
Since \( \frac{h'(\alpha)}{h(\alpha)} \geq 0 \), 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 \( \alpha_s = 1 \) only.

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

If \( h(1) = f(w_o) = 0 \), 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 \( \alpha_s \in (0, \alpha_-) \) such that \( \frac{h'(\alpha_s)}{h(\alpha_s)} = 0 \). That is, \( h'(\alpha) > 0 \) if \( 0 \leq \alpha < \alpha_s \); = 0 if \( \alpha = \alpha_s \); and \( < 0 \) if \( \alpha_s < \alpha < 1 \). Therefore, \( h(\alpha) \) attains its maximum at \( \alpha_s \in (0, 1) \) only.  

\[ \text{Proof of Lemma 4.2:} \] First of all, \( w_* \) exists and is unique. Actually, \( w_* \) exists since \( S = \{ w \in S_0 \mid 0 \leq w_i \leq c_i, i = 1, \ldots, m \} \) is bounded and closed.

Secondly, \( w_* \) is unique and \( f(w_*) > 0 \). Actually, we denote \( S_+ = \{ w \in S \mid f(w) > 0 \} \), which is not empty since \( \sum_{i=1}^m c_i \geq 1 \). Given \( w(i) = (w^{(i)}_1, \ldots, w^{(i)}_m)^T \in S_+ \), \( i = 1, 2 \), by letting \( M_i = \text{diag}\{w^{(i)}_1, \ldots, w^{(i)}_m\} \) in Lemma 3.1, it can be verified that \( \log f(\alpha w(1) + (1 - \alpha) w(2)) > \alpha \log f(w(1)) + (1 - \alpha) \log f(w(2)) \) for all \( \alpha \in (0, 1) \) if \( w(1) \neq w(2) \). In other words, \( \log f(w) \) is strictly concave on \( S_+ \), which leads to the uniqueness of \( w_* \).

Case (i): If without the constraints \( w_i \leq c_i \), \( w_* = (1/m, \ldots, 1/m)^T \) maximizes \( f(w) \) 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 \( w_* \) 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 \( w_* := (c_1, \ldots, c_k, u, \ldots, u)^T \in S \), 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 \( w_* = (c_1, \ldots, c_k, u, \ldots, u)^T \) 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 4 of Algorithm 1, which leads to \( z_* = c_1 \). Note that in this case, \( f_1'(z) = c_i^{-1} \prod_{k=1}^k c_i u^{m-k}(1-c_i)^{1-m}(1-z)^{m-2}(1-mz) \) 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 $r_{ij} = c_i$, $f'_i(z) = \prod_{i=1}^k c_i u^{m-k-1}(1-u)^{1-m}z^{m-2}(1-mz) < 0$ for all $z \in [u, c_i]$, which leads to $z_* = u$ in this case.

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

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

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

By applying Theorem 3.3 to GLMs with $m = p$, it can be verified that $w_*$ maximizes $f(w)$ with $w \in S$.

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

**Proof of Theorem 4.1:** For GLM (5), if $m = p$, then $f(w) = |X^T W X| = |X|^2 \prod_{i=1}^m \nu_i \cdot \prod_{i=1}^m w_i$. According to Lemma 4.2, the constrained uniform allocation $w_*$ maximizes $\prod_{i=1}^m w_i$, $w \in S$. That is, $w_*$ is D-optimal on $S$.

Similarly, since $f_{EW}(w) = |X^T E(W) X| = |X|^2 \prod_{i=1}^m E(\nu_i) \cdot \prod_{i=1}^m w_i$, $w_*$ is EW D-optimal on $S$ as well.

□