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Constructing D-optimal designs for multi-parameter binary regression models: A theoretical characterization of support points

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ABSTRACT

This manuscript presents a comprehensive study on the construction of *D*-optimal designs for multiparameter binary regression models. The aim is to expand and validate the conjectures put forth by Ford et al. (Ford et al., 1992) regarding *D*-optimal designs in generalized linear models with multiple parameters. This is based on a parameter dependent transformation to a weighted regression model and results will be extended to other such models. In this study, building upon the pioneering work by Gunduz and Torsney (Gündüz et al., 2023) in univariate settings with two parameters, we extend their methodology to handle the complexities of multiparameter models. By delving into the intricacies of high-dimensional parameter spaces, we address the challenges associated with constructing *D*-optimal designs for binary regression models, with a specific focus on the rigorous derivation and characterization of the determination of the support points of the design. In summary, our manuscript contributes a significant advancement in the field of experimental design for multiparameter binary regression models. The meticulous mathematical derivations, accompanied by intuitive conceptual plots, provide a comprehensive understanding of our methodology. The compelling simulated examples further emphasize the efficacy of our approach. This work sets the stage for future investigations in adaptive designs, incorporating prior information, and handling complex model structures within the context of *D*-optimal designs.

1. Introduction

This study delves into *D*-optimal designs for binary and weighted linear regression models with multiple design variables. Our main emphasis is on deriving minimal support *D*-optimal designs. Previous scholars such as Ford et al. (1992) considered c-optimal and *D*-optimal designs for generalized linear models with one design variable. Drawing on Silvey's geometrical approach (Silvey, 1972), they proposed that many local *D*-optimal designs in two-parameter models have two support points, and they conjectured what these would be. Building upon this foundation, Sitter and Torsney (1995a, 1995b) extended the investigation to scenarios involving more than two design variables that relate to selected typical binary response models. However, it is important to note that their findings, like those of the earlier work, remain conjectural in nature. Subsequent to the aforementioned studies, Sebastiani and Settimi (1997) considered the design problem of binary logistic regression, offering an analytical validation of the conjectured designs across all design intervals. We extend their work to both a class of binary regression models and to weighted linear regression models. The work contributed to Gündüz (1999), Gündüz and Torsney (2023), Torsney and Gündüz (2001) who, employing geometric and other analytical approaches, extended and substantiated the conjectures presented by Ford et al. (1992). Specifically, their investigations established that *D*-optimal designs for two-parameter generalized linear models possess two support points across all possible design intervals $\mathscr{Z}$. This paper extends these studies to multiparameter models specifically establishing that this result holds true in high dimensional spaces in the generalized linear model (GLM) context. Our work pioneers into high-dimensional spaces, providing a new perspective on *D*-optimality. We believe that our work stands as a significant contribution to the literature on *D*-optimality, broadening our understanding of these complex models and paving the way for future advancements in the field. We believe that our work will be of interest to researchers and practitioners who are involved in the design of experiments involving binary responses. Our new method for constructing *D*-optimal designs provides a valuable tool for improving the precision of parameter estimates in these types of experiments. Additionally, our rigorous and detailed proof of the Ford et al. (1992) conjecture will be of interest to a wider audience of statisticians and mathematicians.

To prowide a clear context of the framework of the present paper, it

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is important to note that several recent and relatively recent studies have provided optimal designs for different models, like the multivariate logistic models by Woods et al. (2006). Also worthy of note are Dror and Steinberg (2006), Lall et al. (2018), and the two-variable logistic model with no interaction by Kabera et al. (2015). *D*-optimal designs for models with restricted design space were given by Sebastiani and Settimi (Sitter & Torsney, 1995b), while other works such as Yang et al. (2011), and Gutiérrez and Martin (2014) have provided valuable insights into different models and design considerations. More recent studies like Hao and Yang (2020), Olamide et al. (2021), and Zhu et al. (2021) have explored novel models, designs, and applications.

As far as really recent related work is concerned, a particularly noteworthy contribution is Bodunwa and Fasoranbaku (2020) who devised a *D*-optimal design within a linear model that incorporates two explanatory variables and accounts for heteroscedasticity. They adopted a sequential method to arrive at the *D*-optimal design. They implemented two distinct structures based on the available literature and found that the optimal design aligns with the extreme values of the design region. The conclusions drawn from their simulated data were further corroborated using real-world data. They explored the kinematic viscosity of a lubricant, measured in stokes, as a function of temperature and pressure, following the discussion in Linssen (1975). Another relevant contribution is Hao and Yang (2020) who addressed the lack of pace in design selection research for multinomial logistic models, despite their widespread application. They highlighted the complexity of studying optimal or efficient designs for these models due to the intricate structure of information matrices and the existence of numerous model variants. A vital step in deriving optimal or efficient designs, they asserted, is determining the number of support points required. In their paper, they thoroughly characterized optimal designs using the complete class framework. Their results applied to any optimal designs, irrespective of the optimality criterion chosen, the parameters of interest, or whether they were one-stage or multi-stage designs. Their work provided theoretical insight into the structure of optimal designs for multinomial logistic models, thereby facilitating subsequent derivations. Even more recently, we have, amongst others, we have Ma et al. (2022) focusing on high-dimensional logistic regression, a common method for analyzing binary outcome data, with their work considering global testing and large-scale multiple testing for regression coefficients in both single and dual-regression scenarios. Also Olamide et al. (2021) who examined a two-variable Poisson regression model for *A*-optimality on a constrained design space, successfully determining the weights of the optimal design points. On the other hand, Freise et al. (2021) provided a comprehensive characterization of *D*-optimal designs in the context of a two-dimensional Poisson regression model with synergetic interaction, backing their findings with an explicit proof. Zhu et al. (2021) tackled the seldom-investigated issue of the *D*-optimal equal allocation design's equivalence theorem for multiresponse mixture experiments. They established that the maximum of the variance function of the equivalence theorem equates to the number of responses, illustrating their findings through two examples. It is also interesting to mention Hooshangifar et al. (2022) who proposed a locally *D*-optimal design for a logistic model. Their work was based on the quasi-information matrix, which they achieved by applying the highly precise Hammersley-Chapman-Robbins lower bound for variance approximation. The work featured in Cui (2022) conducted a systematic exploration of *D*-optimal design for binary regression and quantal response models in toxicology studies. For the two-parameter case, Cui (2022) provided an analytical equation for computing the *D*-optimal design swiftly and introduced particle swarm optimization for instances where an analytical solution was not viable. They also extended their work to the three-parameter case by formulating a concise formula for the determinant of the information matrix. Finally, Zhai et al. (2023) expanded on the work of Kabera et al. (2015), where the model was constrained to positive slopes and negative intercepts, corresponding to an increasing response probability with doses for both drugs. The previous work discussed a design space mainly centered on the set $[0,\infty)\times[0,\infty)$, with a finite rectangular design space only covered in scenarios where the results for the unlimited design space were still suitable. However, Zhai et al. (2023) sought to ease these constraints and discussed the rectangular design spaces for the model where *D*-optimal designs could not be procured. They proposed that their findings could be extended to models where drugs have negative or opposing effects, or models with a positive intercept, by utilizing translation and reflection in the first quadrant.

Spanning several years and a multitude of in-depth studies, the literature on *D*-optimality is extensive and continues to evolve. Ma et al. (2022) explorations in high-dimensional logistic regression to Olamide et al. (2021) investigation of A-optimality in two-variable Poisson regression models, researchers have tirelessly advanced the boundaries of knowledge in the field. Freise and Schwabe's (Freise et al., 2021) detailed characterizations of D-optimal designs in two-dimensional Poisson regression models with synergetic interaction and Zhu et al.'s (2021) invaluable insights on the equivalence theorem of *D*-optimal equal allocation design for multiresponse mixture experiments have expanded the conversation around *D*-optimality, offering new perspectives and considerations. In this rich tapestry of research, Hooshangifaret et al. (2022) study on locally *D*-optimal design in logistic models and Cui's (2022) comprehensive treatment of *D*-optimal design in toxicology studies have made significant contributions. More recently, Zhai et al.'s (2023) work further diversified the landscape by addressing the constraints of previous models and exploring *D*-optimality in rectangular design spaces.

The structure of the paper is as follows: in section 2 we briefly review $k\geq 3$ a parameter (k is the number of parameters) case; the results for optimal design in the three-parameter case heavily depend on a parameter-dependent transformation, as conceived by Ford et al. (1992), which converts the non-linear design problem into a weighted linear design problem; in section 3 we establish that *D*-optimal designs often have 'minimal' supports for many weighted regression models, including those arising from this transformation; in section 4 we establish what these support points can be. Finally the results are discussed in Section 5.

2. Model with ($k\geq 3$) three or more parameters

In the context of multiple binary regression, we commonly examine a model where an observed value u is influenced by a vector of $\underline{x}$ of l explanatory variables $\underline{x}=(x_1,\cdots,x_l)$, selected from a design space $\mathscr{X}\subset R^l$. The binary outcome is characterized by probabilities

$$\Pr(u=1|\underline{x})=\pi(\underline{x})\Pr(u=0|\underline{x})=1-\pi(\underline{x}). \tag{1}$$

In particular, $u\sim Bi(1,\pi(\underline{x}))$. It is assumed that $\pi(\underline{x})=F(\alpha+\beta_1x_1+\cdots+\beta_lx_l)$, where $F(\cdot)$ is a cumulative distribution. As such, this is a GLM under which the dependence of π on $\underline{x}=(x_1,\cdots,x_l)$ is through the linear function

$$z_1=\alpha+\beta_1x_1+\cdots+\beta_lx_l \tag{2}$$

for unknown parameters $\alpha,\beta_1,\cdots,\beta_l$. So

$$\begin{aligned}\mathrm{E}(u|\underline{x})&=\pi(\underline{x})=F(\alpha+\beta_1x_1+\cdots+\beta_lx_l),\\ \mathrm{V}(u|\underline{x})&=\pi(\underline{x})[1-\pi(\underline{x})].\end{aligned} \tag{3}$$

In the aforementioned model, the information matrix for a single replicate can be represented as follows:

$$I(\underline{x},\underline{\theta})=\frac{f^2(z_1)}{F(z_1)[1-F(z_1)]}\begin{pmatrix}1\\x_1\\\vdots\\x_l\end{pmatrix}(1,x_1,\cdots,x_l), \tag{4}$$

where $f(z)=F'(z)$. It is evident that, z_1 has a role akin to $z=\alpha+\beta x$ in both the two and three parameter case. Building upon the same meth-

odology, we apply the transformation to the problem at hand:

$$\begin{pmatrix} 1 \\ z_1 \\ z_2 \\ \vdots \\ z_l \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ \alpha & \beta_1 & \beta_2 & \cdots & \beta_l \\ b_{31} & b_{32} & b_{33} & \cdots & b_{3k} \\ \vdots & \vdots & \vdots & \vdots & \\ b_{k1} & b_{k2} & b_{k3} & \cdots & b_{kk} \end{pmatrix} \begin{pmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_l \end{pmatrix} = \mathscr{B} \begin{pmatrix} 1 \\ x_1 \\ \vdots \\ x_l \end{pmatrix}, \tag{5}$$

where $k = l+1$ and $b_{ij}, i = 3, \cdots, k; j = 1, \cdots, k$ are arbitrary constants for the experimenter to choose and they should be non-singular. Additional variables $z_j, j = 2, \cdots, l$ have been defined new design variables $z_1, \cdots, z_l$ have been transformed to l. The image of $\mathscr{X}$ under the transformation will be their design space. $\mathscr{Z}$ represents this. Thus if

$$\underline{g}(\underline{z}) = \mathscr{B}\underline{v}, \tag{6}$$

Then

$$\underline{g}(\underline{z}) = \frac{f(z_1)}{\sqrt{F(z_1)[1-F(z_1)]}} \begin{pmatrix} 1 \\ z_1 \\ \vdots \\ z_l \end{pmatrix}, \tag{7}$$

and

$$\underline{v} = \mathscr{B}^{-1}\underline{g}(\underline{z}). \tag{8}$$

Now we move on to the D-optimal linear design problem with design vectors

$$\underline{g} = \sqrt{w(z_1)}(1, z_1, \cdots, z_l)^T, (z_1, \cdots, z_l)^T \in \mathscr{Z}, \tag{9}$$

where $w(z_1) = \frac{f^2(z_1)}{F(z_1)(1-F(z_1))}$. This transformation corresponds to a weighted linear regression design problem, where the weight function is defined as $w(z_1)$. The design locus is

$$G = G(Z) = \left\{ \underline{g} = (g_1, \cdots, g_k)^T : g_1 = \sqrt{w(z_1)}, g_j = z_{j-1}\sqrt{w(z_1)}, j = 2, \cdots, k, \underline{z} \in \mathscr{Z} \right\}. \tag{10}$$

We anticipate that the set G must have bounds in order for feasible designs to exist. In practical terms, this will hold true if $\mathscr{X}$ and, consequently, $\mathscr{Z}$ is bounded. Bounds are clearly needed on $z_2 \cdots, z_l$. We contend that the 'largest' possible G is given by

$$G_w = G(z_w) = \left\{ \underline{g} = (g_1, \cdots, g_k)^T : g_1 = \sqrt{w(z_1)}, g_j = z_{j-1}\sqrt{w(z_1)}, z_1 \in I_w, \; -1 \le z_j \le 1, = 2, \cdots, l \right\} \tag{11}$$

where

$$\mathrm{Z_w} = \mathrm{Z}(I_w) = \left\{ (z_1, \cdots, z_l) : z_1 \in I_w, -1 \le z_j \le 1, j = 2, \cdots, l \right\}. \tag{12}$$

All other choices of $\mathscr{Z}$ will align to a subset of G_w. Specifically, we consider

$$G = G_{ab} = G\{\mathscr{Z}(I_{ab})\} = \left\{ \underline{g} = (g_1, \cdots, g_k)^T : g_1 = \sqrt{w(z_1)}, g_j = z_{j-1}\sqrt{w(z_1)}, \; z_1 \in I_{ab} - 1 \le z_j \le 1, j = 2, \cdots, l \right\}. \tag{13}$$

The conclusions regarding D-optimal designs remain consistent with the three-parameter case. A D-optimal design assigns weight exclusively to $z_j = \pm 1, j = 2, \cdots, l$ representing the ridges of G. Additionally, within a single design, the total weight at a given z_1 value is evenly distributed among the combinations of $z_j \pm 1 j = 2, \cdots, l$.

Other potential options for weight assignment include uniform distributions across specific subsets of these combinations, such as sets that form a Hadamard matrix, as explored by Sitter and Torsney (1995a). Therefore, our focus can be directed towards the induced marginal design on z_1, which corresponds to the conditional design on a given 'ridge' comprising design loci $\underline{g} = \sqrt{w(z_1)}(1, z_1, \pm 1, \cdots, \pm 1)$. Our team maintains that $\underline{g} = T(g_1, g_2)^T$ where

$$T = \begin{pmatrix} 1 & 0 & \pm 1 & \cdots & \pm 1 \\ 0 & 1 & 0 & \cdots & 0 \end{pmatrix}, \tag{14}$$

and in this way, the results for 2 dimensions are applicable; of importance is that a conditional D-optimal design is present on the ridge with a maximum of 3 support points. In fact, for many $w(\cdot)$ there will be only two points, resulting in the following form for the design

$$\xi = \begin{pmatrix} z_1 & c & d \\ p_{21} & p_c & p_d \end{pmatrix}, \tag{15}$$

where $p_c, p_d > 0$ and $p_c + p_d = 1$.

When c, d are given, this solution is used for p_c, p_d, i.e.,

$$p_c = \frac{(k-1)(r-1) - 2 + \sqrt{(k-1)^2(r-1)^2 + 4r}}{2k(r-1)}, p_c = 1 - p_c, \tag{16}$$

where $r = \frac{w(c)}{w(d)}$ and $p_d = 1 - p_c$. Remember that $p_c \to \frac{1}{2}$ as $r \to 1$ as is necessary if $w(c) = w(d) = 1$.

Therefore, the values of c and d need to be selected in a way that maximizes the determinant of the information matrix, $\det M(\overline{\zeta})$, where c and d belong to the interval I_{ab} and c is less than d. We will revisit the selection of c and d later in the discussion.

Table 1 lists examples of this kind of weight function (binary regression weight functions) in Group I and non-binary weight functions in Group II. Here, D-optimal designs for these afore mentioned weight functions are explored.

For three parameter case the design locus is

$$G = G(Z) = \left\{ g_z = (g_1, g_2, g_3)^T : g_1 = \sqrt{w(z_1)}, g_2 = z_1\sqrt{w(z_1)}, \; g_3 = z_2\sqrt{w(z_1)}, \underline{z} \in \mathscr{Z} \right\}. \tag{17}$$

Set G must be bounded. g_1 and g_2 can be bounded for all possible z_1, for many $w(z_1)$ just as they can be in the two parameter case. g_3, on the other hand, will be unbounded with unbounded z_2. This variable is an arbitrary linear combination of x_1, x_2. It is safe to assume without loss of generality that $-1 \le z_2 \le 1$. Should $\mathscr{X}$ be bounded (usually it will be rectangular) so too will $\mathscr{Z}$ be and $G(\mathscr{Z})$. In the beginning $\mathscr{Z}$ is assumed to be rectangular for the sake of simplicity, i.e.

$$\mathscr{Z} = \{(z_1, z_2) : z_1 \in I_{ab}, -1 \le z_2 \le 1\} = \mathscr{Z}(I_{ab}) \tag{18}$$

where I_{ab} is the interval $[a, b]$. In this case, the largest possible choice of these sets are $\mathscr{Z} = \mathscr{Z}_w = \mathscr{Z}(I_w), G = G_w = G(\mathscr{Z}(I_w))$ where I_w has the widest possible interval choice for z_1, the sample space of $f(z)$; typically $I_w = \mathscr{R}$ or $\mathscr{R}+$ or $[-1, 1]$.

We assert that every finite selection of $\mathscr{X}$ corresponds to a subset G of G_w. To facilitate our analysis, we initially focus on G_w. Following this, we examine $G_{ab} = G\{\mathscr{Z}(I_{ab})\}$ when $k = 3$ or $l = 2$. Refer to Fig. 1 for visual representations of G_w.

In a number of cases of $F(z)$, the design locus $G(Z_w)$ is a vertical surface with for a given z_2, the set $\left\{ \underline{g} \in G: z_2 = \text{fixed} \right\}$ forming a closed curve. Similar to what was observed in the two parameter case, if $z_2 = 0$ it is the same closed convex curve. If $z_2 = \pm 1$ it is the upper or lower ridge to $G(Z_w)$. The case $G_{ab} = G\{Z(I_{ab})\}$ which corresponds to making vertical cuts to G_w at $z_1 = a, b$ further illustrates this.

From this, we can see that any ellipsoid centered on the origin containing G_w can only touch G_w on these upper and lower ridges. We conclude that D optimal support points lie on these ridges and hence have $z_2 = \pm 1$ since the support points of the D-optimal design are the points of contact between G and the smallest ellipsoid of its kind.

G_w is also symmetric about $g_3 = 0 (z_2 = 0)$. D-optimal supports, then stand to be such that if observations are taken at a particular value of z_1, they are split equally between $z_2 = \pm 1$; (Sitter & Torsney, 1995a). The

Table 1
Considered weight functions.

Group I: Binary Weight Functions:				
NAME	$f(z)$	$F(z)$	$w(\cdot)^*$	$Z_w = [a,b]^{**}$
LOGISTIC	$\frac{e^{-z}}{(1+e^{-2})^2}$	$\frac{1}{1+e^{-2}}$	$\frac{e^2}{(1+e^2)^2}$	$(-\infty,\infty)$
SKEWED LOGISTIC	$m[F_1(z)]^{m-1}f_1(z)$	$(1+e^{-z})^{-m}$	$\frac{me^{-z}}{1+e^{-z}}[(1+e^{-z})^m-1]^{-\frac{1}{2}}]^2$	$(-\infty,\infty)$
GENERALIZED	$(e^z)(\lambda e^z+1)^{-1}-1$	$1-[\lambda e^2+1]^{\frac{1}{\lambda}}$	$\frac{e^{2l}}{(\lambda e^2+1)^2\left[(\lambda e^2+1)^{\frac{1}{\lambda}}-1\right]}$	$(-\infty,\infty)$
COMPLEMENTARY LOG-LOG	$e^{(z-\tau)}$	$1-e^{-r^2}$	$e^{2z}(e^{r^2}-1)^{-1}$	$(-\infty,\infty)$
PROBIT	$\frac{1}{\sqrt{2\pi}}e^{\frac{-x^2}{2}}$	$\int_{-\infty}^{z}\frac{1}{\sqrt{2\pi}}e^{-t^2}\frac{t^2}{2}dt$	$w(.)$	$(-\infty,\infty)$
Group II: Non-Binary weight functions				
BETA	–	–	$(1-z)^{\alpha+1}(1+z)^{\beta+1}\alpha,\beta>-1$	$(-1,1)$
GAMMA	–	–	$z^{\gamma+1}e^{-z}\gamma>-1$	$(0,\infty)$
NORMAL	–	–	e^{-z^2}	$(-\infty,\infty)$

* $w(z) = f^2(z)/F(z)[1-F(z)](F(\cdot)=c.d.f.,f(\cdot)=\dot{F}(\cdot))$.
** Z_v is widest possible design spoce.

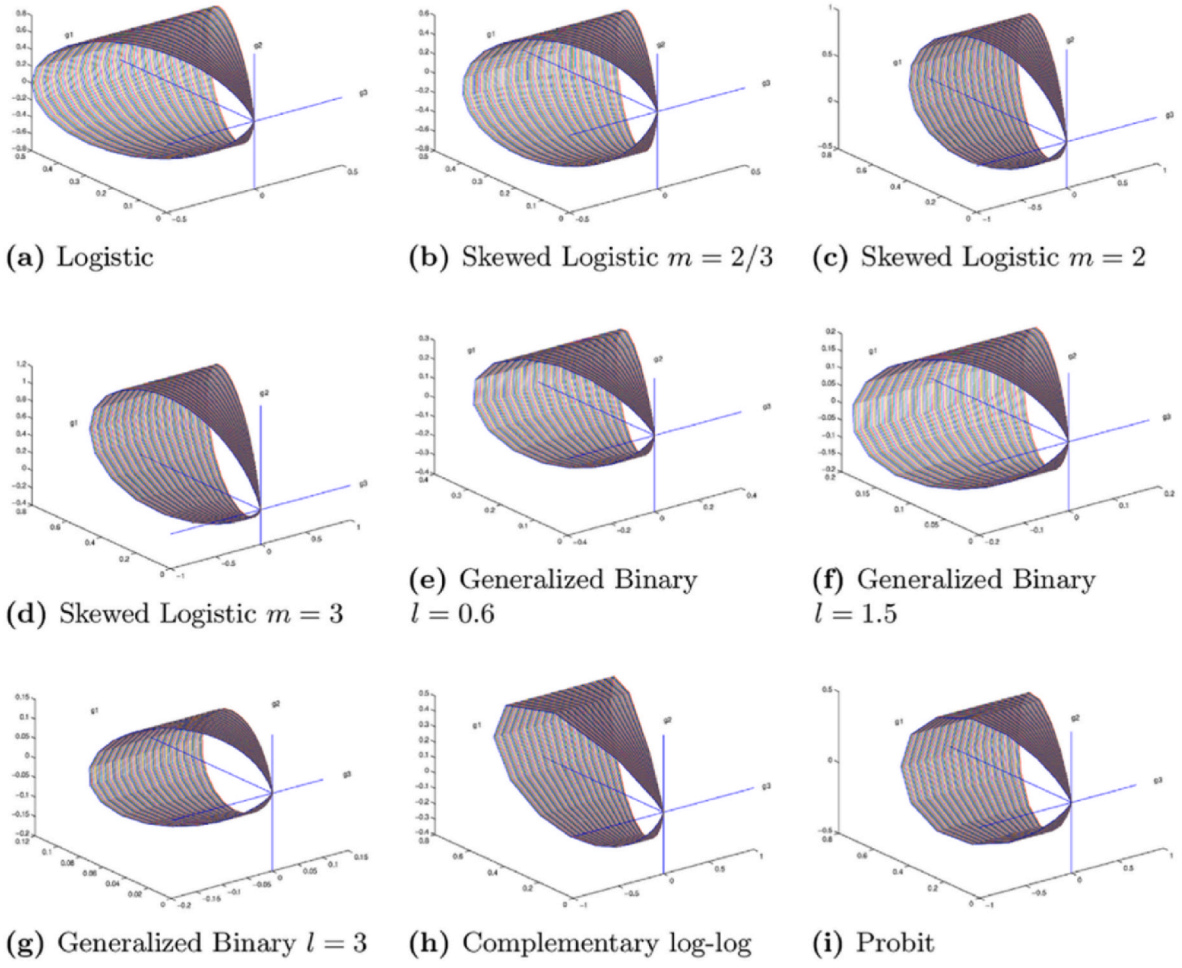


Fig. 1. Group I: Plots of 3-D $G(\mathscr{Z})$ for binary weight functions: $g_1 = \sqrt{w(z_1)}, g_2 = z_1\sqrt{w(z_1)}$ $g_3 = z_2\sqrt{w(z_1)}$ and $-20 \le z_1 \le 20, -1 \le z_2 \le 1$.

marginal design on z_1 can now be our focal point. Caratheodory's theorem tells us that a design necessarily exists of at least 3 and at most 6 points. The marginal distribution on z_1 has 2 or 3 support points as suggested by both this and the previous information. Alternatively, this marginal design is also the conditional design on each ridge. Now on these ridges a design locus $\underline{g} = (g_1, g_2, g_3)$ satisfies $\underline{g} = T(g_1, g_2)^T$ where

$$T=\begin{pmatrix}1 & 0 & \pm 1\\ 0 & 1 & 0\end{pmatrix}^{T}. \tag{19}$$

This is to say the information matrix $M_3(\xi)$ of a conditional design ξ on the ridge satisfies $M_3(\xi) = TM_2(\xi)T^T$, where

$$M_2(\xi)=\mathbb{E}_{\xi}\left\{w(z_1)\begin{pmatrix}1\\ z_1\end{pmatrix}(1,z_1)\right\}. \tag{20}$$

As such, results for 2 dimensions apply. A conditional D-optimal design on a ridge with 2 or 3 support points is an absolute. When we apply Silvey's (1972) minimum ellipsoid argument to G_w the fact remains that the minimum ellipsoid will only touch twice on the two ridges for many $w(z)$. A sufficient condition for this is denoted in parts to follow. The marginal distribution on z_1 then has two supports, for example c, d and takes the form

$$\xi=\begin{pmatrix}z_1 & c & d\\ p_{z_1} & p_c & p_d\end{pmatrix}, \tag{21}$$

where $p_c, p_d > 0$ and $p_c + p_d = 1$. Therefore, it is necessary to choose c, d, p_c, p_d for a D-optimal design on I_{ab}. For a given c,d, an explicit solution is available for the optimal values of p_cp_d as follows:

$$p_c=\frac{(r-2)+\sqrt{(r-1)^2+r}}{3(r-1)}, p_d=1-p_c \tag{22}$$

where $r=\frac{w(c)}{w(d)}$. It is important to point out that if $r\to 1, p_c\to\frac{1}{2}$ by L'Hospital's rule. It is not surprising to consider if $w(c) = w(d).c$ and d as choices will be looked at further in sections to follow.

3. Determination of support points

Based on the equivalence theorem, a design λ is considered D-optimal for any $\mathcal{Z}$ if and only if

$$\begin{aligned}w(z_1)(1,z_1,\cdots,z_l)M^{-1}(\lambda)(1,z_1,\cdots,z_l)^T &\le k\forall(z_1,\cdots,z_l)\in\mathcal{Z},\\ &= k \text{ if}\lambda(z_1,\cdots,z_l)>0.\end{aligned} \tag{23}$$

If λ is one of the potential optimal designs described above and $\mathcal{Z} = \mathcal{Z}(I_{ab})$, then it transforms to the following condition on the induced marginal design $\overline{\zeta}$ of z_1 :

$$\begin{aligned}v(z_1)=\frac{1}{k}Q(z_1)-\frac{1}{w(z_1)} &\le 0 z_1\in I_{ab}\\ &= 0 \text{if}\xi(z_1)>0,\end{aligned} \tag{24}$$

where $Q(z_1) = (1, z_1, \pm 1, \cdots, \pm)M^{-1}(\lambda)(1, z_1, \pm 1, \cdots, \pm 1)^T$, a quadratic function of z_1.Considering a potential design $\overline{\zeta}$ is optimal for its support, meaning it has optimal weights, then $v(z_1) = 0$ if it is a support point. It is evidenced that support points are maximal turning points of $v(z_1)$ except for in cases where they are endpoints of $\mathcal{Z}$. Because

$$v'(z_1)=L(z_1)-H(z_1), \tag{25}$$

where $H(z)=\frac{-w'(z)}{[w(z)^2]}$ and $L(z_1)=\frac{1}{k}Q(z_1)$ is an upward sloping line the turning points (TP) of $v(z_1)$ correspond to points where $L(z_1)$ crosses $H(z_1)$. The significance of $H(z)$ becomes apparent through the following reasoning. An upper limit of 3 crossings of this kind are permitable. No more than this are allowed if $H(z_1)$ meets the properties of the lemma.

Take for instance is $I_w = [A, B]$. Then $\text{Lim}_{z\to A} H(z) = -\infty$ and $\text{Lim}_{z\to B} H(z) = +\infty$.$H(A) = -\infty H(B) = +\infty$ and $H(z_1)$ is written as concave increasing up to some point and thereafter convex increasing. Additional limits are $H'(A) = \infty, H'(B) = \infty$. For the complementary log-log binary weight function of Group I which is given in Table 1, an example of the $H(z)$ function plot is given in Gündüz and Torsney (2023).

As demonstrated by Gündüz and Torsney (2023) and Torsney and Gündüz (2001), $H(z_1)$ satisfies these conditions for various choices of $w(z_1)$ and was further expanded to include polygonal $\mathcal{Z}$.As the marginal design on z_1 for any interval $l \subseteq I_w$ has two support points, the optimal design takes the form

$$\xi=\begin{pmatrix}z_1 & c & d\\ p_{z_1} & p_c & p_d\end{pmatrix}. \tag{26}$$

The optimal weights are

$$p_c=\frac{(k-1)(r-1)-2+\sqrt{(k-1)^2(r-1)^2+4r}}{2k(r-1)}, \tag{27}$$

with $r=\frac{w(c)}{w(d)}$. The joint design produced on G should be written as $\lambda(\overline{\zeta})$ and in order to optimize on I_{ab}, c, d has to maximize $\det\{M(\lambda(\xi))\}$ over $a \le c \le d \le b$. The following conjecture illustrates about this. Allow a^*, b^* to be the values of c, d which maximize $\det M(\lambda(\xi))$ over l_w.

Allow $b^*(a)$ maximize $\det(M(\lambda(\xi)))$ in relation to d (over $\ge a$) where ξ is the design.

$$\xi=\begin{pmatrix}z_1 & a & d\\ p_{z_1} & p_a & p_d\end{pmatrix}, \tag{28}$$

and allow $a^*(b)$ maximize $\det(M(\lambda(\xi)))$ in relation to c (over $c \le b$) where ξ is the design

$$\xi=\begin{pmatrix}z_1 & c & b\\ p_{z_1} & p_c & p_b\end{pmatrix}. \tag{29}$$

It is clear that $a^*(b)$ solve $h(a) = b$ and $b^*(a)$ solves $h(b) = a$, while a^*, b^* solves $h(b^*) = a^*, b^* = h(a^*)$.

Now, a conjecture is given for the support points on I_{ab} for all $a, b \in I_w$ and $< b$:

- Case 1: $I = I_w$ Supp $(\widetilde{\xi}) = \{a^*, b^*\}$.
- Case 2: $I = I_{abr}$ $a \le a^*b \ge b^*$. The D-optimal design remains unchanged as stated previously, as $\mathcal{Z}$ encompasses the support points mentioned above.
- Case 3: $I = I_{ab}, a \ge a^*, b \ge b^*$ Supp $(\overline{\zeta}) = \{a, \min\{b, b^*(a)\}\}$, $(b^*(a) > b^*)$.
- Case 4: $I = I_{abr}, a \le a^*b \le b^*$ Supp $(\xi) = \{\max\{a, a^*(b)\}, b\}$, $(a^*(b) < a^*)$.
- Case 5: $I = I_{ab}, a \ge a^*b \le b^*$ Supp $(\widetilde{\zeta}) = \{a, b\}$.

If we can demonstrate that the variance function $v(z)$ exhibits either a zero or negative derivative at the lower support point and a zero or positive derivative at the upper support point, these assertions will hold. Different scenarios are depicted in Gündüz and Torsney (2023). It is important to note that Cases 1 and 2 are already established, as the derivatives at the respective support points are zero according to the definition of a^* and b^*. The subsequent theorem, Theorem 1, further substantiates these conclusions in the remaining scenarios.

Theorem 1. *Let*

$$h_y(z_1)=z_1+\frac{2w(z_1)}{kp_y(z_1)w'(z_1)}, \tag{30}$$

where $p_y(z)$ represents the optimal weight assigned to z under a marginal design focusing on z_1, with support points z and y, illustrated by

$$p_y(z)=\frac{(k-1)(r-1)-2+\sqrt{(k-1)^2(r-1)^2+4r}}{2k(r-1)} \tag{31}$$

in which $r=\frac{w(z)}{w(y)}$. In addition to the properties required by $H(z)$, a sufficient condition for the validity of the conjecture is the differentiability

and uni-modality of the weight function $w(z)$, with a maximum at $z_{\max}$. Furthermore, the function $h_u(z)$ must meet the following two conditions:

- $h_u(z_1)$ is increasing in z_1 over $z_1 \le z_{\max}$ and $z_1 \ge z_{\max}$ for eadh u.
- For all $z_1 \le z_{\max}, h_u(z_1)$ decreases in u over $u \ge z_{\max}$, and for all $z_1 \ge z_{\max}, h_u(z_1)$ decreases in u over $u \le z_{\max}$.

These will be discussed more in coming sections.

Proof 1. The relevance of $h_u(z)$ is first seen from two different standpoints. We can immediately show from two points of view the releuance of $h_y(z_1)$. To start the derivatives of $\ln\{\det(M(\lambda(\xi)))\}$ are

$$\begin{aligned}\frac{\partial[\ln\det M(\lambda(\overline{\zeta}))]}{\partial c} &= \frac{p_c w'(c)2^{(k-2)}k}{w(c)(d-c)}[d-h_d(c)] \quad (\text{if} w'(c)\neq 0)\\ \frac{\partial[\ln\det M(\lambda(\overline{\zeta}))]}{\partial d} &= \frac{p_d w'(d)2^{k-2}k}{w(d)(d-c)}[h_c(d)-c] \quad (\text{if} w'(d)\neq 0).\end{aligned} \tag{32}$$

Next look at the variance function $v(z)$ under the aforementioned design (so that $(c) = v(d) = 0$). After this,

$$\begin{aligned}v'(c) &= \frac{k2^{(k-2)}w'(c)}{[w(c)]^2(d-c)}[d-h_d(c)]\\ v'(d) &= \frac{k2^{(k-2)}w'(d)}{[w(d)]^2(d-c)}[h_c(d)-c].\end{aligned} \tag{33}$$

The theorem can now be proven if look at four sets of conditions on the interval I_{ab} and corresponding choices for the marginal z_1-support points c, d. We establish that the derivative $v'(c)$ is negative (or zero, depending on the context), and the derivative $v'(d)$ is positive (or zero, depending on the context). Collectively, these findings provide evidence for the various scenarios proposed in the conjecture. In the first two cases, only one of these conditions is explicitly specified.

Condition Set I: $c = a > z_{\max}, d = b > a$. Demonstrating $v'(c) = v'(a) < 0$, in which when provided $d = b$,

$$v'(a) = \frac{6w'(a)}{[w(a)]^2(b-a)}[b-h_b(a)]. \tag{34}$$

If we consider $a > z_{\max}$, you get $w'(a) < 0$. As $v'(a) < 0$ is true if $[b - h_b(a)] > 0$.

$$b - h_b(a) = (b-a) - \frac{2w(a)}{6p(a)w'(a)} \tag{35}$$

The equation is always positive on the right side, since $a < b$ and $w'(a) < 0$. Such that $v'(c) = v'(a) < 0$. $d = b < z_{\max}, c = a < b$. One can see that $v'(d) = v'(b) > 0$, in instance where you have $c = a$,

$$v'(b) = \frac{6w'(b)}{[w(b)]^2(b-a)}[h_a(b)-a] \tag{36}$$

Hence $w'(b) > 0$. So $v'(b) > 0$ is true if $[h_a(b) - a] > 0$.

$$h_a(b) - a = (b-a) + \frac{2w(b)}{6p(b)w'(b)} \tag{37}$$

$[h_a(b) - a]$ always produces positive values, as $a < b$ and $w'(b) > 0$. For this reason, $v'(d) = v'(b) > 0$.

Condition Set II: $a^* < a < z_{\max} < b < b^*$ $c = a, d = b$.
As $a < z_{\max}$ and $b > z_{\max}, w'(a) > 0$ and $w'(b) < 0$.

- $[b - h_b(a)] < [b^* - h_b(a)]$ because $b < b^*$. $[b^* - h_b(a)] < [b^* - h_{b^*}(a)]$ because $h_u(z_1)$ decreases in u by (ii). $[b^* - h_{b^*}(a)] < [b^* - h_{b^*}(a^*)]$ by (i) $[b^* - h_{b^*}(a)] < [b^* - h_{b^*}(a^*)] = 0$. Hence $v'(c) = v'(a) < 0$.
- $[h_a(b) - a] < [h_a(b) - a^*]$ as $a^* < a$. $[h_a(b) - a^*] < [h_{a^*}(b) - a^*]$ as $h_u(z_1)$ decreases in u by (ii). $[h_{a^*}(b) - a^*] < [h_{a^*}(b^*) - a^*]$ by (i). As a result, $v'(d) = v'(b) > 0$.

Condition Set III: $a^* \le a \le z_{\max} \le b = b^*(a)$ $(b^*(a) > b^*)$ $c = a, d = b^*(a)$.One can see that $v'(d) = 0.w'(a) > 0$. If we would like $v'(c) = v'(a)$ to be negative, the derivative of $v'(a)$ should be examined.

$$\begin{aligned}v'(a) &= \frac{w'(a)}{[w(a)]^2(b-a)}\left[b^*(a) - h_{b^*(a)}(a)\right]\\ v'(a) &\propto w'(a)\left[b^*(a) - h_{b^*(a)}(a)\right]\end{aligned} \tag{38}$$

where $w'(a) > 0$ since $a^* \le a \le z_{\max}$. Due to this, we must insist that

$$D = b^*(a) - h_{b^*(a)}(a) < 0 \forall a^* \le a \le z_{\max}$$

As (a^*, b^*) is the unique solution, $a = a^*$ is the only solution to $D = 0$. Furthermore, considering $a = z_{\max}$, the result of $h_{b^*(z_{\max})}(z_{\max}) = \infty$ and $b^*(z_{\max})$ is finite. Hence $D < 0$ at $a = z_{\max}$ and thus over $a^* \le a \le z_{\max}$. The result is $v'(c) = v'(a) < 0$. For $b > b^*(a)$, this design also applies and provides D-optimality.

Condition Set IV: $a^* \le a \le z_{\max}, b^* < b < b^*(a)$ $c = a, d = b$.

Denoting $w'(a) > 0$ then $[b - h_b(a)] < b^*(a) - h_b(a) < b^*(a) - h_{b^*(a)}(a)$. At the top $b^*(a) - h_{b^*}(a) < 0$, so $v'(c) = v'(a) < 0$. In addition, it should be demonstrated that $v'(d) = v'(b) > 0$. As $b \ge z_{\max}, w'(b) < 0$. An assumption is made that $b < b^*(a)$. If $h_a(\cdot)$ is an increasing function, $h_a(b) < h_a(b^*(a)) = a$. In this way, $h_a(b) - a < [h_a(b^*(a)) - a] = 0$. Therefore $v'(d) = v'(b) > 0$.

4. Study of $h_y(z)$: General observations

We shift our focus to the examination of $h_y(z)$. Initially, we visually demonstrate that for numerous selections of $w(z)$, the conditions outlined in the theorem are satisfied. While some conditions can be established via analysis, others are confirmed empirically. Figs. 2 and 3, respectively, depict some $h_y(z)$ for the logistic weight function for different values of k (the number of parameters) and y (the end point support point). Some pairs of values (y_1, y_2) of y with $y_1 < z_{\max} < y_2$ exist such that

$$h_{y_1}(z) = h_{y_2}(z) \forall z. \tag{39}$$

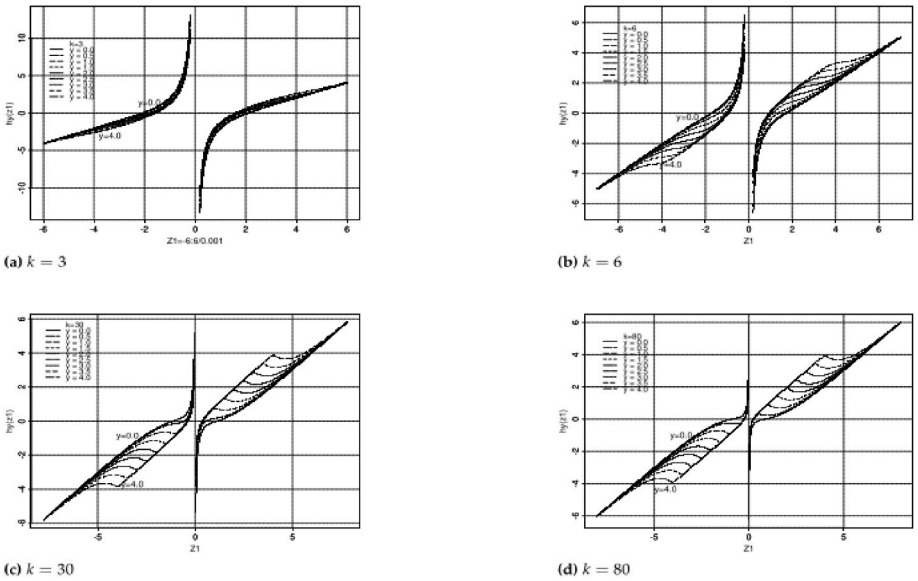
This follows since $w(z)$ is unimodal. The condition of $w(y_1) = w(y_2)$ must be met. If $w(z)$ is symmetric about zero then $y_1 = -y_2$. In most cases, numerical methods are necessary to determine the value of y_2, given a specific y_1, since analytical solutions are not readily available. However, it is worth noting that an exception to this situation arises when $y = z_{\max}$.

In the context of our analysis, it is important to assign different y-values to a given function $h_y(z)$ depending on whether it is evaluated above or below $z_{\max}$. Specifically, we label the higher y-values corresponding to values of z above $z_{\max}$, and the lower y-values corresponding to values of z below $z_{\max}$. These labels are utilized in the Figs. 2–4 for clarity and reference. Two situations are generally observed:

i. For low dimensions $k \le 6, h_u(z_1)$ is increasing in z_1 over $z_1 \le z_{\max}$ and $z_1 \ge z_{\max}$ for each u; but for higher dimensions $h_u(z)$ can have two TP's: a maximal then a minimal one.
ii. It is worth noting that a slightly less stringent condition, yet still sufficient to support the conjecture, is also satisfied. Specifically, for $b > z_{\max}, h_b(z) > b$ for $a^*(b) < z < z_{\max}$, while, for $a < z_{\max}, h_a(z) < a$ for $z_{\max} < z < b^*(a)$. It is important to highlight that there exists only one solution in each of these ranges, $z < z_{\max}$ and $z > z_{\max}$ satisfying the equation

$$h_y(z) = y. \tag{40}$$

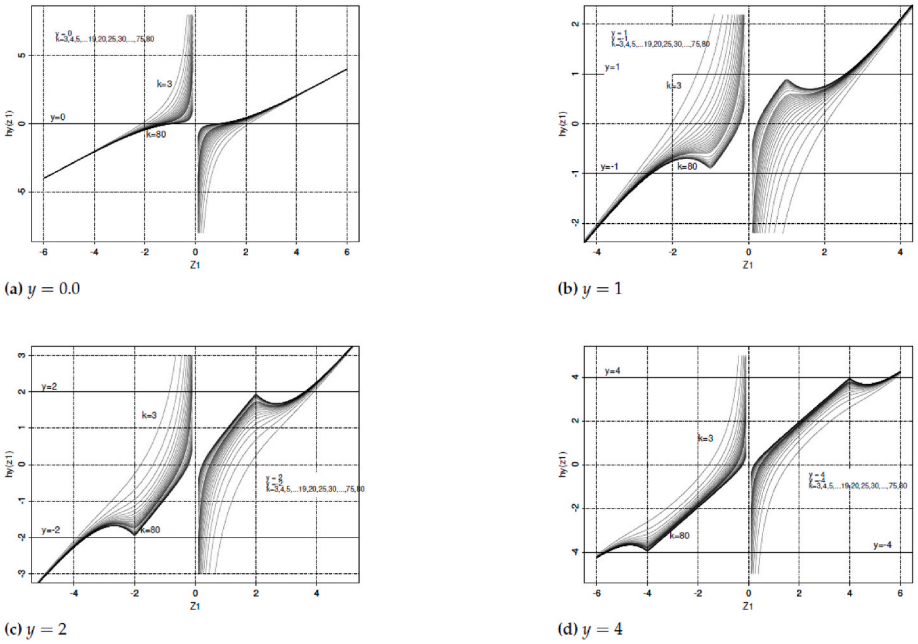
While we will have a closer look at $h_y(z)'$ s dependence on z, y and k respectively, we also continue to look at $z < z_{\max}$ in the course of this analysis.



(a) $k = 3$ (b) $k = 6$

(c) $k = 30$ (d) $k = 80$

Fig. 2. Plots of $h_y(z)$ for the Logistic weight function k= 3, 4, 19, 20, 25, …, 75, 80 for each of $y = 0, 1.0, 2.0, 4.0$.



(a) $y = 0.0$ (b) $y = 1$

(c) $y = 2$ (d) $y = 4$

Fig. 3. Plots of $h_y(z)$ for the Logistic weight function k= 3, 4, 19, 20, 25, …, 75, 80 for each of $y = 0, 1.0, 2.0, 4.0$.

5. Conclusion

In our study, we introduced a technique for the development of *D*-optimal designs for binary regression models, accommodating any number of parameters. This innovative method combines both analytical and numerical strategies, providing the most comprehensive and systematic approach available to date. We are confident that the depth of our derivation and the direct applicability of our design's support points distinguishes our work in this area. Our in-depth exploration of *D*-optimality relays heavily on the use of multiparameter design problems also transformed to weighted regression design problems. Our results indicate that optimal designs for many weight functions can be a two-point design, with support points following the provided formulas, which are contingent on certain mathematical criteria being met.

We anticipate that this research will appeal to both researchers and practitioners invested in experimental design involving binary responses. Our newly devised method offers a powerful tool to enhance the accuracy of parameter estimations within these experiments. Moreover, the extensive detail and rigor we applied to substantiate the Ford et al. (1992) conjecture should interest mathematicians and statisticians alike.

The significance of our work lies not only in its immediate application but also in its potential for future expansion and development. We foresee potential extensions of our method to other regression models, such as Poisson regression models and other members of the exponential family of distributions. Furthermore, we are interested in exploring the application of our method in more intricate experimental designs, like factorial and multi-stage experiments. We also aim to cultivate mone efficient algorithms for executing our method.

We also investigated scenarios with multiple design variables,

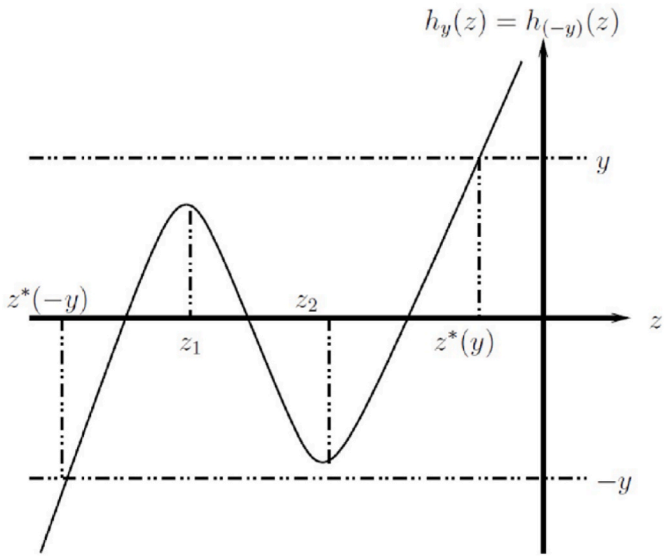


Fig. 4. Plot of arbitrary $h_y(z)$ function.

transforming these multi-parameter design issues into weighted regression design problems with rectangular design spaces. We found that optimal designs usually involve making observations at two values satisfying the given conjecture, with one specific design distributing the total weight at each of these values across all combinations of additional parameters.

Our research also extended into bounded design spaces, where we found optimal designs for two design variables when their design space is a polygon, with certain conditions extending from previous results. We also improved and reported new results focusing on optimal designs for the second bid of a double bounded study, given the response at the first bid.

On the other hand, *D*-optimal designs for multi-parameter binary regression models can be extended to ordinal outcomes in weighted linear regression models. However, adjustments to the construction of D-optimal designs and their optimality criteria may be necessary to accommodate ordinal data. Ordinal responses require a cumulative or adjacent categories modelling approach. In essence, integrating ordinal outcomes into weighted linear regression models represents an intriguing avenue for future research.

In conclusion, our work represents a significant step forward in the realm of experimental design. It is our hope that it will stimulate further investigation in this area, paving the way for the development of even more powerful and efficient methods for constructing optimal designs. We have critically analyzed the use of optimal designs in the Contingent Valuation (CV) literature and proposed new designs for future research. There is still much work to be done, including deriving designs with respect to ' *D*-optimal' and 'median' oriented criteria in both stages of a double bounded CV study, and for the bivariate approach when the dependence parameter is unknown.

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