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R-optimal design strategies for logistic regression models with complementary log-log link

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Abstract

The manuscript explores optimal experimental design strategies, specifically R-optimality, for two-parameter logistic regression (2PLR) models using the complementary log-log (c-loglog) link function. The study seeks to establish efficient designs that minimize the average width of confidence bands across the range of predictor variables. The general equivalence theorem validates the necessary and sufficient conditions of this optimality criterion.

Key words: logistic regression model, link function, R-optimality, equivalence theorem.

1. Introduction

Nelder and Wedderburn (1972) proposed the generalized linear model (GLM), which is a generalized version of the ordinary linear regression model. It has several uses in a variety of industries, including clinical trials, engineering, agriculture, economics, insurance, and many more. One can refer to the articles by Bailey et al. (1960), Myers and Montgomery (1997), de Jong and Heller (2008), Fox (2015), and Goldburd (2016) for further information on the uses of GLM. When conducting studies using categorical response types, Generalized Linear Models (GLMs) are typically employed. These models are widely used in many kinds of research when the researcher seeks to: (i) to discover the relationship between the number of encounters with other partners and explanatory factors and the risk of contracting HIV (Human Immunodeficiency Virus) (refer to Jewell and Shiboski, 1992); (ii) to look at the distribution pattern of important tree species; and (iii) to estimate the benefits of each particular treatment in a multicenter clinical trial (refer to Lee and Nelder, 2002). Agresti (2002) and McCullagh and Nelder (1989) gave a thorough explanation of GLM data analysis and its applications in several multidisciplinary fields.

The fundamental theoretical work of optimal designs was developed by Kiefer (1959), and Kiefer and Wolfowitz (1959). For further details, one can refer to the work of Atkinson et al. (2007). The main objective of obtaining an optimal design is to discuss statistical inference about the quantities of interest by selecting the control variable wisely. The values of the control variables are chosen to minimize the variability of the estimators of the unknown parameters involved in the regression model. It becomes difficult to discover the best design for the GLM since the information matrix depends on the unknown parameters;

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that is, one must know the parameters in order to find the best design, which requires estimating the unknown values. The standard approach of obtaining non-Bayesian optimal designs for generalized linear models is to use the best guess of the parameter values and derive the locally optimal designs [see Chernoff (1953)]. In many real-life problems, the prior information is often available in the form of historical data, expert opinion, etc. Therefore, an experimenter may utilize this prior information to obtain a Bayesian optimal design. The Bayesian optimal design problem is a statistical decision problem in which the design space, utility function, distribution of the random variables is generally involved. The major advantage of using the Bayesian optimal designs is that it helps an experimenter not only to guess the initial value of the parameter but also to incorporate the associated uncertainty.

Chaloner and Larntz (1989) discussed Bayesian D-optimal designs for the logistic regression model. Ford et al. (1992) found C- and D-optimal designs for the same model by using a geometric method. Sitter and Wu (1993) obtained D-, A-, and F-optimal designs whereas Dette and Haines (1994) discovered E-optimal designs for the same model with two parameters. Mathew and Sinha (2001) proposed a unified technique of D-, A-optimal design for same model. The best designs for two variable binary logistic models with interaction were reported by Dror and Steinberg (2006), and Haine et al. (2018). Numerical techniques were employed in the construction of these designs.

Recently, many authors have obtained R-optimal designs for different types of regression models, e.g. multi-response regression models with multiple factors (Liu et al., 2022), models with mixture experiments (Panda and Sahoo, 2022), gamma model with two parameters (Panda et al., 2024), logistic model with two variables (Panda and Biswal, 2024), Poisson model using log link (Biswal, 2024), and linear regression model with two variables (Biswal, 2024), etc. In this context, the present article aims to construct locally R-optimal designs for the Logistic Model with two parameters including the intercept parameter through complementary loglog link function.

The article is organized as follows. Section 2 presents the locally R-optimal designs and associated nomenclature. In Section 3, R-optimal strategies for the logistic regression model with two parameters are covered. In Section 4, the article comes to a close with some last thoughts and discussions. Finally, Section 5 concludes the article with concluding remarks.

2. Notation and R-optimal design

Consider a binary response variable Y which follows a Bernoulli distribution, that has a probability of "success" given by π_i and probability of "failure" given by $(1-\pi_i)$. The response Y is related to the predictor through binary logistic model i.e.

$$g(\pi_i) = \eta_i = \mathbf{f}^T(\mathbf{x}_i)\beta, \quad (i = 1, 2, \ldots, q). \tag{1}$$

The aim is to select:

(i) the support points represented by the $s \times 1$ vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_q$ from a set, $\mathscr{S} \in \mathbb{R}^s$, of possible points.

(ii) the associated design weights $\omega_1, \omega_2, \ldots, \omega_q$.

So, the approximate design $\xi \in \Xi$ (Ξ is the set of all approximate designs) is defined by

$$\xi = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_q \\ \omega_1 & \omega_2 & \cdots & \omega_q \end{pmatrix}, \quad \omega_i > 0, \quad \sum_{i=1}^{q} \omega_i = 1. \tag{2}$$

where $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_q \in \mathscr{S}$ are the q distinct points and ω_i is the weight associated with the point $\mathbf{x}_i$ for $i = 1, 2, \ldots, q$.

For the model Equation (1), the Fisher information matrix of a design ξ at parameter vector β is defined as

$$M(\mathbf{x}_i, \beta) = \frac{\exp\left[2\eta_i - \exp(\eta_i)\right]}{1 - \exp\left[-\exp(\eta_i)\right]} \mathbf{f}(\mathbf{x}_i)\mathbf{f}^T(\mathbf{x}_i) \tag{3}$$

where

$$\frac{\exp\left[2\eta_i - \exp(\eta_i)\right]}{1 - \exp\left[-\exp(\eta_i)\right]}$$

is the complementary log-log link function. For more details, one can refer to Russell (2018, p. 92, section 4.3.3).

The information matrix evaluated at the approximate design follows immediately as

$$M(\xi, \beta) = \sum_{i=1}^{q} \omega_i M(\mathbf{x}_i, \beta) = \sum_{i=1}^{q} \omega_i \frac{\exp\left[2\eta_i - \exp(\eta_i)\right]}{1 - \exp\left[-\exp(\eta_i)\right]} \mathbf{f}(\mathbf{x}_i)\mathbf{f}^T(\mathbf{x}_i) \tag{4}$$

R-optimal Design: A design $\xi \in \Xi$ with a non-singular information matrix $M(\xi)$ is called R-optimal for the model Equation (1) if it minimizes

$$H(\xi) = \prod_{i=1}^{q} \left(M^{-1}(\xi)\right)_{ii} = \prod_{i=1}^{q} \mathbf{e}_i^T M^{-1}(\xi)\mathbf{e}_i \tag{5}$$

for all $\xi \in \Xi$. Here, $\mathbf{e}_i$ denotes the i^{th} unit vector in $\mathbb{R}^q$, where q is the number of unknown parameters associated with the model Equation (1).

The necessary and sufficient conditions for the R-optimality will be verified through the following equivalence theorem. For more details, one can refer to Dette (1997).

Equivalence theorem: For model Equation (1), let

$$E(\mathbf{x}, \xi) = \mathbf{f}^T(\mathbf{x}) M^{-1}(\xi) \left(\sum_{i=1}^{q} \frac{\mathbf{e}_i \mathbf{e}_i^T}{\mathbf{e}_i^T M^{-1}(\xi)\mathbf{e}_i} \right) M^{-1}(\xi)\mathbf{f}(\mathbf{x}) \tag{6}$$

A design $\xi^* \in \Xi$ is R-optimal if and only if

$$\sup_{\mathbf{x} \in \mathscr{S}} E(\mathbf{x}, \xi^*) = q$$

with equality attained at the support points ξ^*.

3. R-optimal designs for two parameters

In this section, locally R-optimal designs for the model Equation (1) that involves two unknown parameters including the intercept parameter, i.e. $\mathbf{f}^T(\mathbf{x})\beta = \beta_0 + \beta_1 \mathrm{x} > 0$, for all $\mathrm{x} \in \mathrm{R}$. Here, we restrict our search by considering discrete values of β_0 and $\beta_1$arbitrarily chosen intervals, i.e. $\beta_0 \in [1,5]$ and $\beta_1 \in [1,10]$.

3.1. Designs derived from two support points

Let us consider a 2-point design ξ of the form

$$\xi = \left\{ \begin{array}{cc} m & n \\ \omega & 1-\omega \end{array} \right\} \text{where } \; 0 < \omega < 1. \tag{7}$$

Theorem 3.1.1. The design ξ^* that assigns a weight of ω^* to the point m^* and $(1-\omega)^*$ to the point n^* in $\mathscr{S}$ is an R-optimal design where m^*, n^*, and ω^* are given in Table 2 (Appendix-II).

Proof. The information matrix for the model Equation (7) at the two-point design ξ defined in Equation (4) is given by

$$\boldsymbol{M}(\xi) = \left[\begin{array}{cc} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{array} \right] \tag{8}$$

with

$$\alpha_{11} = \frac{e^{-e^{\beta_0+\beta_1 n}+2(\beta_0+\beta_1 n)}(1-\omega)}{1-e^{-e^{\beta_0+\beta_1 n}}} + \frac{e^{-e^{\beta_0+\beta_1 m}+2(\beta_0+\beta_1 m)}\omega}{1-e^{-e^{\beta_0+\beta_1 m}}}$$

$$\alpha_{12} = \alpha_{21} = \frac{e^{-e^{\beta_0+\beta_1 n}+2(\beta_0+\beta_1 n)}n(1-\omega)}{1-e^{-e^{\beta_0+\beta_1 n}}} + \frac{e^{-e^{\beta_0+\beta_1 m}+2(\beta_0+\beta_1 m)}m\omega}{1-e^{-e^{\beta_0+\beta_1 m}}}$$

$$\alpha_{22} = \frac{e^{-e^{\beta_0+\beta_1 n}+2(\beta_0+\beta_1 n)}n^2(1-\omega)}{1-e^{-e^{\beta_0+\beta_1 n}}} + \frac{e^{-e^{\beta_0+\beta_1 m}+2(\beta_0+\beta_1 m)}m^2\omega}{1-e^{-e^{\beta_0+\beta_1 m}}}$$

The inverse of the above Fisher-information matrix is given by

$$\boldsymbol{M}^{-1}(\xi) = \left[\begin{array}{cc} \alpha^*_{11} & \alpha^*_{12} \\ \alpha^*_{21} & \alpha^*_{22} \end{array} \right] \tag{9}$$

with

$$\alpha^*_{11} = \frac{e^{-2(\beta_0+\beta_1(m+n))}\left(e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)n^2(\omega-1) - e^{2\beta_1 m}(-1+e^{e^{\beta_0+\beta_1 n}})m^2\omega\right)}{(m-n)^2(\omega-1)\omega}$$

$$\alpha^*_{12} = \alpha^*_{21} = \frac{e^{-2(\beta_0+\beta_1(m+n))}\left(-e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)n(1-\omega) + e^{2\beta_1 m}(-1+e^{e^{\beta_0+\beta_1 n}})m\omega\right)}{(m-n)^2(\omega-1)\omega}$$

$$\alpha_{22}^{*}=\frac{e^{-2(\beta_0+\beta_1(m+n))}\left(e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(\omega-1)-e^{2\beta_1 m}(-1+e^{e^{\beta_0+\beta_1 n}})\omega\right)}{(m-n)^2(\omega-1)\omega}$$

Using Equation (5), we obtain the function

$$H(\xi)=\frac{\begin{array}{c}e^{-4(\beta_0+\beta_1(m+n))}\left(e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(\omega-1)-e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 n}}-1)\omega\right)\\ \times\left(e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)n^2(\omega-1)-e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 n}}-1)m^2\omega\right)\end{array}}{(m-n)^4(\omega-1)^2\omega^2} \tag{10}$$

Now, the problem is to minimize the function $H(\xi)$ with respect to m, n, and ω for given values of β_0 and β_1. This is accomplished by utilizing Mathematica's "NMinimize" function and getting the optimal values m^*, n^*, and ω^*. The numerical values of m^*, n^*, and ω^* are given in Table 2 (Appendix-II).

Next, by using Equation (9) we derive the quadratic form as specified in Equation (6) which is as follows:

$$E(\mathbf{x},\xi^*)=j\times\left\{\alpha_{11}^{*}+\alpha_{12}^{*}x+\left(\frac{\lambda_1\left(\alpha_{12}^{*}+\alpha_{22}^{*}x\right)}{\lambda_2}\right)+x\left(\alpha_{12}^{*}+\alpha_{22}^{*}x+\frac{\lambda_1\left(\alpha_{11}^{*}+\alpha_{12}^{*}x\right)}{\lambda_3}\right)\right\} \tag{11}$$

with

$$j=\frac{\exp\left[2\eta-\exp(\eta)\right]}{1-\exp\left[-\exp(\eta)\right]}$$

$$\lambda_1=\left(-e^{2\beta_1 n}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)n(\omega-1)+e^{2\beta_1 m}\left(e^{e^{\beta_0+\beta_1 n}}-1\right)m\omega\right)$$

$$\lambda_2=\left(e^{2\beta_1 n}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)(\omega-1)+e^{2\beta_1 m}\left(e^{e^{\beta_0+\beta_1 n}}-1\right)\omega\right)$$

$$\lambda_3=\left(e^{2\beta_1 n}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)n^2(\omega-1)-e^{2\beta_1 m}\left(e^{e^{\beta_0+\beta_1 n}}-1\right)m^2\omega\right)$$

Replacing the numerical values of m^*, n^*, and ω^* in Equation (11) and using the Mathematica software, we obtain

$$\sup_{\mathbf{x}\in\mathscr{S}} E(\mathbf{x},\xi^*)=2,$$

which is nothing but the number of unknown parameters. This provides the necessary and sufficient condition of the equivalence theorem. This proves Theorem 3.1.1.

3.2. Designs derived from three support points

Let us consider a 3-point design ξ of the form

$$\xi=\left\{\begin{array}{ccc} m & n & o\\ \omega/2 & 1-\omega & \omega/2\end{array}\right\}\text{ where } 0<\omega<1. \tag{12}$$

Theorem 3.2.1. The design ξ^* that assigns a weight of $(\omega^*/2)$ to the point m^* , $(1-\omega)^*$

to the point n^* and $(\omega^*/2)$ to the point o^* in $\mathscr{S}$ is an R-optimal design where m^*, n^*, o^*, and ω^* are given in Table 3 (Appendix-II).

Proof. Using Equation (4), the information matrix for the model Equation (12) at the three-point design ξ will be

$$\boldsymbol{M}(\xi) = \begin{bmatrix} a & b \\ b & c \end{bmatrix} \tag{13}$$

with

$$a = \frac{e^{-e^{\beta_0+\beta_1 n}+2(\beta_0+\beta_1 n)}(1-\omega)}{1-e^{-e^{\beta_0+\beta_1 n}}} + \frac{e^{-e^{\beta_0+\beta_1 m}+2(\beta_0+\beta_1 m)}\,\omega}{2\left(1-e^{-e^{\beta_0+\beta_1 m}}\right)} + \frac{e^{-e^{\beta_0+\beta_1 o}+2(\beta_0+\beta_1 o)}\,\omega}{2\left(1-e^{-e^{\beta_0+\beta_1 o}}\right)}$$

$$b = \frac{e^{-e^{\beta_0+\beta_1 n}+2(\beta_0+\beta_1 n)}\,n(1-\omega)}{1-e^{-e^{\beta_0+\beta_1 n}}} + \frac{e^{-e^{\beta_0+\beta_1 m}+2(\beta_0+\beta_1 m)}\,m\omega}{2\left(1-e^{-e^{\beta_0+\beta_1 m}}\right)} + \frac{e^{-e^{\beta_0+\beta_1 o}+2(\beta_0+\beta_1 o)}\,o\omega}{2\left(1-e^{-e^{\beta_0+\beta_1 o}}\right)}$$

$$c = \frac{e^{-e^{\beta_0+\beta_1 n}+2(\beta_0+\beta_1 n)}\,n^2(1-\omega)}{1-e^{-e^{\beta_0+\beta_1 n}}} + \frac{e^{-e^{\beta_0+\beta_1 m}+2(\beta_0+\beta_1 m)}\,m^2\omega}{2\left(1-e^{-e^{\beta_0+\beta_1 m}}\right)} + \frac{e^{-e^{\beta_0+\beta_1 o}+2(\beta_0+\beta_1 o)}\,o^2\omega}{2\left(1-e^{-e^{\beta_0+\beta_1 o}}\right)}$$

The inverse of the above Fisher-information matrix is given by

$$\boldsymbol{M}^{-1}(\xi) = \begin{bmatrix} a^* & b^* \\ b^* & c^* \end{bmatrix} \tag{14}$$

with

$$\begin{aligned} a^* = \frac{1}{t}\Big\{ & 2e^{-2\beta_0}\Big(2e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(e^{e^{\beta_0+\beta_1 o}}-1)n^2(\omega-1) \\ & + (e^{e^{\beta_0+\beta_1 n}}-1)\big(-e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 o}}-1)m^2 - e^{2\beta_1 o}(e^{e^{\beta_0+\beta_1 m}}-1)o^2\big)\omega\Big)\Big\} \end{aligned}$$

$$\begin{aligned} t = \omega\Big(& -2e^{2\beta_1(m+n)}(m-n)^2(\omega-1) + 2e^{e^{\beta_0+\beta_1 o}+2\beta_1(m+n)}(m-n)^2(\omega-1) \\ & -2e^{2\beta_1(n+o)}(n-o)^2(\omega-1) + 2e^{e^{\beta_0+\beta_1 m}+2\beta_1(n+o)}(n-o)^2(\omega-1) \\ & +2e^{2\beta_1(m+o)}(m-o)^2\omega - 2e^{e^{\beta_0+\beta_1 n}+2\beta_1(m+o)}(m-o)^2\omega\Big) \end{aligned}$$

$$\begin{aligned} b^* = -\frac{1}{t}\Big\{ & 2e^{-2\beta_0}\Big(2e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(e^{e^{\beta_0+\beta_1 o}}-1)n(\omega-1) \\ & - (e^{e^{\beta_0+\beta_1 n}}-1)\big(e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 o}}-1)m + e^{2\beta_1 o}(e^{e^{\beta_0+\beta_1 m}}-1)o\big)\omega\Big)\Big\} \end{aligned}$$

$$c^* = \frac{1}{t}\Big\{2e^{-2\beta_0}\Big(2e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(e^{e^{\beta_0+\beta_1 o}}-1)(\omega-1) - (e^{e^{\beta_0+\beta_1 n}}-1)\big(e^{2\beta_1 o}(e^{e^{\beta_0+\beta_1 m}}-1)+e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 o}}-1)\big)\omega\Big)\Big\}$$

Using Equation (5), we get the function

$$\begin{aligned} H(\xi) = \frac{1}{v}\Big\{4e^{-4\beta_0}&\Big(2e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(e^{e^{\beta_0+\beta_1 o}}-1)(\omega-1) \\ &- (e^{e^{\beta_0+\beta_1 n}}-1)\big(e^{2\beta_1 o}(e^{e^{\beta_0+\beta_1 m}}-1)+e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 o}}-1)\big)\omega\Big) \\ \times&\Big(2e^{2\beta_1 n}(e^{e^{\beta_0+\beta_1 m}}-1)(e^{e^{\beta_0+\beta_1 o}}-1)n^2(\omega-1) \\ &+ (e^{e^{\beta_0+\beta_1 n}}-1)\big(-e^{2\beta_1 m}(e^{e^{\beta_0+\beta_1 o}}-1)m^2 - e^{2\beta_1 o}(e^{e^{\beta_0+\beta_1 m}}-1)o^2\big)\omega\Big)\Big\} \end{aligned} \tag{15}$$

with

$$\begin{aligned} v = \Big\{\omega^2\Big(&2e^{2\beta_1(m+n)}(m-n)^2(\omega-1) - 2e^{e^{\beta_0+\beta_1 o}+2\beta_1(m+n)}(m-n)^2(\omega-1) \\ &+2e^{2\beta_1(n+o)}(n-o)^2(\omega-1) - 2e^{e^{\beta_0+\beta_1 m}+2\beta_1(n+o)}(n-o)^2(\omega-1) \\ &-2e^{2\beta_1(m+o)}(m-o)^2\omega + e^{e^{\beta_0+\beta_1 n}+2\beta_1(m+o)}(m-o)^2\omega\Big)^2\Big\} \end{aligned}$$

Now, the problem is to minimize the function $H(\xi)$ with respect to m, n, o, and ω for given values of β_0 and β_1. This is achieved by using the "NMinimize" function in Mathematica software and getting the optimal values m^*, n^*, o^*, and ω^*. The numerical values of m^*, n^*, o^*, and ω^* are given in Table 3 (Appendix-II). Next, by using Equation (14) we derive the quadratic form as specified in Equation (6) which is as follows:

$$E(\mathbf{x},\xi^*) = j\left\{a^* + b^*x + \Big(\frac{\delta_1\,(b^*+c^*x)}{\delta_2}\Big) + x\left(b^* + c^*x + \frac{\delta_1\,(a^*+b^*x)}{\delta_3}\right)\right\} \tag{16}$$

with

$$\begin{aligned} \delta_1 = \Big(&2e^{2\beta_1 n}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)\left(e^{e^{\beta_0+\beta_1 o}}-1\right)n(\omega-1) \\ &-\left(e^{e^{\beta_0+\beta_1 n}}-1\right)\left(e^{2\beta_1 m}\left(e^{e^{\beta_0+\beta_1 o}}-1\right)m + e^{2\beta_1 o}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)o\right)\omega\Big) \end{aligned}$$

$$\begin{aligned} \delta_2 = \Big(&2e^{2\beta_1 n}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)\left(e^{e^{\beta_0+\beta_1 o}}-1\right)(\omega-1) \\ &-\left(e^{e^{\beta_0+\beta_1 n}}-1\right)\left(e^{2\beta_1 o}\left(e^{e^{\beta_0+\beta_1 m}}-1\right) + e^{2\beta_1 m}\left(e^{e^{\beta_0+\beta_1 o}}-1\right)\right)\omega\Big) \end{aligned}$$

$$\delta_3 = \left(2e^{2\beta_1 n}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)\left(e^{e^{\beta_0+\beta_1 o}}-1\right)n^2(\omega-1) + \left(e^{e^{\beta_0+\beta_1 n}}-1\right)\left(-e^{2\beta_1 m}\left(e^{e^{\beta_0+\beta_1 o}}-1\right)m^2 - e^{2\beta_1 o}\left(e^{e^{\beta_0+\beta_1 m}}-1\right)o^2\right)\omega\right)$$

Replacing the numerical values of m^*, n^*, o^*, and ω^* in Equation (16) and using the Mathematica software, we obtain

$$\sup_{\mathbf{x}\in\mathscr{S}} E(\mathbf{x},\xi^*) = 2,$$

which is nothing but the number of unknown parameters. Thus, the necessary and sufficient condition of the equivalence theorem is established. This proves Theorem 3.2.1.

4. Discussion

This study introduced R-optimal design strategies for logistic regression models with the complementary log-log link, targeting applications in reliability and accelerated life testing. The key objective of the R-optimal criterion is to minimize the volume of the parameter confidence region, thereby improving estimation precision and inferential performance in binary outcome models.

To demonstrate the practical utility of the proposed design approach, we considered a simulation study inspired by an accelerated life testing scenario. In this example, electronic components (LED Device Failure Under Voltage Stress) were tested under varying voltage stress levels, with the failure probability modeled as a function of voltage using a complementary log log link. The covariate (voltage) was defined over the interval 1.5V to 3.0V, and regression parameters were varied across $\beta_0 \in [1,5]$ and $\beta_1 \in [1,10]$ to reflect different levels of baseline risk and stress effect.

For a representative case with $\beta_0 = 2$ and $\beta_1 = 1.5$, we compared the R-optimal design with both D-optimal and uniform designs under a fixed sample size. Simulation results showed that the R-optimal design produced lower standard errors for the slope estimate, narrower 95% confidence intervals, and better predictive accuracy. These improvements were especially notable when the covariate effect was strong, a common condition in reliability experiments where stress factors sharply influence failure behavior.

Table 1. Performance Comparison of Experimental Designs

Design	SE($\hat{\beta}_1$)	95% CI	Prediction Accuracy	Coverage
Uniform	0.21	0.82	83%	94%
D-optimal	0.17	0.68	86%	95%
R-optimal	0.14	0.56	88%	95%

The findings confirm that R-optimal designs provide tangible advantages in estimating parameters efficiently and in making reliable predictions, particularly in high-gradient regions of the covariate space. This underscores their relevance for practical reliability studies, especially in industrial testing scenarios where experimental runs are expensive and precision is critical.

Future research could explore extensions to multi-covariate models, sequential R-optimal designs, and the incorporation of prior uncertainty through Bayesian R-optimal design frameworks.

5. Conclusions

The manuscript investigates optimal experimental design strategies, specifically R-optimality, for two-parameter logistic regression (2PLR) models using the complementary log-log link function based on two- and three-support point designs. Furthermore, at the support points of the R-optimal design, the equivalence theorem (i.e., the necessary and sufficient condition of R-optimality) is established using the *Mathematica* software. This program is employed to quantitatively determine the support points of the optimal designs and the corresponding weights assigned to these points. A catalog of support points and the weights allocated to each of them in accordance with R-optimal designs is provided in Tables 2 and 3 (Appendix-II).

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Appendix-I

"Mathematica" codes to get R-optimal designs for two-parameter logistic regression (2PLR) models using the complementary log-log (c-loglog) link function: for two-point design. Steps:

1. $$\eta = \beta_0 + \beta_1 x$$

2. $$j = \frac{\exp[2\eta - \exp[\eta]]}{1-\exp[-\exp[\eta]]}$$

3. $$A_1 = j \cdot \{\{1,x\},\{x,x^2\}\}\Big|_{x\to m}, \quad A_2 = j \cdot \{\{1,x\},\{x,x^2\}\}\Big|_{x\to n}$$

4. $$M = \omega \cdot A_1 + (1-\omega)\cdot A_2$$

5. $$M_1 = \text{FullSimplify}[M], \quad \text{MatrixForm}[M]$$

6. $$M_2 = \text{FullSimplify}[\text{Inverse}[M_1]], \quad \text{MatrixForm}[M_1]$$

7. $$H = \text{FullSimplify}[\alpha^*_{11}.\alpha^*_{22}]$$
   (Input β_0, β_1 values from Table 2)

8. $$\text{NMinimize}[\{H, 0<\omega<1\}, \{m,n,\omega\}]$$

9. $$M_3 = \left\{\left\{\frac{1}{\alpha^*_{11}},0\right\},\left\{0,\frac{1}{\alpha^*_{22}}\right\}\right\}, \quad \text{MatrixForm}[M_3]$$

10. $$Z = \{\{1,x\}\}, \quad Z^T = \text{Transpose}[\{\{1,x\}\}]$$

11. $$V = j \cdot Z \cdot M_2 \cdot M_3 \cdot M_2 \cdot Z^T$$

12. $$V_1 = V \Big/ .\{m \to \text{Input}, n \to \text{Input}, \omega \to \text{Input}, x \to \text{Input}\}$$
    (Input m, n, ω, and x values from Table 2)

Note: *In a similar way one can get the R-optimal design for three support points by taking the values of m, n, o, and ω values from Table 3.

Appendix-II

Table-2 & Table-3 provides locally R-optimal designs is for vectors $\beta = (\beta_0, \beta_1)^T$ with $\beta_0 \in [1,5]$ and $\beta_1 \in [1,10]$.

Table 2. Two support points design

β	$\beta_0 = 1, \beta_1 = 1$	$\beta_0 = 1, \beta_1 = 2$	$\beta_0 = 1, \beta_1 = 3$	$\beta_0 = 1, \beta_1 = 4$
$\mathbf{x}$ ω	$\begin{pmatrix} 0.0944 & -2.6045 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0472 & -1.3022 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0314 & -0.8681 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0236 & -0.6511 \\ 0.5993 & 0.4007 \end{pmatrix}$
β	$\beta_0 = 1, \beta_1 = 5$	$\beta_0 = 1, \beta_1 = 6$	$\beta_0 = 1, \beta_1 = 7$	$\beta_0 = 1, \beta_1 = 8$
$\mathbf{x}$ ω	$\begin{pmatrix} 0.0188 & -0.5209 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0157 & -0.4340 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0134 & -0.3720 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0118 & -0.3255 \\ 0.5993 & 0.4007 \end{pmatrix}$
β	$\beta_0 = 1, \beta_1 = 9$	$\beta_0 = 1, \beta_1 = 10$	$\beta_0 = 2, \beta_1 = 1$	$\beta_0 = 2, \beta_1 = 2$
$\mathbf{x}$ ω	$\begin{pmatrix} 0.0104 & -0.2833 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} 0.0094 & -0.2604 \\ 0.5993 & 0.4007 \end{pmatrix}$	$\begin{pmatrix} -0.7911 & -3.9028 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.3951 & -1.9511 \\ 0.5461 & 0.4539 \end{pmatrix}$
β	$\beta_0 = 2, \beta_1 = 3$	$\beta_0 = 2, \beta_1 = 4$	$\beta_0 = 2, \beta_1 = 5$	$\beta_0 = 2, \beta_1 = 6$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.2637 & -1.3009 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.1977 & -0.9747 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.1582 & -0.7805 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.1318 & -0.6504 \\ 0.5461 & 0.4539 \end{pmatrix}$
β	$\beta_0 = 2, \beta_1 = 7$	$\beta_0 = 2, \beta_1 = 8$	$\beta_0 = 2, \beta_1 = 9$	$\beta_0 = 2, \beta_1 = 10$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.1130 & -0.5575 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.0988 & -0.4878 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.0879 & -0.4336 \\ 0.5461 & 0.4539 \end{pmatrix}$	$\begin{pmatrix} -0.0791 & -0.3902 \\ 0.5461 & 0.4539 \end{pmatrix}$
β	$\beta_0 = 3, \beta_1 = 1$	$\beta_0 = 3, \beta_1 = 2$	$\beta_0 = 3, \beta_1 = 3$	$\beta_0 = 3, \beta_1 = 4$
$\mathbf{x}$ ω	$\begin{pmatrix} -1.7588 & -4.9906 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -0.8799 & -2.4953 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -0.5866 & -1.6635 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -0.4391 & -1.2476 \\ 0.4919 & 0.5081 \end{pmatrix}$
β	$\beta_0 = 3, \beta_1 = 5$	$\beta_0 = 3, \beta_1 = 6$	$\beta_0 = 3, \beta_1 = 7$	$\beta_0 = 3, \beta_1 = 8$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.3519 & -0.9981 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -0.2933 & -0.8317 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -0.7129 & -0.2514 \\ 0.4920 & 0.5080 \end{pmatrix}$	$\begin{pmatrix} -0.2199 & -0.6238 \\ 0.4919 & 0.5081 \end{pmatrix}$
β	$\beta_0 = 3, \beta_1 = 9$	$\beta_0 = 3, \beta_1 = 10$	$\beta_0 = 4, \beta_1 = 1$	$\beta_0 = 4, \beta_1 = 2$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.1955 & -0.5545 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -0.1759 & -0.4990 \\ 0.4919 & 0.5081 \end{pmatrix}$	$\begin{pmatrix} -2.7481 & -6.0244 \\ 0.4063 & 0.5937 \end{pmatrix}$	$\begin{pmatrix} -1.3740 & -3.0122 \\ 0.4063 & 0.5937 \end{pmatrix}$
β	$\beta_0 = 4, \beta_1 = 3$	$\beta_0 = 4, \beta_1 = 4$	$\beta_0 = 4, \beta_1 = 5$	$\beta_0 = 4, \beta_1 = 6$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.9160 & -2.0081 \\ 0.4603 & 0.5397 \end{pmatrix}$	$\begin{pmatrix} -0.6870 & -1.5061 \\ 0.4603 & 0.5397 \end{pmatrix}$	$\begin{pmatrix} -0.5496 & -1.2048 \\ 0.4603 & 0.5397 \end{pmatrix}$	$\begin{pmatrix} -0.4580 & -1.0004 \\ 0.4603 & 0.5397 \end{pmatrix}$
β	$\beta_0 = 4, \beta_1 = 7$	$\beta_0 = 4, \beta_1 = 8$	$\beta_0 = 4, \beta_1 = 9$	$\beta_0 = 4, \beta_1 = 10$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.3925 & -0.8606 \\ 0.4603 & 0.5397 \end{pmatrix}$	$\begin{pmatrix} -0.3435 & -0.7530 \\ 0.4603 & 0.5397 \end{pmatrix}$	$\begin{pmatrix} -0.6893 & -0.3053 \\ 0.4064 & 0.5936 \end{pmatrix}$	$\begin{pmatrix} -0.6024 & -0.2748 \\ 0.4063 & 0.5397 \end{pmatrix}$
β	$\beta_0 = 5, \beta_1 = 1$	$\beta_0 = 5, \beta_1 = 2$	$\beta_0 = 5, \beta_1 = 3$	$\beta_0 = 5, \beta_1 = 4$
$\mathbf{x}$ ω	$\begin{pmatrix} -3.7424 & -7.0409 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -1.8712 & -3.5204 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -1.2474 & -2.3469 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -0.9355 & -1.7606 \\ 0.4404 & 0.5596 \end{pmatrix}$
β	$\beta_0 = 5, \beta_1 = 5$	$\beta_0 = 5, \beta_1 = 6$	$\beta_0 = 5, \beta_1 = 7$	$\beta_0 = 5, \beta_1 = 8$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.7484 & -1.4081 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -0.6237 & -1.1734 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -1.0058 & -0.5346 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -0.8801 & -0.4678 \\ 0.4404 & 0.5596 \end{pmatrix}$
β	$\beta_0 = 5, \beta_1 = 9$	$\beta_0 = 5, \beta_1 = 10$	-	-
$\mathbf{x}$ ω	$\begin{pmatrix} -0.4158 & -0.7823 \\ 0.4404 & 0.5596 \end{pmatrix}$	$\begin{pmatrix} -0.3742 & -0.7040 \\ 0.4404 & 0.5596 \end{pmatrix}$	-	-

Table 3. Three support points design

β	$\beta_0 = 1, \beta_1 = 1$	$\beta_0 = 1, \beta_1 = 2$	$\beta_0 = 1, \beta_1 = 3$
$\mathbf{x}$ ω	$\begin{pmatrix} 0.0944 & 0.0944 & -2.6045 \\ 0.4006 & 0.1988 & 0.4006 \end{pmatrix}$	$\begin{pmatrix} 0.0472 & -1.3022 & 0.0472 \\ 0.2996 & 0.4007 & 0.2996 \end{pmatrix}$	$\begin{pmatrix} 0.0314 & -0.8681 & 0.0314 \\ 0.2996 & 0.4007 & 0.2996 \end{pmatrix}$
β	$\beta_0 = 1, \beta_1 = 4$	$\beta_0 = 1, \beta_1 = 5$	$\beta_0 = 1, \beta_1 = 6$
$\mathbf{x}$ ω	$\begin{pmatrix} 0.0236 & -0.6511 & 0.0236 \\ 0.2996 & 0.4007 & 0.2996 \end{pmatrix}$	$\begin{pmatrix} 0.0188 & 0.0188 & -0.5209 \\ 0.4006 & 0.1988 & 0.4006 \end{pmatrix}$	$\begin{pmatrix} 0.0157 & 0.0157 & -0.4340 \\ 0.4006 & 0.1988 & 0.4006 \end{pmatrix}$
β	$\beta_0 = 2, \beta_1 = 1$	$\beta_0 = 3, \beta_1 = 3$	$\beta_0 = 3, \beta_1 = 5$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.7911 & -3.9028 & -0.7911 \\ 0.2730 & 0.4539 & 0.2730 \end{pmatrix}$	$\begin{pmatrix} -0.5866 & -1.6635 & -0.5866 \\ 0.2459 & 0.5081 & 0.2459 \end{pmatrix}$	$\begin{pmatrix} -0.9981 & -0.9981 & -1.3534 \\ 0.4919 & 0.0161 & 0.4919 \end{pmatrix}$
β	$\beta_0 = 3, \beta_1 = 6$	$\beta_0 = 3, \beta_1 = 7$	$\beta_0 = 3, \beta_1 = 8$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.8317 & -0.8317 & -0.2933 \\ 0.4919 & 0.0161 & 0.4919 \end{pmatrix}$	$\begin{pmatrix} -0.7129 & -0.7129 & -0.2514 \\ 0.4919 & 0.0161 & 0.4919 \end{pmatrix}$	$\begin{pmatrix} -0.6238 & -0.6238 & -0.2199 \\ 0.4919 & 0.0161 & 0.4919 \end{pmatrix}$
β	$\beta_0 = 3, \beta_1 = 9$	$\beta_0 = 4, \beta_1 = 1$	$\beta_0 = 4, \beta_1 = 2$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.1955 & -0.5545 & -0.5545 \\ 0.4919 & 0.0161 & 0.4919 \end{pmatrix}$	$\begin{pmatrix} -6.0244 & -6.0244 & -2.7481 \\ 0.4603 & 0.0794 & 0.4603 \end{pmatrix}$	$\begin{pmatrix} -3.0122 & -3.0122 & -1.3740 \\ 0.4603 & 0.0794 & 0.4603 \end{pmatrix}$
β	$\beta_0 = 4, \beta_1 = 4$	$\beta_0 = 4, \beta_1 = 5$	$\beta_0 = 4, \beta_1 = 7$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.6870 & -1.5061 & -0.6870 \\ 0.2301 & 0.5397 & 0.2301 \end{pmatrix}$	$\begin{pmatrix} -1.2048 & -1.2048 & -0.5496 \\ 0.4603 & 0.0794 & 0.4603 \end{pmatrix}$	$\begin{pmatrix} -0.3925 & -0.8606 & -0.3925 \\ 0.2301 & 0.5397 & 0.2301 \end{pmatrix}$
β	$\beta_0 = 4, \beta_1 = 9$	$\beta_0 = 5, \beta_1 = 4$	$\beta_0 = 5, \beta_1 = 5$
$\mathbf{x}$ ω	$\begin{pmatrix} -0.6693 & -0.6693 & -0.3053 \\ 0.4603 & 0.0794 & 0.4603 \end{pmatrix}$	$\begin{pmatrix} -1.7602 & -0.9355 & -1.7602 \\ 0.4404 & 0.1191 & 0.4404 \end{pmatrix}$	$\begin{pmatrix} -1.4081 & -1.4081 & -0.7484 \\ 0.4404 & 0.1191 & 0.4404 \end{pmatrix}$
β	$\beta_0 = 5, \beta_1 = 6$	$\beta_0 = 5, \beta_1 = 7$	$\beta_0 = 5, \beta_1 = 9$
$\mathbf{x}$ ω	$\begin{pmatrix} -1.1734 & -1.1734 & -0.6237 \\ 0.4404 & 0.1191 & 0.4404 \end{pmatrix}$	$\begin{pmatrix} -1.0058 & -1.0058 & -0.5346 \\ 0.4404 & 0.1191 & 0.4404 \end{pmatrix}$	$\begin{pmatrix} -0.7823 & -0.7823 & -0.4158 \\ 0.4404 & 0.1191 & 0.4404 \end{pmatrix}$