D-OPTIMAL DESIGNS FOR POLYNOMIAL POISSON REGRESSION MODELS ON CONSTRAINED DESIGN SPACE

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ABSTRACT: This research considers Polynomial Poisson regression models with orders two and three in one variable for design optimization using constrained design space [0, 1]. The D-optimality criterion is explicitly examined in this study. Imperialist competitive algorithmic procedure was used to generate the optimal design points and weights. The quadratic Poisson regression model was found to be D-optimal at 3-design points: 0.0000, 0.4142 and 1.0000 with design weights 0.3333, 0.3333 and 0.3333 respectively. The cubic Poisson regression model was optimal at 4-design points 0.0000, 0.2204, 0.6596 and 1.0000, each with design weights of 0.25. The constructed D-optimal designs were verified using the general equivalence theorem via the maximum sensitivity function of each model.
Keywords: D-optimality, Design Point, Fisher Information Matrix and Polynomial Poisson Regression Model

1. INTRODUCTION

Optimal designs depict the presence of highly efficient designs in relation to some statistical criteria. Classification of optimal designs is systematically conceptualized from design efficiency through available information. Improvement in statistical power and precise estimation of model parameters are aided by optimal designs through minimization of the variances of estimators [9].

Generation of G-optimum designs for a polynomial of order six in one variable serves as a foundational study on design optimization [10].

D-optimal designs were comparatively constructed by [11] via the determinant of Fisher information matrix.

Construction of D-optimal designs from a model involving variables of first-order term was considered by [2] and biases were evaded from the omission of higher-order terms through design rotation.

Smith's findings on G-optimum designs pertaining to polynomial model in one variable were generalized and the support points were the roots of the Legendre polynomial [7].

Demonstration of non-linear models with Chemical kinetics for the generation of locally D-optimum designs was illustrated by [3].

Exact D-optimal designs of experiments involving nonlinear regression models through the minimization of determinant of approximate variance-covariance matrix of the estimates of parameters can be obtained. The intrinsic and nonlinearity in the parameter-effects accounts for the inability of the determinant in giving a correct suggestion about the size of combined inferential region for the parameters. Investigations of experimental designs that aid the minimization of second-order volume approximations were examined and the dependence of the investigated designs on the noise, confidence levels and parameterization used were also evaluated. When sequential procedure is employed, the quadratic designs are dependent on the residuals from previous experiments and on the kind of inference [8].

Linear models involving a discrete factor and some continuous factors were studied by [12]. A considerable optimal design problem was facilitated through the imposition of restriction of equal regression design measure on all treatment levels. The development of a basically complete class as regards D-optimality for inference on the treatment effects, the regression parameters, and the combined parameter vector by the product designs was presented. Characterizations of optimal designs in terms of optimality for pure regression settings were produced using the theorems.

Regression models involving low-degree polynomial terms using the theoretical approach of canonical moments produce D-optimal designs. When the number of unknown model parameters is even, equal weights are placed by the optimal design on each zero of the polynomial of Jacobi. Also, when the number of unknown model parameters is odd, the technique and illustrations on the constructions of optimal designs and weights are presented [5].

Certain logistic regression models with quadratic terms and varying sample sizes were studied by [4] for the derivation of D-optimal designs. The performances of the designs as regards maximum likelihood estimation of model parameters, as well as the estimation of optimum response function were examined using various sample sizes and compared with some non-optimal designs. The asymptotic and small sample distributions of the maximum likelihood estimator were observed to be inconsistent. Evaluations of the designs were examined depending on the level to which they suffered from the problem of absence of maximum likelihood estimator. The various designs were compared for the probability of the presence of maximum likelihood estimate. Absence of maximum likelihood estimate has been established as a difficulty in estimating quadratic logistic model.
[6] investigated Poisson regression models containing three binary predictor variables. Application of the models was considered on rule-based problems in educational and psychological testing. Locally D-optimal designs were generated to provide efficient estimation for the parameters of the models. For the active models, eight out of seventy saturated designs were shown to exhibit local D-optimality. The classical fractional factorial designs which are two additional saturated designs exhibited local-D-optimality for vanishing effects.
Ordered categorical responses and cumulative link models were studied by [13] for the generation of D-optimal designs. The conditions that are essential, as well as adequate for a design allocation to be locally D-optimal were derived for a predetermined set of design points and algorithms that are efficient in constructing approximate and exact designs were developed. The dependence of the quantity of design points in a design that is minimally supported on the number of predictors that can be much less than the number of parameters in the model was established. Non-uniformity in the allocation of a minimally D-optimal design on its support points was established.
Solutions in an obvious, succinct and effective manner are aided through a properly planned experiment. Additional information to simple plots is usually needed for the initial analysis in revealing the nature of dependence of responses on design factors. Parameters dependence can be demonstrated through the estimation of parameters via least squares method. Good experiments are expected to produce results of estimated parameters with minimum variances and covariances. Functions of variances are minimized by optimally designing experiments, thereby aiding provision of reasonable parameter estimates and predictions of responses [1].
Optimal experimental designs play vital roles in several fields of applications. For instance, it can be widely applied when conducting research in medicine, biology, agriculture and industries. Generation of optimal experimental designs is model-dependent and optimization process involves the Fisher information matrix. For example, when examining a compound in dose-response studies, good knowledge, in addition with proper characterization of dose linked with its reaction is a major step to be considered because poor knowledge about the dose response record can have an undeviating effect when estimating the chosen level of dose.
In the case of drug development setting, choosing a very high quantity of dose may lead into intolerable toxicity and harmfulness while selecting too little quantity of dose can reduce the possibility of having effectiveness in the confirmatory stage, this can therefore reduce the possibility of obtaining endorsement and approval for the drug from the regulatory body. Different levels of penalties exist for choosing an incorrect dose level when a new compound is to be developed.
The Poisson regression model has a basic assumption - the distribution of the response variable follows a Poisson distribution and the expectation of the response variable can be linearly molded with the unknown coefficients through logarithmic transformation.
Poisson regression models are nonlinear in nature; they fit in the set of generalized linear models. The log link function describes the linear relationship between the mean response and the predictors.
This study considers the construction of D-optimal designs for Quadratic and Cubic Poisson regression models in one variable.
The paper is organized as follows. The introduction is presented in section 1 where the aim, scope and literature review are discussed. Materials and methods are presented in the second section which contains the Poisson regression model and the procedures for the construction of D-optimal designs are discussed. Section 3 presents the results and discussions while the conclusion is presented in section 4.

2. MATERIALS AND METHODS

2.1 Poisson Regression Model

Generally, the Poisson regression model can be written as equation (1)

$$y_{ij} \sim Poisson\ (\mu_i) \qquad (1)$$

The mean response, μ_i, can be expressed as equation (2)

$$\mu_i = exp(X_i'\ \beta) \qquad (2)$$

where,
y_{ij} are the response variables,

μ_i is the expectation of the response variable at the i^{th} design point,
X_i' is the design matrix containing factors, X_i, (i = 1, 2, …), and
β is a vector of parameters.
This research is aimed at developing D-optimal experimental designs for the Polynomial Poisson regression models in equations (3) and (4) respectively.

$$\mu_i = exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2) \quad (3)$$
$$\mu_i = exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3) \quad (4)$$

A general assumption for a Poisson regression model is that the response variables are nonnegative. An approximate or a near-optimal design, $\xi \in \Xi$, in design space, χ, containing definite design points is denoted by equation (5)

$$\xi = \begin{Bmatrix} x_1, x_2, \cdots, x_s \\ w_1, w_2, \cdots, w_s \end{Bmatrix} \quad (5)$$

where,
$x_i \in \chi$ (are the design points),
$\boldsymbol{\chi}$ is a compact subset of real numbers, and
w_i are the weights of the design at each design point satisfying $0 < w_i \le 1$ and $\sum_{i=1}^{s} w_i = 1$.

2.2 Construction of D-optimal Designs

The D-optimum design searches for the maximization of the determinant of the Fisher information matrix or equivalently searches for the minimization of the determinant of the inverse of the Fisher information matrix. Mathematically, if the dimension of β is $p \times 1$, the Fisher information matrix, $\mathrm{I}(X,\beta)$ is a $p \times p$ matrix denoted in (6)

$$I\,(\mathrm{X},\beta) = -E\left[\frac{\partial^2 \log(L(\mathrm{X},\beta))}{\partial\beta\partial\beta'}\right] \quad (6)$$

where,

$(L(\mathrm{X}, \beta)$ is the likelihood function of the data, and
X, is the design matrix.
The general D-optimal criterion searches for the minimization of the generalized variance of $\hat{\beta}$, equivqlently maximizing the determinant of the Fisher information matrix.
The commonly used D-optimal criterion is defined by (7)

$$\max_{X \in \mathcal{D}} det\left[\frac{\mathrm{I}\,(\mathrm{X},\beta)}{n}\right], \quad (7)$$

where,
n is the total sample size, and
$\boldsymbol{\mathcal{D}}$ is the set of all possible designs.
Since n is usually fixed, the D-optimal design is obtained by maximizing the determinant of the Fisher information matrix in (6).

The information matrix is specifically defined in terms of a design measure as $\mathrm{M}(\xi;\ \beta)$.
D-optimal= min[(|(X'X)|)$^{-1}$] or max[|(X'X)|].

Considering the model in (3),

$$ln\,\mu_i = \eta_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 \quad (8)$$

Here,
$$f'\,(x_i) = (1, \quad x_i, \quad x_i^2) \quad (9)$$

where,
$f'(x_i)$ is the i^{th} row of X, a known function of predictor variables.
The element of the Fisher information matrix obtained is expressed in (10)

$$\mathrm{M} = \mathrm{X'X} = \begin{bmatrix} 1 & x_i & x_i^2 \\ x_i & x_i^2 & x_i^3 \\ x_i^2 & x_i^3 & x_i^4 \end{bmatrix} \quad (10)$$

and the information matrix in terms of a saturated design is presented in equation (11)

$$\mathrm{M}(\xi;\ \beta_0, \beta_1, \beta_2) = \begin{bmatrix} \sum_{i=1}^{3} w_i\mu_i & \sum_{i=1}^{3} w_i\mu_i\, x_i & \sum_{i=1}^{3} w_i\mu_i\, x_i^2 \\ \sum_{i=1}^{3} w_i\mu_i\, x_i & \sum_{i=1}^{3} w_i\mu_i\, x_i^2 & \sum_{i=1}^{3} w_i\mu_i x_i^3 \\ \sum_{i=1}^{3} w_i\mu_i\, x_i^2 & \sum_{i=1}^{3} w_i\mu_i x_i^3 & \sum_{i=1}^{3} w_i\mu_i x_i^4 \end{bmatrix} \quad (11)$$

The D-optimal design maximizes $\mathrm{M}(\xi;\ \beta_0, \beta_1, \beta_2)$ of (11).
The Fisher information matrix can be expressed in compact form as equation (12)

$$\mathrm{M}(\xi;\ \beta_0, \beta_1, \beta_2) = \sum w_i\mu_i f(x_i)\, f'(x_i) \quad (12)$$

and more compactly, as equation (13)

$$\mathrm{M}(\xi;\ \beta_0, \beta_1, \beta_2) = X'WX \quad (13)$$

where,
w_i represent the weights of the support points,
$\mu_i = \exp\,(\eta_i)$, is the mean response of the i^{th} design point,
ξ is the design measure, and

$W = diag\{w_i\,\mu_i\}$, and
$X = [f(\mathrm{x_i}),\ f(x_i^2)]$.

Considering the cubic Poisson regression model, the information matrix for the model in equation (4) is obtained as equation (14)

$$M(\xi;\ \beta_0,\beta_1,\beta_2,\beta_3) = \begin{bmatrix} \sum_{i=1}^{4} w_i\mu_i & \sum_{i=1}^{4} w_i\mu_i x_i & \sum_{i=1}^{4} w_i\mu_i {x_i}^2 & \sum_{i=1}^{4} w_i\mu_i {x_i}^3 \\ \sum_{i=1}^{4} w_i\mu_i x_i & \sum_{i=1}^{4} w_i\mu_i {x_i}^2 & \sum_{i=1}^{4} w_i\mu_i {x_i}^3 & \sum_{i=1}^{4} w_i\mu_i {x_i}^4 \\ \sum_{i=1}^{4} w_i\mu_i {x_i}^2 & \sum_{i=1}^{4} w_i\mu_i {x_i}^3 & \sum_{i=1}^{4} w_i\mu_i {x_i}^4 & \sum_{i=1}^{4} w_i\mu_i {x_i}^5 \\ \sum_{i=1}^{4} w_i\mu_i {x_i}^3 & \sum_{i=1}^{4} w_i\mu_i {x_i}^4 & \sum_{i=1}^{4} w_i\mu_i {x_i}^5 & \sum_{i=1}^{4} w_i\mu_i {x_i}^6 \end{bmatrix} \quad (14)$$

The D-optimal design for (4) is the function that satisfies equation (15)

$$|\,M(\xi^*;\ \beta_0,\beta_1,\beta_2,\beta_3)| = \max_{\xi\in\Xi}|M(\xi;\ \beta_0,\beta_1,\beta_2,\beta_3)| \quad (15)$$

3. RESULTS AND DISCUSSION

3.1 D-optimal Designs for Quadratic Poisson Regression Model

The result of D-optimal designs relating to the Poisson regression model with one predictor variable involving a quadratic term is hereby presented. For the model in (3), the assumption is that

$x_i \in [0,1]\ (i = 1,\cdots,p+1)$, and
$\beta = (1,\ 2,\ 1)^T$.

The D-optimal design relating to the model is therefore constructed as (16)

$$\xi_D^* = \begin{Bmatrix} (0.000) & (0.4142) & (1.0000) \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{Bmatrix} \quad (16)$$

Considering this model, the design is found to be optimal at 3-design points. After 1000 iterations, the optimal design points are $x = 0.0000$, $x = 0.4142$ and $x = 1.0000$ with each generated design weight of $\frac{1}{3}$.

This implies that 33.33% of the total experimental runs are allocated to each optimal design point. The maximum sensitivity function for this model is 1.081764e-08, which confirms that the design is indeed D-optimal at 3-design points.

Figure 1 in the appendix shows the D-criterion value for the quadratic Poisson regression model. The positive criterion value corroborates the choice of the restricted design space.

3.2 D-optimal Designs for Cubic Poisson Regression Model

The result of D-optimal designs relating to Cubic Poisson regression model with one predictor variable is hereby presented. Considering the model in equation (4), suppose $x_i \in [0,1]\ (i = 1,\cdots,p+1)$, and $\beta = (1,\ 2,\ 2,\ 1)^T$; the D-optimal design for the model is constructed and expressed in equation (17)

$$\xi_D^* = \begin{Bmatrix} (0.000) & (0.2204) & (0.6596) & (1.0000) \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{Bmatrix} \quad (17)$$

For a Poisson regression model involving cubic polynomial term in the predictor variable, the design is optimal at 4-design points. After 1000 iterations, optimal design points: $x = 0.0000$, $x = 0.2204$, $x = 0.6596$ and $x = 1.0000$ were obtained. Each of the optimal design points has equal optimal design weight of $\frac{1}{4}$.

This implies that 25% of the total experimental runs are allocated to each optimal design point.

The maximum sensitivity function for the model is 2.320493e-07, which confirms the D-optimality of the design.

CONCLUSION

This research investigates and constructs D-optimal experimental designs for Poisson regression models containing quadratic and cubic terms in one variable. In the case of the quadratic Poisson regression model, it can be seen that the design is optimal at 3-design points with generated equal weights of 0.3333; the cubic Poisson regression model is optimal at 4-design points with generated equal weights of 0.25. This implies that equal proportional allocation of treatments is allotted to each of the constructed D-optimal design point with respect to the orders of polynomial in the Poisson regression models.

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Appendix

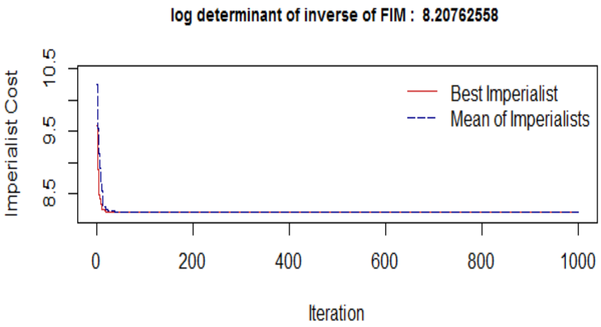

Figure 1: D-optimal Designs for a Quadratic Poisson Regression Model in One Variable