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HETEROSCEDASTIC D-OPTIMAL DESIGN IN REGRESSION MODELS WITH APPLICATION IN KINEMATIC VISCOSITY DATA

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ABSTRACT

In real life situations, the assumption of homogeneity is often violated and the variances of the error terms are not the same which is termed heteroscedasticity. In this work, D-optimality criterion was used when there is heterocedsasticity in the data set and when the data had been corrected using different methods for correction thereby making the variance of the error structure to be equal. Comparing the result for the two models used, when there is heteroscedasticity and when it has been corrected, the variances and the determinants of dispersion matrices shows that D-optimal design when the data set has been corrected is more efficient than when there is heteroscedastic

Key words: D-optimal, Heteroscedasticity, Experimental Design, Regression model

INTRODUCTION

Experimentation is the process of planning a study to meet specified objectives which constitutes a foundation of the empirical sciences (Zhu, 2012). One major advantage of experiment is its ability to control the experimental conditions; as well as to determine the variables to include in a study (Fackle Fornius, 2008). Since the introduction of experimental design principle in the first half of the 1930, optimal experimental designs have been gaining attention and had become useful tools among researchers in various fields (Atkinson and Donev, 1992; Atkinson, 1996; Atkinson, Donev and Tobias, 2007; Berger and Wong, 2009).

There are various design criteria, D-optimality has been the most frequently used; and often performs better than other criteria (Zocchi and Atkinson, 1999; Atkinson *et al.*, 2007). Hence, the D-optimality has become one of the most popular criteria which involve designs that minimize the generalized variance of the parameter vector. The D-optimal designs seek to minimize $|(X'X)^{-1}|$ (dispersion matrix) or equivalently maximize the determinant of the information matrix $(X'X)$ of the design through some forms of statistical modeling such as regression model. The information matrix (also called Fisher information matrix) measures the amount of information that random variable, X affects an unknown parameter θ of a distribution. One of the important assumptions of the standard regression model is that the variance of the error terms (disturbance term, u_i) must be equal across the observations which is refers to as homoscedastic $[E(u_i^2) = \sigma^2 \quad i = 1,2,\cdots,n]$. However, in real life situations, this assumption is often violated and the variances of the error terms are not the same. The condition where error terms have different

variances is termed heteroscedasticity $\left[E\left(u_i^2\right) = \sigma_i^2 \quad i = 1,2,\cdots,n\right]$ that is, unequal variance across the observations (Lambert, 2013; Knaub, 2017). Heteroscedasticity, which is often referred to as a "problem" that needs to be "solved" or "corrected" is the change in variance of predicted y, given different values of the independent variables (Knaub, 2011, 2017). This study will therefore, adopt D-optimal designs otherwise known as D-optimality criterion in the presence of Heteroscedasticity due to it's widely selection to provide the most globally accurate estimates of model parameters.

MATERIALS AND METHOD

The sequential method for getting D-optimal design was used to achieve the results in this work. The data is from secondary source on the kinematic viscosity of a lubricant (response variable) in stokes as a function of temperature (o_C) and the pressure in atmosphere (atm), were obtained by Linssen (1975). The data set which violated the assumption of homoscedasticity was coded between $-1 \leq x \leq 1$. Linear and polynomial models were used and we found D-optimal design for each model when there is heteroscedasticity and when it has been corrected.

Heteroscedasticity was corrected using the following steps;

i. Run the OLS of the model and obtain the estimated residuals
ii. Obtain the log of the squared residuals
iii. Correction methods are

Method 1 regress $log\hat{e}_i^2\ on\ (x_1, x_2)$

Method 2 regress $log\hat{e}_i^2\ on\ (x_1,\ x_2, x_1^2, x_2^2\ )$

Method 3 regress$log\hat{e}_i^2\ on\ (x_1,\ \ x_2, x_1^2,\ \ x_2^2,\ x_1x_2)$

RESULT AND DISCUSSION

The linear (first) model is

$$y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + e_i \qquad (1)$$

The partial derivative for the model is

$$f'(x_i) = (1,\ x_1,\ x_2) \qquad (2)$$

The information matrix is now

$$M(\xi) = \sum w_i\, f(x_i)\ f'(x_i) \qquad (3)$$

The corresponding 3×3 design matrix for the model is

$$X_3 = \begin{bmatrix} 1.000000 & 1.000000 & 0.322035 \\ 1.000000 & -0.494439 & 0.413935 \\ 1.000000 & -0.235592 & -0.026634 \end{bmatrix} \qquad (4)$$

It should be noted that the procedure requires a sufficient number of observation because we have to ensure that the inverse $|X_N' X_N|^{-1}$ exist. A simple condition that will guarantee the inverse exist is to have the number of different design points greater than or equal to the number of parameters, that is $N \geq p$. The design points are selected within the range of $-1 \leq x \leq 1$ for the variables. The maximum $s(x_a, \xi)$ is found for $x_1 = 1.00000\ and\ x_2 = -1.000000$, so these design points were added to design matrix X_3 and the design matrix is now

$$X_4 = \begin{bmatrix} 1.000000 & 1.000000 & 0.322035 \\ 1.000000 & -0.494439 & 0.413935 \\ 1.000000 & -0.235592 & -0.026634 \\ 1.000000 & 1.000000 & -1.000000 \end{bmatrix} \qquad (5)$$

The process continued until the condition for getting optimal design was reached. The maximum $s(x_a, \xi)$ value decreases as N increases, according to the general equivalence theorem (Kiefer and Wolfowitz, 1960), a D-optimal design satisfies the condition that $s(x_a, \xi) \leq p$.

Table 1 shows the D-optimal design when there is heteroscedasticity. It means that if there are 100 experimental units, 20 should be allocated to when $x_1 = -1$ and $x_2 = 1$, also when $x_1 = 1$ and $x_2 = 1$. In the same vein, 30 should be allocated to when $x_1 = -1$ and $x_2 = -1$, also when $x_1 = 1$ and $x_2 = -1$

Table1: Sequential construction of a D-optimal design for the linear (first) model

N	x_{1N+1}	x_{2N+1}	$s(x_a,\xi)$	D_{eff}
3	1.0000	−1.0000	49.5896	0.000819
4	−1.0000	−1.0000	13.9742	0.002128
5	−1.0000	1.0000	7.2029	0.003511
6	1.0000	1.0000	6.0575	0.004728
7	−1.0000	−1.0000	4.3792	0.005966
8	1.0000	−1.0000	4.3516	0.007015
9	−1.0000	1.0000	4.2274	0.008169
10	1.0000	1.0000	3.7240	0.00931
903	−1.0000	−1.0000	3.009	1

The D-optimal design for the model is

$$\xi^* = \begin{Bmatrix} (-1,1) & (1,1) & (-1,-1) & (1,-1) \\ \frac{2}{10} & \frac{2}{10} & \frac{3}{10} & \frac{3}{10} \end{Bmatrix} \quad (6)$$

Comparison for D-optimal designs when there is heteroscedaticicty and when it has been corrected was presented in Table 2 for linear model. The Mean and Variance for these were shown. The correction methods used here were three and this was done for polynomial model.

Table 2: D-optimal designs for model 1 $y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + e_i$ (Linear Model)

Model	D-optimal Designs	Mean	Variance
Uncorrected	$\begin{Bmatrix} (-1,1) & (1,1) & (-1,-1) & (1,-1) \\ \frac{2}{10} & \frac{2}{10} & \frac{3}{10} & \frac{3}{10} \end{Bmatrix}$	**2.7**	**8.5**
Corrected 1	$\begin{Bmatrix} (-1,1) & (1,1) & (-1,-1) & (1,-1) \\ \frac{5}{20} & \frac{5}{20} & \frac{5}{20} & \frac{5}{20} \end{Bmatrix}$	**2.5**	**7.5**
2	$\begin{Bmatrix} (-1,1) & (1,1) & (-1,-1) & (1,-1) \\ \frac{5}{20} & \frac{6}{20} & \frac{4}{20} & \frac{5}{20} \end{Bmatrix}$	**2.45**	**7.25**
3	$\begin{Bmatrix} (-1,1) & (1,1) & (-1,-1) & (1,-1) \\ \frac{5}{20} & \frac{5}{20} & \frac{5}{20} & \frac{5}{20} \end{Bmatrix}$	**2.5**	**2.5**

From Table 2, the mean and variance for the D-Optimal design when there is heteroscedasticity and it has been corrected were shown. The results show that the variance of the D- Optimal when there is heteroscedasticity is higher than when it has been corrected, which show the efficiency of the corrected one. Similarly, Table 3 also show same results for the second model used.

The polynomial model considered in this work is $y_i = \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 + \beta_3 x_2 + e_i$

Table 3: D-optimal designs for model 2 (Polynomial Model)

Model	D-optimal Designs	Mean	Variance
Uncorrected	$\begin{Bmatrix}(-1,1) & (1,1) & (-1,-1) & (1,-1) & (-0.2356,1) & (-0.2356,-1)\\ \frac{3}{20} & \frac{3}{20} & \frac{3}{20} & \frac{4}{20} & \frac{3}{20} & \frac{4}{20}\end{Bmatrix}$	**3.65**	**16.25**
Corrected 1	$\begin{Bmatrix}(-1,1) & (1,1) & (-1,-1) & (1,-1) & (-0.2356,1) & (-0.2356,-1)\\ \frac{4}{20} & \frac{4}{20} & \frac{2}{20} & \frac{3}{20} & \frac{4}{20} & \frac{3}{20}\end{Bmatrix}$	**3.4**	**14.3**
2	$\begin{Bmatrix}(-1,1) & (1,1) & (-1,-1) & (1,-1) & (-0.2356,1) & (-0.2356,-1)\\ \frac{4}{20} & \frac{4}{20} & \frac{2}{20} & \frac{3}{20} & \frac{4}{20} & \frac{3}{20}\end{Bmatrix}$	**3.4**	**14.7**
3	$\begin{Bmatrix}(-1,1) & (1,1) & (-1,-1) & (1,-1) & (-0.2356,1) & (-0.2356,-1)\\ \frac{4}{20} & \frac{4}{20} & \frac{4}{20} & \frac{4}{20} & \frac{2}{20} & \frac{2}{20}\end{Bmatrix}$	**3.1**	**12.1**

Table 3 below shows the D-optimal design and the comparison is based on the mean and the variance of the design knowing fully well that for a good estimator, efficiency must be ascertained which is relevant to minimum variance. Therefore, the D-optimal design when there is no heteroscedasticity is the best in experimental design. Table 4 further established the effect of heteroscedasticity on D-optimal design for it minimizes the determinant of dispersion matrix or maximize the information matrix, meaning that the smaller the determinant, the better the design. Model 1 can be considered to have performed best in relative to this fact

Table 4: Comparison of D-optimal designs in relative to the determinants of dispersion matrices

Model	heteroscedasticity	No Heteroscedasticity		
		Correction Method 1	2	3
Model 1	$3.331295e^{-11}$	$3.331158e^{-11}$	$3.329784e^{-11}$	$3.323053e^{-11}$
Model 2	$2.498338e^{-11}$	$2.498807e^{-11}$	$2.499842e^{-11}$	$2.4987226e^{-11}$

CONCLUSION

In regression model, presence of heteroscedasticity makes the estimator unbiased but not efficient when ordinary
least squares (OLS) approach is used. The outcome of experiment has shown that D-optimal design when Heteroscedasticity has been corrected is better than when left uncorrected. In optimality criterion too, presence of this phenomenon will also affect
the D-optimal design that an experimenter wishes to achieve.

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