Journal of the Nigerian Association of Mathematical Physics
***Volume* 18 (May, 2011), pp 611 – 616**
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Optimal 3-Point Symmetric Quadratic Regression Designs for the Number of Trials, N ≤ 7.

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Abstract

Optimal 3-point symmetric quadratic regression designs were constructed in the experimental domain $[-1, 1]$ ***with the regression range*** $\chi = \left\{\left(1,\ x, x^2, \cdots, x^k\right): x \in D\right\}$.

For the symmetric design d_3^****, the information matrix,*** $M\left(d_3^*\right)$ ***and standardized variance,*** $\tilde{V}\left(x, d_3^*\right)$ ***were exploited to identify optimal 3-point symmetric quadratic regression designs based on optimality criteria.***

The design points $\left\{(-1,\ 0,\ 1) \in D\right\}$ ***and the weights*** $w_1,\ w_2,\ w_3$ ***for the number of trials*** $N \leq 7$ ***were used for the construction of the optimal designs. Some A-, V-, and D-optimal 3-point symmetric quadratic regression designs for the number of trials*** $N \leq 7$ ***are highlighted***

Keywords: Optimal, 3-point**,** regression, design, symmetric, weights, matrix, domain, quadratic**.**

1.0 Introduction:

Consider the kth degree polynomial model [6]

$$Y_{ij} = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_k x_i^k + e_{ij}\ , \quad i = 1,\ 2, \cdots, n\ \ ;\ \ j = 1,\ 2, \cdots, N \tag{1.1}$$

with

$$E\left(Y_{ij}\right) = \sum_{j=0}^{k} \beta_j x_i^j \quad and \quad Var\left(Y_{ij}\right) = \sigma^2 \tag{1.2}$$

In a compact form (1.1) is re-written as

$$Y = X\beta + e \tag{1.3}$$

where $X = \left(1,\ x_i\ ,\ x_i^2, \cdots, x_i^k\right)$

and

$$\beta = \left(\beta_0\ ,\ \beta_1,\ \beta_2, \cdots, \beta_k\right)^T \tag{1.4}$$

Theorem: Gauss Markov Theorem [10].

For the full mean parameter system: Let X be an $n \times K$ matrix with full column rank K, *and* V be a nonnegative definite $n \times n$ matrix.

A left inverse L of X attains the minimum of LVL^T over all left inverses L of X

$$LVL^T = \underset{\substack{L \in R^{k \times n} \\ LX = I_k}}{Min} LVL^T$$

if and only if $LVR^T = 0$, where R is a projector given by $R = I_n - XG$ for some generalized inverse G of X .

A minimizing left inverse L exists; a particular choice is G-GVR^{T}HR, with any generalized inverse H of RVR^T. The minimum admits the representation

$$\underset{\substack{L \in R^{k \times n} \\ LX = I_k}}{Min} LVL^T = \left(X^T V^{-1} X\right)^{-1}$$

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and is attained by any matrix $L = \left(X^T V^{-1} X\right)^{-1} X^T H$, where H is any generalized inverse of V .

By the theorem, the optimal estimator of β is given by

$$\hat{\beta} = \left(X^T X\right)^{-1} X^T Y \tag{1.5}$$

with the dispersion matrix

$$V\left(\hat{\beta}\right) = \sigma^2 \left(X^T X\right)^{-1} \tag{1.6}$$

which depends on the values $x_1, x_2, x_3, \cdots, x_n$ of x, and the number of replications $N_1, N_2, N_3, \cdots, N_n$ such that $\sum_{i=1}^{n} N_i = N$ (N is the total number of observations)

Given the experimental design

$$d_n = \{x_1, x_2, x_3, \cdots, x_n; N_1, N_2, N_3, \cdots, N_n\} \tag{1.7}$$

with a finite N and finite number $n(n \geq k+1)$ of distinct regression values in the interval $[a, b]$, the regression vector $x_i = \left(1, x_i, x_i^2, \cdots, x_i^k\right)^T$, $i = 1, 2, \cdots$ are called the support of d_n written as:

$$\text{supp } d_n = \{x_1, x_2, \cdots, x_n\} \tag{1.8}$$

Accordingly, the matrix

$$X^T X = \sum_{i \leq x} N_i x_i x_i^T \tag{1.9}$$

is called the information matrix of d_n and is denoted by $M\left(d_n\right)$ (See [8])

Since matrix inversion is antitonic [1] the inverse dispersion matrix is

$$V^{-1}\left(\hat{\beta}\right) = \frac{1}{\sigma^2}\left(X^T X\right) = \frac{1}{\sigma^2}\sum_{i \leq x} N_i x_i x_i^T = \frac{1}{\sigma^2} M\left(d_n\right)$$

Hence

$$V^{-1}\left(\hat{\beta}\right) = \frac{N}{\sigma^2}\sum_{i \leq x} M\left(\frac{d_n}{N}\right) \tag{1.10}$$

is the precision matrix for the design d_n in the experimental domain $D = [a, b]$ and corresponding range $\chi = \left[\left(1, x, x^2, \cdots, x^k\right): x \in D\right] \in \mathbb{R}^{k+1}$.

Clearly, if the weights $w_i = \frac{N_i}{N}$, $i = 1, 2, \cdots, n$ are placed on the regression vectors, they vary continuously in the closed interval $[0, 1]$ such that $w_1 + w_2 + w_3 + \cdots + w_n = 1$. Thus the precision matrix becomes.

$$V^{-1}\left(\hat{\beta}\right) = \frac{N}{\sigma^2}\sum_{i \leq k} w_i x_i x_i^T \tag{1.11}$$

and the design (1.7) becomes

$$d_n = \{x_1, x_2, \cdots, x_n; w_1, w_2, \cdots, w_n\} \tag{1.12}$$

where $n > k+1$

For simplicity [12, 13], take $\sigma^2 = I$, the dispersion matrix for design (1.12) is

$$V\left(\hat{\beta}\right) = \left(X^T D_n X\right)^{-1} \tag{1.13}$$

and the information matrix

$$M\left(d_n\right) = X^T D_n X \tag{1.14}$$

where $$X = \begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^k \\ 1 & x_2 & x_2^2 & \cdots & x_2^k \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^k \end{pmatrix} \quad and \quad D_n = diag\,(w_1,\ w_2, \cdots, w_n)$$

2.0 Materials and Methods

Define the experimental symmetric domain $D = [1, -1]$ [10] with the regression range $\chi = \{(1,\ x,\ x^2, \cdots, x^k)^T : x \in D\}$ Let d_n^R be the reflected design for (1.1) with respect to (1.2).

$$d_n^R = (-x_1\ ,\ x_2, \cdots, -x_n\ ;\ w_1,\ w_2, \cdots, w_n) \tag{2.1}$$

Accordingly, the design d_n *and* d_n^R have the same even moments while the odd moments of d^R have a reversed sign. (See [4])

Let $M(d_n^R)$ be the information $(k+1) \times (k+1)$ matrix of the design d_n^R.

$$M(d_n^R) = QM(d_n)Q \tag{2.2}$$

where $Q = diag(-1,\ 1,\ -1, \cdots, \pm 1)$ is a diagonal matrix. Hence, the symmetric design

$$d_n^* = \frac{1}{2}(d_n + d_n^R) = \left\{ \pm\ x_i\ ,\ \frac{w_i}{2}, \frac{w_i}{2} / \ i = 1,\ 2, \cdots, n \right\} \tag{2.3}$$

assigns the weights $\frac{w_i}{2}$ to x_i *and* $-x_i$ for each i. Clearly, the information matrix for d_n^* is

$$\begin{aligned} M(d_n^*) &= \frac{1}{2}[M(d_n) + M(d_n^R)] \\ &= \frac{1}{2}[M(d_n) + QM(d_n)Q] \end{aligned} \tag{2.4}$$

By similarity transformation $M(d_n)$ *and* $M(d_n^R)$ have the same eigenvalue. Since optimality criterion, ϕ is super-additive (Atkinson and Donev, 2002; Atkinsion et al, 2007)

$$\phi[M(d_n^*)] = \phi\left[\frac{1}{2}[M(d_n) + M(d_n^R)]\right] \geq \phi[M(d_n)] \tag{2.5}$$

which according to Pukelsheim (2006) shows that symmetrization improves the value of the criterion ϕ or at least it guarantees the same value as long as ϕ is supper-additive and invariant with respect to the reflection.

According to [7], comparison of designs is based on dispersion matrices of the estimator of the regression parameters. Let $\hat{\beta}_1$ *and* $\hat{\beta}_2$ be the esimators of β under designs d_1 *and* d_2. If $V(\hat{\beta}_1) \leq V(\hat{\beta}_2)$, we say that the design d_1 dominates design d_2. Pukelsheim and Studden [9] define optimality criterion ϕ as supper-additive function from the closed cone of nonnegative definite matrix into a real line. The most prominent optimality criteria are the matrix means ϕ_p for $p \in (-\infty, 1)$. The classical $A-,\ D-,\ V-,\ E-$ *and* T criteria are special cases of matrix means (see [10]).

According to [4, 11], the standardized variance for comparing designs is

$$\tilde{V}(x,\ d_n^*) = \frac{V(\hat{Y})}{\sigma^2} \tag{2.6}$$

where

$$V(\hat{Y}) = \sigma^2 f^T(x)\ M^{-1}(d_n^*) f(x), \text{ provided } \left| M(d_n^*) \right| \neq 0 \tag{2.7}$$

$$f(x) = (1,\ x,\ x^2, \cdots, x^k)^T$$

Fedorov [3] and Kiefer [5] established the following equivalence conditions for d_n^*

(i) the design d_n^* minimizes $\phi\left[M\left(d_n^*\right)\right]$

(ii) the minimum of $\tilde{V}\left(x,\, d_n^*\right) \geq 0$ for $x \in D$

(iii) the variance $\tilde{V}\left(x,\, d_n^*\right)$ achieves its minimum at the points of the design, d_n^* .

By condition (ii), the design d_n^* is D-optimum if $\max\limits_{x\in D} \tilde{V}\left(x,\, d_n^*\right) \leq p$, where p is the number of support points of the design, d_n^*. The design d_n^* is $A-,\ V-,\ \text{and}\ D-\text{optimal}$ in the class of designs if d_n^* has

(i) $\min\ tr\left(X^T D_T X\right)^{-1}$

(ii) $\underset{x\in D}{Min}\, V\left(\hat{Y}\right)$

(iii) $Min\left[\underset{x\in D}{Max}\, \tilde{V}\left(x, d_n^*\right)\right]$, respectively.

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oint Symmetric Quadratic Regression Designs

3-point symmetric Quadratic Regression Designs d_3^* on [-1, 1]	Information matrix $M\left(d_3^*\right)$	$M^{-1}\left(d_3^*\right)$	$\left\|M\left(d_3^*\right)\right\|$	Trace of $M^{-1}\left(d_3^*\right)$	$V\left(\hat{Y}\right)$	$\min_{x\in D} V\left(\hat{Y}\right)$	$\tilde{V}\left(x, d_3^*\right)$	min $_{x\in D}$
$\left\{-1, 0, 1; \frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right\}$	$\frac{1}{3}\begin{pmatrix} 3 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 2 \end{pmatrix}$	$\frac{3}{2}\begin{pmatrix} 2 & 0 & -2 \\ 0 & 1 & 0 \\ -2 & 0 & 3 \end{pmatrix}$	$\frac{4}{27}$	9	$\frac{\sigma^2}{2}(9x^4 - 9x^2 + 6)$	$3\sigma^2$	$\frac{1}{2}(9x^4 - x^2 + 6)$	**D-o**
$\left\{-1, 0, 1; \frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right\}$	$\frac{1}{2}\begin{pmatrix} 2 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & -2 \\ 0 & 2 & 0 \\ -2 & 0 & 4 \end{pmatrix}$	$\frac{1}{8}$	8	$2\sigma^2(2x^4 - x^2 + 1)$	$2\sigma^2$	$2(2x^4 - x^2 + 1)$	**A-o**
$\left\{-1, 0, 1; \frac{1}{5}, \frac{3}{5}, \frac{1}{5}\right\}$	$\frac{1}{5}\begin{pmatrix} 5 & 0 & 2 \\ 0 & 2 & 0 \\ 2 & 0 & 2 \end{pmatrix}$	$\frac{5}{6}\begin{pmatrix} 2 & 0 & -2 \\ 0 & 3 & 0 \\ -2 & 0 & 5 \end{pmatrix}$	$\frac{12}{125}$	$\frac{25}{3}$	$\frac{5\sigma^2}{6}(5x^4 + 2)$	$\frac{5\sigma^2}{3}$	$\frac{5}{6}(5x^4 + 2)$	
$\left\{-1, 0, 1; \frac{2}{5}, \frac{1}{5}, \frac{2}{5}\right\}$	$\frac{1}{5}\begin{pmatrix} 5 & 0 & 4 \\ 0 & 4 & 0 \\ 4 & 0 & 4 \end{pmatrix}$	$\frac{5}{4}\begin{pmatrix} 4 & 0 & -4 \\ 0 & 1 & 0 \\ -4 & 0 & 5 \end{pmatrix}$	$\frac{16}{125}$	$\frac{25}{2}$	$\frac{5\sigma^2}{6}(5x^4 - 7x^2 + 4)$	$\frac{5\sigma^2}{2}$	$\frac{5}{4}(5x^4 - 7x^2 + 4)$	**D-o**
$\left\{-1, 0, 1; \frac{1}{6}, \frac{2}{3}, \frac{1}{6}\right\}$	$\frac{1}{3}\begin{pmatrix} 3 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$	$\frac{3}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 3 \end{pmatrix}$	$\frac{1}{9}$	9	$\frac{3\sigma^2}{2}(3x^4 + 1)$	$\frac{3}{2}\sigma^2$	$9(3x^4 + 1)$	**V-o**
$\left\{-1, 0, 1; \frac{1}{3}, \frac{1}{2}, \frac{1}{6}\right\}$	$\frac{1}{6}\begin{pmatrix} 6 & -1 & 3 \\ -1 & 3 & -1 \\ 3 & -1 & 3 \end{pmatrix}$	$\frac{1}{4}\begin{pmatrix} 8 & 0 & -8 \\ 0 & 9 & 3 \\ -8 & 3 & 17 \end{pmatrix}$	$\frac{1}{9}$	$\frac{17}{2}$	$\frac{\sigma^2}{4}(17x^4 + 6x^3 -$ $25x^2 + 8)$	$\frac{3}{2}\sigma^2$	$\frac{3}{2}(17x^4 + 6x^3 -$ $25x^2 + 8)$	**D-o** **V-o**
$\left\{-1, 0, 1; \frac{3}{7}, \frac{1}{7}, \frac{3}{7}\right\}$	$\frac{1}{7}\begin{pmatrix} 7 & 0 & 6 \\ 0 & 6 & 0 \\ 6 & 0 & 6 \end{pmatrix}$	$\frac{7}{6}\begin{pmatrix} 6 & 0 & -6 \\ 0 & 1 & 0 \\ -6 & 0 & 7 \end{pmatrix}$	$\frac{36}{343}$	$\frac{49}{3}$	$\frac{7\sigma^2}{6}(7x^4 - 6x^2 + 6)$	$7\sigma^2$	$\frac{49}{6}(7x^4 - 6x^2 + 6$	

4.0 Discussion

Clearly, we have constructed a 3-point symmetric quadratic regression design $\left\{-1, 0, 1, \frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right\}$, which is A-optimal. Also the 3-point symmetric quadratic regression designs $\left\{-1, 0, 1, \frac{2}{5}, \frac{1}{5}, \frac{2}{5}\right\}$, $\left\{-1, 0, 1, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right\}$, and $\left\{-1, 0, 1, \frac{1}{3}, \frac{1}{2}, \frac{1}{6}\right\}$ are D-optimal. But the designs $\left\{-1, 0, 1, \frac{1}{6}, \frac{2}{3}, \frac{1}{6}\right\}$ and $\left\{-1, 0, 1, \frac{1}{3}, \frac{1}{2}, \frac{1}{6}\right\}$ are V-optimal among the class of designs constructed.

References

[1]. Atkinson, A. C. and Donev, A. N. (2002), Optimum Experimental Designs, Oxford University Press Inc., New York, pp. 93-133.

[2]. Atkinson, A. C., Donev, A. N., and Tobias R. D. (2007), Optimum Experimental Designs with SAS, Oxford University Press, N. Y., pp. 53-64.

[3]. Fedorov, V. V. (1972), Theory of Optimal Experiments, Academic Press, N. Y., pp. 76-95.

[4]. Goos, P., Tack, L. and Vandebrowk, M. (2001), Optimal Designs for Variance Function Estimation using Sample Variances, Journal Stat. Planning and Inference 92: pp. 233-252.

[5]. Kiefer, J. C. (1974), General Equivalence Theory for Optimum Designs, Annal. Stat. 2, 849-879.

[6]. Kiefer, J. C. (1961), Optimal Designs in regression Problems II, Annals. Math. Stat. 32, 298-325.

[7]. Kiefer, J. C. and Wolfowitz, J. (1959), Optimum Designs in regression Problems, Annals. Math. Stat. 30, 271-294.

[8]. Pukelsheim, F. (1980), On Linear Regession Designs which maximize Information matrix, Journal Stat. Planning and Inference 4: 339-364.

[9]. Pukelsheim, F. and Studden, W. J. (1993), E-Optimal Designs for Polynomial regression, Annals Stat. 21; 402-415.

[10]. Pukelsheim, F. (2006), Optimum Design of Experiments, Society for Industrial and Applied Mathematics, Wiley, USA, pp. 1-34.

[11]. Trinca, I. A. and Gilmour, S. A. (1999), Difference Variance Dispersion Graphs for Comparing Response Surface Designs, Applied Stat. 48, 441-455.

[12]. Wierich, W. (1987), On Optimal Designs and Complete Class Theorems for experiments with Continuous and Discrete Factors Influence, Journal. Stat. Planning and Inference, 15; 19-27.

[13]. Wu, C. F. J. and Hamada, M (2002), Experiments, Planning, strategies, and parameter design Optimization, Wiley USA, pp. 10-24.