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SEGMENTED LINE SEARCH METHOD FOR CONSTRUCTING D-OPTIMAL EXACT DESIGNS IN CONTINUOUS EXPERIMENTAL AREAS

F.I Nsude

Department of Statistics

Akanu Ibiam Federal Polytechnic, Unwana, Ebonyi State, Nigeria

P.E. Chigbu

Department of Statistics, University of Nigeria, Nsukka, Enugu State, Nigeria

Abstract
An effective segmented line search technique for constructing D-optimal exact designs in a polynomial response function of degree **z** is presented in this paper. The direction of search is a weighted average from all segments of the experimental trials; the weight being proportional to the mean square errors from the segments. The method is rapidly convergent and its application in continuous experimental areas is shown.
Key words: variance function, Exact Designs, Continuous design, Exchange algorithm.

1. Introduction

The method reported here is a segmented line search procedure for constructing D-optimal exact designs in a continuous experimental region. In this search system, variance of polynomial response function of degree **z** is approximated by a polynomial function of degree 2**z**. Maximizer of this polynomial is determined by segmenting the experimental area into segments. Thereafter, this maximizer is used to replace the point of minimum prediction variance amongst the points already in the design. The search method is via the Super Convergent line Search Series reported by Onukogu (1997) [8] which has shown to have rapid convergence capability; see Onukogu and Chigbu (2002, p. 112) [9], and Ugbe and Chigbu (2014) [11].

Every line search technique has four characteristics sequence as follows: (a) the starting point, $\underline{\bar{x}}$, which is an n-component vector, $\underline{X}$; (b) an n-component direction vector, $\underline{d}$; (c) the step-length, ρ; and (d) Movement to the iterate, ($\underline{x} = \underline{\bar{x}} + \underline{d}\rho$). This set of sequential activities applies as well to this technique herein reported.

This search method also makes use of variance exchange of points procedure which is originally reported by Fedorov (1972) [5], and modified severally over decades before the Variance Exchange Method reported by Atkinson and Donev (1989) [1].

2. Design Background Problem

Given the basic experimental triple $\{\tilde{X}, F_X, \Sigma_X\}$, where F_x is the response functions, which is a space of finite dimensional linear function and continuous in $\tilde{X}$; $\tilde{X}$ is a collection of factor levels $\underline{X}$, which constitutes a compact, continuous and metric space, and at each point, $\underline{x} \in \tilde{X}$, the response is observed with a random error, e_x, which is a point in the space, $\sum_x$ which is a non-negative continuous function, define in $\tilde{X}$ (Chigbu and Oladugba, 2010) [4].

In this study, treatment or support point, $\underline{X}$, was selected such that each element of $\underline{x}_i$, is attached a weigh $\mathrm{w_i}; \mathrm{w_i} \geq 0$ and $\sum_{\mathrm{i=1}}^{\mathrm{n}} \mathrm{w_i} = 1$, where n is the number of support points in the design. From a collection of n support points we form a design matrix, X, as well as normalized Fisher's information matrix, $M(\xi_n) = \frac{X_\xi' X_\xi \sigma^2}{n}$, where X is the design matrix of the model terms (the columns) evaluated at specific point/treatment in the design space (the rows), $X_\xi' X_\xi$ is a non-singular matrix (information matrix) and $\sigma^2(X_\xi' X_\xi)^{-1}$ is the variance-covariance matrix of the least square estimate of the response parameters.

Our interest is to find n-points design, $\underline{x}_i \in \tilde{X}, i = 1, 2, \ldots, n$, such that the resultant information matrix $(X_\xi' X_\xi)$ is maximized. A design criterion that maximizes the determinant of the information matrix $|X_\xi' X_\xi|$ or, equivalently, minimizes $|X_\xi' X_\xi|^{-1}$ is referred to as D-optimality. Other optimality criteria have been reported severally (Atkinson and Donev, (1992) [2]; Onukogu and Chigbu (2002) [9]).

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Therefore in this paper, the intention is to present a search method which seeks iteratively an n-point design measure, ξ_n that maximizes the determinant of $M(\xi^*)$; i.e $Max|\ M(\xi^*)|$; $M(\xi_n) \in S^{p\times p}$, where $S^{p\times p}$ is a set of all non-singular p x p information matrices defined in $\tilde{X}$.

3. **Theoretical Framework**

The method is summarized by the following sequence of steps.

3.1. Pick at random an initial n-point design of nonsingular information matrix.

3.2. Obtain its extended design matrix, X, according to the model terms, and the Fisher's information matrix, $X_\xi' X_\xi = M(\xi)$.

3.3. From the above, compute standardized generalized variance function of degree 2**z** as

$$d(\underline{x}, \xi) = n\underline{x}' M^{-1}(\xi)\underline{x}, \qquad (3.1)$$

$$= g(\underline{x}) \qquad (3.2)$$

$$= \beta_0 + \sum_{i=1}^m \beta_i x_i + \sum_{i=1}^m \beta_i x_i + \sum_{i=1}^{m-1}\sum_{i<j}^m \beta_i x_i x_j \ \dots$$

$$\underline{x}'_{1\times p} = (1\ \ x_{1i}\ \ x_{2i}\ \ . . .\ \ x_{1i}\, x_{2i}\ \ \ x_{1i}x_{3i}\ \ . . . x_{1i}^2\ \ \ x_{2i}^2 . . .)$$

Note that the number of factor interaction is $\frac{m(m-1)}{2}$, where m is the number of factors or variables.

3.4. Partition the experimental region,$\tilde{X}$, either into $S_k; k = 1,2. . ., s$ non-overlapping segments such that $S_1 \cap S_2\ . . .\cap S_s = \emptyset$, and $S_1 \cup S_2 . . .\cup S_s \leq \tilde{X}$; or with common boundary such that $S_1 \cap S_2\ . . .\cap S_s \neq \emptyset$, and $S_1 \cup S_2 . . .\cup S_8 \leq \tilde{X}$: See (Ugbe and Chigbu (2014) [11].

3.5. From each k^{th} segment, pick or select n_k supports points, $n_k \geq m+1, k = 1,2,. . . s$; $\sum_{k=1}^s n_k = N_0$, the total number of selected points in all the segments.

3.6. Obtain the design matrix, X_k, $k = 1, 2,. . ., s$, for each segment, and the information matrices,

$$\overline{\underline{X}}_k = X_k' X_k \qquad (3.3)$$

3.7. Compute $Xb_{k,}$ the matrices of interaction/biasing effect of the variable for each segment; where k = 1, 2, . . ., s; and the vector of coefficient of interaction/biasing terms of $g(\underline{x})$ is given by $\underline{c}_b$. Matrix of mean square error of each of the k^{th} segment is given by

$$\overline{M}_k = \overline{\underline{X}}_k^{-1} + \overline{\underline{X}}_k^{-1} X_k' X b_k \underline{c}_b \underline{c}_b' X' b_k X_k \overline{\underline{X}}_k^{-1} \qquad (3.4)$$

where $\overline{\underline{X}}_k = X_\kappa' X_\kappa$, and $\overline{M}_k$ is an (m+1) x (m + 1) matrix, m being the number of factors/variables.

3.8. The average mean square error is minimized to obtain the matrix of convex combination, H_k; Thus, min $(\overline{M}(dt)) = \min(\sum_{k=1}^s h_{tk}\, \alpha_{tk})$ and as the cross terms are zero; we have

$$\min\left(\overline{M}(dt)\right) = min\ \sum_{k=1}^s h_{tk}^2\, \overline{M}(a_{tk}) \qquad (3.5)$$

where $d_t = \sum_{k=1}^s h_{tk}\, a_{tk}$; $\sum_{k=1}^s h_{tk} = 1; t = 0, 1, \dots, m, h_{tk} \geq 0.$

The values, h_{tk}, are obtained by taking partial derivatives of $\overline{M}(d_t)$ with respect to h_{tr} of equation (3.5), equating to zero, and solving.

3.9. The average information matrix from all the segments is given by

$$M_d = H\underline{X}'\underline{X}\, H'$$

$$= \sum_k^s H_k\, X_k' X_k H_k'$$

Where H is a matrix of convex combination, and H = $(H_1, H_2, . . . , H_s)$

$$\underline{X}'\underline{X} = diag\ (X_1'X_1, X_2'X_2, \dots, X_s' X_s\ );$$

3.10. The response vector, $\underline{z}$, is obtained from the variance function, g ($\underline{x}$). Hence,

$$\underline{z} = (z_0, z_1, \dots, z_m)';\ z_i = g(\eta_{ij}), \qquad (3.6)$$

$$i = 0, 1, \dots, m; j = 1, 2, \dots, m;$$

Where η_{ij} is the ith and jth element of the average information matrix, M_d.

3.11. Obtain the vector, starting point $(\overline{\underline{x}}_j^*)$,

$$\overline{\underline{x}}_j^* = \sum_{i=1}^{N_0} w_i\, \underline{x}_i;\ w_i = \frac{a_i^{-1}}{\sum_{i=1}^{N_0} a_i^{-1}};$$

$$a_i = \underline{x}_i'\, M^{-1}(\xi_N)\underline{x}_i; \qquad (3.7)$$

And the direction vector $(\underline{d}^*)$ is,

$$\underline{\hat{d}} = M_d^{-1}\underline{z} \tag{3.8}$$

$\underline{d} = (d_0, d_1, \ldots, d_m)'$ and normalized such that $\underline{\hat{d}}'^{*}\underline{\hat{d}}^{*} = 1$. Thus, $\underline{d}^{*} = \underline{d}(\underline{d}'\ \underline{d})^{-\frac{1}{2}}$; and the optimal step-length (ρ^{*}), $g(\rho) = g(\underline{\bar{x}}_j + \rho\underline{d})$, and by taking derivatives of the function with respect to ρ, we have

$$\frac{d[g(\rho)]}{d\rho} = 0;$$

3.12. The new point is $\underline{x}_j = \underline{\bar{x}}^{*} + \rho^{*}\underline{d}^{*}, j = 1, 2, \ldots$

3.13. Take the point, $\underline{x}_1$, to step (3.5) above and add it to the segment it falls into, so that the number of support points for the segment is $(n_k + 1)$, and follow the steps down to obtain a second point $\underline{x}_2$. Again, add the points, $\underline{x}_2$, to the segments it falls, and continue with the steps to obtain a third pint, $\underline{x}_3$, etc. This process is continued until it converges to a point, $\underline{x}_j^{*}$.

3.14. Compute the prediction variance of each design points as $\underline{x}_i' M^{-1}(\xi^0)\underline{x}_i$; i = 1, 2, . . . , n and select the one with minimum prediction variance $V(\underline{x}_{min}) = \underline{x}_{min}' M^{-1}(\xi^0)\underline{x}_{min}$. Add the point $\underline{x}_j'$ row vector to augment the n rows extended matrix, and remove the point with minimum predicted variance in the design to have the determinant as

$$\left|M(\xi^0) + \underline{x}_j\underline{x}_j' - \underline{x}_{min}\underline{x}_{min}'\right|$$

$$= |M(\xi^0)|\{1 + \Delta(\underline{x}_j, \underline{x}_{min})\}$$

Note that $\underline{x}_{min}$ is the point of minimum prediction variance in the design and x_j^{*} is the point of maximum prediction variance from the experimental region, $\tilde{X}$.

3.15. With the new point in the design, compute the inverse information matrix, and the variance function, $g(\underline{x})$, and continue the other processes of the steps to obtain another converging point, which is exchanged with a point of minimum prediction variance from the design.

3.16. Is $\left|\det M_j(\xi)\right| - \det\ M_{j-1}(\xi)\ |$

$\leq \epsilon; \epsilon \geq 0$?

Yes; stop and $M_j(\xi)$ is D-optimal.

4. **Convergence of the sequence**

Given a line sequence $\underline{x}_j = \underline{\bar{x}}_j + \rho_j\underline{d}_j; j = 1, 2, \ldots$; then, $\{\underline{x}_j\}_{j=1}^{\infty} = \{\underline{\bar{x}}_j + \rho_j\underline{d}_j\}_{j=1}^{\infty}$

$\Rightarrow \{\underline{x}_j\}_{j=1}^{\infty} = \underline{x}_r$

Proof

Define the information matrix at the j[th] iteration as

$M_j(\xi_n) = \sum_{i=1}^{n} \underline{x}_i\underline{x}_i'(\xi_n)$: See Gaffke and Krafft(1982) [7] , then

$$M_j = \underline{x}_1\underline{x}_1' + \underline{x}_2\underline{x}_2' + \ldots + \underline{x}_r\underline{x}_r' + \ldots \underline{x}_n\underline{x}_n'$$

$\Rightarrow \sum_{i=1}^{n-1} x_i\,\underline{x}_1' + \underline{x}_r\underline{x}_r'$

Set $M_0 = \sum_{i=1}^{n-1} x_i\,\underline{x}_1'$

$M_j = M_0 + \underline{x}_r\underline{x}_r'$,

Then the determinant becomes

$|M_j| = |M_0 + \underline{x}_r\underline{x}_r'|$

$$\Rightarrow |M_0(1 + \underline{x}_r' M_0^{-1}\underline{x}_r)| \tag{4.1}$$

The information matrix at the (j-1) iteration is $M_{j-1} = M_0 + \underline{x}_k\underline{x}_k'$

$\Rightarrow |M_{j-1}| = |M_0 + \underline{x}_k\underline{x}_k'|$

$$|M_{j-1}| = |M_0(1 + \underline{x}_k' M_0^{-1}\underline{x}_k)| \tag{4.2}$$

By comparing equation (4.1) and (4.2), the sequence moves from a point of low variance to a point of high variance, therefore

$$\underline{x}_k' M_0^{-1}\underline{x}_k \leq \underline{x}_r' M_0^{-1}\underline{x}_r$$

$$\Rightarrow \underline{x}_{j-1}' M_{j-1}^{-1}\underline{x}_{j-1} \leq \underline{x}_j' M_j^{-1}\underline{x}_j, \tag{4.3}$$

Since $M_0 = \sum_{i=1}^{n-1} x_i\,x_i'$ is the same in both equations $\left|M_0(1 + \underline{x}_r' M_0^{-1}\underline{x}_r)\right| \geq \left|M_0(1 + \underline{x}_k' M_0^{-1}\underline{x}_k)\right|$

$\Rightarrow |M_j| \geq |M_{j-1}|$

Then, since $\underline{x}_k' M_0^{-1}\underline{x}_k \leq \underline{x}_r' M_0^{-1}\underline{x}_r$, it follows from equation (4.3) that the point $\{\underline{x}_j' M_j^{-1}\underline{x}_j\}_{j=1}^{\infty}$, is monotonically increasing, and is sure to converge to a point, $\underline{x}_r$.

=> $\{\underline{x}_j\}_{j=1}^{\infty} = \underline{x}_r$. Therefore, the Kolmogrov's condition for convergence with probability one is assured, see Feller (1966, pg 259), and Onukogu and Nsude (2014) [10].

The sequence has the following attributes:

(i) The direction vector is a weighted average from all segments; the weight being proportional to the mean square errors from the segments; see equation (3.7) and the sequence converges with minimax point; see Atkinson and Donev (1992, chapt. 11) [2].

(ii) Again, the response function was not use, only its variance function.

(iii) Division of experimental region into s over-lapping or non-overlapping segments avoids the use of second derivative in obtaining Hessian matrix which at times constitutes problem of inevitability in most line search algorithms, eg. Newton's method is achieved.

5. Numerical Demonstrations

The problems below are used to illustrate the numerical behavior of the search system.

Problem 1: Consider a polynomial regression function, $f(\underline{x}) = \beta_0 + \beta_1 x + \beta_2 x^2, -1 < x < 1$; obtain a 4-point exact D-optimal design. (Atkinson and Donev, 1992) [2]; (Atkinson, Donev and Tobias, 2006) [3] used this problem to find exact D-optimal design of a quadratic polynomial of a single factor. Begin with initial design points as

$$\xi^0 = \{-1, -0.3333, 0.3333, 1\}$$

The extended design matrix is,

$$X(\xi^0) = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -0.3333 & .1111 \\ 1 & 0.3333 & .1111 \\ 1 & 1 & 1 \end{pmatrix};$$

$$X'X(\xi^0) = M(\xi^0)$$

$$= \begin{pmatrix} 4.0000 & 0 & 2.2222 \\ 0 & 2.2222 & 0 \\ 2.2222 & 0 & 2.0247 \end{pmatrix}$$

The variance-covariance matrix is

$$M^{-1}(\xi^0) = \begin{pmatrix} 0.6404 & 0 & -0.7031 \\ 0 & 0.4500 & 0 \\ -0.7031 & 0 & 1.2656 \end{pmatrix};$$

$$det M(\xi^0) = 7.0233$$

The standardized general variance function is given by

$$g(\underline{x}) = n\underline{x}' M^{-1}(\xi^0)\underline{x} = \beta_0 + \sum_{i=1}^{4} \beta_0 \, x^i$$

Thus, the variance function is

$$g(\underline{x}) = 2.5624 - 3.8249x^2 + 5.0624x^4$$

Now partition the experimental region $-1 \leq x \leq 1$ into k=2 non over-lapping segments; $-1 \leq S_1 \leq -0.25$, and $0.25 \leq S_2 \leq 1$ and in the k^th^ segment, $g(\underline{x})$ is approximated by a first-order linear function.

Thus, $y_k = \beta_{00} + \beta_{0k} x \,; k = 1, 2.$

Pick points in the s_k segments, and obtain the X_k design matrices as thus:

$$X_1 = \begin{pmatrix} 1 & -1.0000 \\ 1 & -0.7500 \\ 1 & -0.5000 \\ 1 & -0.2500 \end{pmatrix}; \; X_2 = \begin{pmatrix} 1 & 0.2500 \\ 1 & 0.5000 \\ 1 & 0.7500 \\ 1 & 1.0000 \end{pmatrix}$$

and their information matrices are respectively given as

$$\underline{\bar{X}_1} = \begin{pmatrix} 4 & -2.5000 \\ -2.5000 & 1.8750 \end{pmatrix};$$

$$\underline{\bar{X}_2} = \begin{pmatrix} 4 & 2.5000 \\ 2.5000 & 1.8750 \end{pmatrix};$$

where $\underline{\bar{X}_1} = X_1' X_1$ and $\underline{\bar{X}_2} = X_2' X_2$

The matrices of biasing terms, x^2, x^4, of the variance function, $g(\underline{x})$, of each segment are

$$Xb_1 = \begin{pmatrix} 1.0000 & 1.0000 \\ 0.5625 & 0.3164 \\ 0.2500 & 0.0625 \\ 0.0625 & 0.0156 \end{pmatrix};$$

$$Xb_2 = \begin{pmatrix} 0.0625 & 0.0156 \\ 0.2500 & 0.0625 \\ 0.5625 & 0.3164 \\ 1.0000 & 1.0000 \end{pmatrix}$$

and the coefficient of biasing terms is

$$\underline{c_b} = \begin{pmatrix} -3.8248 \\ 5.0625 \end{pmatrix}$$

The matrix of mean square error of each of the k^th^ segment is given by

$$\overline{M}_k = \underline{\overline{X}}_k^{-1} + \underline{\overline{X}}_k^{-1} X_k' X b_k \underline{c_b} \underline{c_b}' X' b_k X_k \underline{\overline{X}}_k^{-1}$$

$$\Rightarrow \; \overline{M}_1 = \begin{pmatrix} 2.7070 & 3.8821 \\ 3.8821 & 6.1347 \end{pmatrix}; \text{and}$$

$$\overline{M}_2 = \begin{pmatrix} 2.7070 & -3.8821 \\ -3.8821 & 6.1347 \end{pmatrix}$$

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The matrices of convex combination of the segments are $H_1 = diag(0.5, 0.5)$ and $H_2 = (1 - H_1) = diag(0.5, 0.5)$. These matrices are normalized to have

$H_1^* = diag(0.7071, 0.7071)$, and

$$H_2^* = diag(0.7071, 0.7071).$$

The direction vector $\hat{\underline{d}}$, is $\hat{\underline{d}} = M_d^{-1}\underline{z}$

$$\underline{d} = \begin{pmatrix} d_0 \\ d_1 \end{pmatrix}; \hat{\underline{d}} = \begin{pmatrix} 0.6406 \\ 27.5654 \end{pmatrix}$$

and the normalized direction vector, $\hat{\underline{d}}$, such that $\hat{\underline{d}}' \hat{\underline{d}} = 1$ is

$$\hat{\underline{d}} = \begin{pmatrix} 0.0232 \\ 0.9997 \end{pmatrix}$$

Then, the optimal starting point is

$$\overline{\underline{x}}_j = \sum_{i=1}^{8} w_i \underline{x}_i$$

$$\overline{\underline{x}}_0 = \begin{pmatrix} 1.0000 \\ 0.0000 \end{pmatrix}$$

Compute the optimal step-length, ρ_0, by substituting the values of $\overline{\underline{x}}_0 = 0$ and $\hat{\underline{d}} = 0.9997$ in the variance function, we have

$$g(\rho_0) = 2.5624 - 3.8248(0 + .9997\rho_0)^2 + 5.0624(0 + 0.9997\rho_0)^4$$

and solve for ρ_0 to have

$$\hat{\rho}_0 = 0; or$$
$$\hat{\rho}_0 = 0.6148; or$$

$$\hat{\rho}_0 = 0.6148$$

Make a move to obtain a point,

$$\underline{x}_1 = \overline{\underline{x}}_0 + \hat{\rho}_0 \hat{\underline{d}}$$

Thus, substituting the three values of $\hat{\rho}_0$, and have

$$\underline{x}_1 = 0; or$$

-0.6148; or

0.6148.

Checking the prediction variance at each of these three points, we have

$\underline{x}_1 = 0 = \underline{x}_{max.}$

Beginning another iteration in this iteration cycle, we add the point, $\underline{x}_{max}$= 0, to the second segment (S_2) and repeat the process. The points in the first segment are the same as to the first iteration, whereas the second segment is increased by the new point.

This is because; this point falls in the second segment.

Thus, a MATLAB program was developed for this work and the result of the iteration cycles is present in the table 5.1 below.

Table 5.1: The iteration sequence of D-optimal design in (-1, 1), for a quadratic single factor polynomial function

Iteration	Design Points				$\det M\ (\xi)$	ϵ
0	-1	-.3333	.3333	1	7.0233	0
1	-1	-.3333	0	1	7.4074	.3841
2	-1	.0191	0	1	7.9978	.5904
3	-1	.0096	0	1	7.9994	.0016
4	-1	.0048	0	1	7.9999	.0005

In this table, the value of $\epsilon = 0.0005$ is considered very small, meaning that the optimal design is achieved. Therefore, the optimal design points are, (-1, 0.0048, 0, 1).

Problem 2

Let us consider the most general second-order polynomial in two factors with a known solution. Thus, $f(\underline{x}) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2$, $-1 \leq x_1, x_2 \leq 1$; to obtain a 6-point exact D-optimal design.

In the experimental region, $\widehat{X}$, pick the following points.

$$\begin{pmatrix} x_1 & -1 & -1 & 1 & 1 & 0 & -.25 \\ x_2 & 1 & -1 & -1 & 1 & -1 & .25 \end{pmatrix}$$

Then, the extended design matrix is

$$X(\xi^0) = \begin{pmatrix} 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & -.25 & .25 & -.0625 & .0625 & .0625 \end{pmatrix}$$

and the information matrix is

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$X'X = M(\xi^0)$

$$= \begin{pmatrix} 6 & -.25 & -.75 & -.0625 & 4.0625 & 5.0025 \\ -.25 & 4.0625 & -0.625 & .0156 & -.0156 & -.0156 \\ -.75 & -.0625 & 5.0625 & -.0156 & .0156 & -.9844 \\ -.0625 & .0156 & -.0156 & 4.0039 & -.0039 & -.0039 \\ 4.0625 & -.0156 & .0156 & -.0039 & 4.0039 & 4.0039 \\ 5.0625 & -.0156 & -.9844 & -.0039 & 4.00039 & 5.0039 \end{pmatrix}$$

The variance-covariance matrix is

$M^{-1}(\xi^0)$

$$= \begin{pmatrix} 1.1756 & .0667 & -.0667 & .0167 & .05 & -1.2422 \\ .0667 & .2500 & 0.0 & 0.0 & 0.0 & -.0667 \\ -.0667 & 0.0 & .25 & 0.0 & -.25 & .3167 \\ .0167 & 0.0 & 0.0 & .2500 & 0.0 & -.0167 \\ .0500 & 0.0 & -.25 & 0.0 & 1.5000 & -1.3 \\ -1.2422 & -.0667 & .3167 & -.0167 & -1.3 & 2.5589 \end{pmatrix};$$

$$DetM\,(\xi^0) = 225.000$$

The standardized general variance function is

$$d(\underline{x}, \xi_0) = n\underline{x}' M^{-1}(\xi^0)\underline{x}, = g(\underline{x})$$

$$= \beta_0 + \sum_{i=1}^{m} \beta_i x_i + \sum_{i=1}^{m-1}\sum_{i<j}^{m} \beta_{ij} x_i x_j + \sum_{i=1}^{m} \beta_{ii} x_i^2 + \dots$$

Where

$$\underline{x}'_{1\times p} = (1 \quad x_1 \quad x_2 \quad x_1x_2 \quad x_1^2 \quad x_2^2\,)$$

Thus, the variance function is

$$\begin{aligned} g(\underline{x}) = 7.0536 + .80042x_1 - .8004x_2 + .2004x_1x_2 \\ + 2.1x_1^2 - 13.4064x_2^2 - .8002x_1x_2^2 \\ - 3x_1^2x_2 + 3.8004x_2^3 - 14.1x_1^2x_2^2 \\ - .002x_1x_2^3 - .1002x_1^3x_2 + 9x_1^4 \\ + 15.3534x_2^4 \end{aligned}$$

We now partition the experimental region $-1 \le x_1, x_2 \le 1$ into k-segments, k=2 with common boundary as

$S_1 = \{-1 \le x_1 \le 0, -1 \le x_2 \le 1\}$ and $S_2 = \{0 \le x_1 \le 1, -1 \le x_2 \le 1\}$, and in the kth segment, $g(\underline{x})$ is approximated by a first-order linear function.

Thus, $y_k = \beta_{00} + \beta_{1k}x_{1+}\,\beta_{2k}x_{2;}$ k=1, 2.

Pick points in the S_k segments, and obtain the X_k design matrices as thus

$$X_1 = \begin{pmatrix} 1 & -1 & 1 \\ 1 & -1 & 0 \\ 1 & -1 & -1 \\ 1 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix}; X_2 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 1 & -1 \\ 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

and their information matrices are respectively given as

$$\underline{\bar{X}}_1 = \begin{pmatrix} 6 & -3 & 0 \\ -3 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}; \underline{\bar{X}}_2 = \begin{pmatrix} 6 & 3 & 0 \\ 3 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix};$$

Where $\underline{\bar{X}}_1 = X_1'X_1$ and $\underline{\bar{X}}_2 = X_2'X_2$

The matrices of biasing terms, $x_1x_2, x_1^2, \dots, x_2^4$, of the variance function of each segment are

$$Xb_1 = \begin{pmatrix} -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}$$

and

$$Xb_2 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 1 \end{pmatrix}$$

while the coefficient of biasing terms is

$\underline{c}_b' = (.2004\ \ 2.1000 - 13.4064 - .8004 - 3.000 - 3.8004\ - 14.1000 - .002\ - .1002\ \ 9.0000\ \ 15.3534\,)$

The matrix of mean square error of each of the kth segment is given by

$$\overline{M}_k = \underline{\overline{X}}_k^{-1} + \underline{\overline{X}}_k^{-1} X_k' X b_k \underline{c}_b \underline{c}_b' X' b_k X_k \underline{\overline{X}}_k^{-1}$$

$$=> \overline{M}_1 = \begin{pmatrix} 2.0181 & -2.5659 & 2.9859 \\ -2.5659 & 5.6556 & -5.1382 \\ 2.9895 & -5.1382 & 5.5418 \end{pmatrix}; and$$

$$\overline{M}_2 = \begin{pmatrix} 2.0181 & 1.1807 & 2.9895 \\ 1.1807 & 2.0272 & 2.6832 \\ 2.9859 & 2.6832 & 5.5418 \end{pmatrix}$$

The matrices of convex combination of the segments are arranged in the H_i matrices as follows

$$H_1 = \begin{pmatrix} .5000 & 0 & 0 \\ 0 & .2639 & 0 \\ 0 & 0 & .5000 \end{pmatrix};$$

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$$H_2 = \begin{pmatrix} .5000 & 0 & 0 \\ 0 & .7361 & 0 \\ 0 & 0 & .5000 \end{pmatrix}$$

and the normalized H_i are:

$$H_1^* = \begin{pmatrix} .7071 & 0 & 0 \\ 0 & .3374 & 0 \\ 0 & 0 & .7071 \end{pmatrix};$$

$$H_2^* = \begin{pmatrix} .7071 & 0 & 0 \\ 0 & .9414 & 0 \\ 0 & 0 & .7071 \end{pmatrix}$$

The direction vector $\underline{\hat{d}}$, is

$$\underline{\hat{d}} = M_d^{-1}\underline{z}$$

$$= \begin{pmatrix} -0.1069 \\ 9.4973 \\ -52.6626 \end{pmatrix}$$

and normalized the direction vector, $\underline{\hat{d}}$,

such that $\underline{\hat{d}}'\ \underline{\hat{d}} = 1$ is

$$\underline{\hat{d}} = \begin{pmatrix} -.0020 \\ .1775 \\ -.9841 \end{pmatrix}$$

Then, the optimal starting point is

$$\underline{\overline{x}}_j = \sum_{i=1}^{12} w_i \underline{x}_i$$

$$\underline{\overline{x}}_0 = \begin{pmatrix} 1.0000 \\ -0.0031 \\ -0.1166 \end{pmatrix}$$

Compute the optimal step-length ρ_0, by substituting the values of $\underline{\overline{x}}_0$ and $\underline{\hat{d}}$ in the variance function, and thereafter differentiate with respect to ρ_0, equate to zero and solve for $\hat{\rho}_0$, to obtain

$$\rho_0 = .6483, or\ \hat{\rho}_0 = -.7296; or\ \hat{\rho}_0 = -.0835$$

Make a move to obtain a point

$$\underline{x}_1 = \underline{\overline{x}}_0 + \hat{\rho}_0 \underline{\hat{d}}$$

Then, substituting the value of $\hat{\rho}_0$, we have

$$\underline{x}_1 = \begin{pmatrix} .1119 \\ -.7546 \end{pmatrix}; or\ \underline{x}_1 = \begin{pmatrix} -.1326 \\ .6015 \end{pmatrix};\ or\ \underline{x}_1 = \begin{pmatrix} -.0180 \\ -.0344 \end{pmatrix}$$

The point of maximum prediction variance among the three points is

$$\underline{x}_1^* = \begin{pmatrix} -.0180 \\ -.0344 \end{pmatrix}$$

Add this point $\underline{x}_1^*$, to the second segment (S_2) of the experimental region and repeat the process. Notice that the points in the first segment have increased by the addition of the new point, whereas the points in the second segment remain the same.

The summary of the iteration cycles is given in the table below.

Table 5.2: The iteration sequence of D-optimal design in [-1, 1], for a quadratic polynomial function of two factors

Iteration	Design points	$Det\ M(\xi)$	ϵ
0	-1,1 -1,-1 1,-1 1,1 0,-1 -25, .25	225.0000	-
1	-1,1 -1,-1 1,-1 1,1 0,-1 -.0140, -.0345	255.3910	30.3910
2	-1,1 -1,-1 1,-1 1,1 0,-1 -.018 .0049	255.9877	.5967
3	-1,1 -1,-1 1,-1 1,1 0,-1 -.0178, -.0007	255.9997	.0012
4	-1,1 -1,-1 1,-1 1,1 0,-1 -.0178, .0001	256.0000	.0003

The value of $\epsilon = .0003$ is considered very small, meaning that the optimal design is reached.

Atkinson and Donev (1992) used KL exchange method to solve the problem for generating an exact D-optimal design for this regression model and obtain the same result which Box and Draper (1971) obtained via a computer hill-climbing search.

Their D-optimal design is

$$n = (-1,-1),(1,-1),(-1,1),(-.1315,-.1315),(.3945,1),(1,.3945)$$

5.2 Assessment of the search method

The assessment of this method was considered in two folds. The first one is the computer execution

time (c. e. t.) of the algorithm to get to D-optimal design. In this paper, a Matlab program of this algorithm was developed and average of twenty running time of each model is presented in the table below. All runs were performed in a Presario CQ56 laptop computer.

The second other way of assessment is through D-efficiency. D-efficiency is a relative measure of how design compares with the D-optimum design for a specific design experimental region. Design efficiency is used to compare user-specified design to the optimal design. Theoretically, design efficiency lies between 0 and 1, and the closer the efficiency to 1, the better the arbitrary design. If information matrix for optimal design is $M(\xi_1)$, and suppose an arbitrary information matrix of a design is $M(\xi_2)$. Then the D-efficiency of the arbitrary design is defined as

$D_{eff} = \{\frac{|M(\xi_2)|}{|M(\xi_1)|}\}^{\frac{1}{p}}$, where p is the number of model parameters: see Atkinson and Donev (1989).

The table below shows how the method compares with the KL-exchange method reported by Atkinson and Donev.

Table 5.3: The performance of method

Design problem			Performance of line search	Performance relative to KL exchange	Execution time
m	p	n	$\lvert M(\xi)\rvert$	D_{eff}	In seconds
1	3	3	7.9999	1.0000	0.08
2	6	6	256.0000	0.9924	2.24

The table 5.3 above shows that the method is efficiently equal to what Atkinson, Donev and Tobias reported for a single factor quadratic polynomial function. In the same way, the new method is highly efficient as the result reported using KL exchange method for two factor quadratic polynomial models. Again, the new method reached the optimal design points in only four iteration cycles in each of the example with minimal execution time.

6. Conclusion

A line search method for constructing D-optimal exact designs for a polynomial response function f($\underline{x}$) of degree **z,** where the factor levels $\underline{x}$ are defined in continuous geometry is shown. Under this search method, variance of the regression function is approximated by a polynomial function of degree 2**z**. A maximizer of this polynomial is determined by segmented line search technique. Thereafter, this maximizer is used to replace the point of minimum prediction variance from amongst the point already in the design. This exchange of points is continued until the sequence converges to D-optimal design.

The search method compares favorably with the method of KL-Exchange Algorithm reported by Atkinson and Donev. We affirm that the new search method is a single search system, in contrast to the “Adjustment Algorithm” of Atkinson and Donev (1992, Chapter 15), where a secondary search is required at the end of the primary one before the search terminates.

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