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VARIANCE GRADIENT-BASED LINE SEARCH ALGORITHM FOR CONSTRUCTING *D*-OPTIMAL EXACT DESIGNS IN CONTINUOUS EXPERIMENTAL REGION

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Abstract

The method presented here is a variance gradient based approach for constructing exact D-optimal designs. Variance of regression function is approximated by a polynomial function of degree $2n'$. Maximizer of this polynomial is determined by a variance modulated line search. Thereafter, this maximizer is used to replace the point of minimum prediction variance amongst the points already in the design. This exchange of points is continued until the sequence converges to D-optimal design. This method has a rapid convergence and compares with the method reported by Atkinson and Donev. Finally, the computer execution time of this method is highly encouraged.

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1. Introduction

Construction of D-optimal exact designs involves selection of n-support points or treatments $(\underline{x})$ from a given space of trials $\widetilde{X}$, $\underline{x} \in \widetilde{X}$, such that the determinant of the Fisher's information matrix $|X'X|$ is optimized.

In this study, treatments or support points, $\underline{x}_i$, were selected such that each element of $\underline{x}_i$, is attached a weight w_i; $w_i \geq 0$ and $\sum_{i=1}^{n} w_i = 1$, 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 term (the columns) evaluated at specific treatments 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, $\underline{x}_i \in \widetilde{X}$, $i = 1, 2, \ldots, n$, 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. This criterion has attracted interest from many authors. For instance, Boon [4] noted that in many cases of optimal experiments, D-optimality criterion is simply used to minimize post-experiment uncertainty in the model parameters. Again, Montgomery [9] describe D-optimality criterion as the most popular and mathematically tractable for which minimizing $|X'_\xi X_\xi|^{-1}$ (or maximizing $|X'_\xi X_\xi|$) results in minimizing the generalized variance of the estimated coefficients and

minimizing the volume of the confidence ellipsoid of parameter, β. Some of the influential qualities of D-optimality criterion has been given by Mitchell [8] as low variances for the parameters, low correlations among parameters, and low maximum variance $(\text{var}(\underline{x}))$ over the experimental region, $\widetilde{X}$. Other optimality criteria have been reported severally (Atkinson and Donev [2]; Onukogu and Chigbu [11]).

Therefore, in this paper, the intention is to develop a new algorithm called a variance gradient-based algorithm which seeks iteratively an n-point design measure, ξ_n that maximizes the determinant of $M(\xi^*)$; i.e., $\text{Max}|M(\xi^*)|$; $M(\xi_n) \in S^{p\times p}$, where $S^{p\times p}$ is a set of all non-singular $p \times p$ information matrices defined in $\widetilde{X}$.

There are many algorithms developed for the construction of D-optimal exact designs. For instance, Fedorov [7] reported a sequence of continuous design algorithm based on sequential addition of points to initial starting design. This algorithm was called Fedorov exchange algorithm (FEA). The Fedorov's algorithm calculates delta function for all possible exchange couples during one iteration but only uses one of the values that maximizes the determinant of the information matrix to perform an exchange. This algorithm is computationally intensive and time waste. Due to the Fedorov [7] drawback which borders on the explosion of candidate list of points as the factor increases, Cook and Nachtsheim [6] modified the Fedorov's procedure by reducing the number of calculations, where each iteration is broken down into n-stages, one for each support point in the design. This method also calculates the delta functions, but does it in stages. In the last two decades, Atkinson and Donev [1] have also reported KL-exchange algorithm for constructing D-optimal exact designs. The idea of the KL-exchange algorithms is to remove or add support points to the initial design matrix and determine the effect of the modification. This algorithm begins with non-singular

n-point designs and then new points from the experimental region, $\widetilde{X}$, are added and existing design points deleted in an effort to improve the value of the determinant.

Recently, Onukogu [10] reported methods for locating optimum of constrained as well as unconstrained optimization problems. The methods favoured classical line search techniques with significant differences in its approach to estimate the key parameters. Generally, most gradient line search techniques adopt three common parts such as the initial point $(\underline{\bar{x}}_k)$, direction vector $(\underline{d}_k)$, and step-length (ρ_k), yielding a new point, $(\underline{x}_{k+1} = \underline{\bar{x}}_k + \rho_k \underline{d}_k)$; and the process is then repeated.

This set of sequential activities applies as well to the new technique herein introduced. Again, the new method also adopts the use of variance exchange of points procedure, which is originally reported by Fedorov [7], and modified severally over decades before Atkinson and Donev [1] KL-exchange algorithm.

2. Theoretical Framework

Let us assume a p parameter polynomial function, and we are desired to select n point that would give a D-optimal exact design.

The following steps summarize the method:

(1) Obtain a collection of $N > n$ support points from the experimental region, $\widetilde{X}$ as follows, $\underline{x}_1, \underline{x}_2, \ldots, \underline{x}_N$, where $\underline{x}_i = (x_{i1}, x_{i2}, \ldots, x_{im})$, $i = 1, 2, \ldots, N$.

(2) Group the candidates points into g_k groups with n_k elements, $k = 1, 2, \ldots, h$, according to their relative distance, d_k, from the center of the experimental region, $\widetilde{X}$.

Thus,

$$g_1 = \begin{pmatrix} \underline{x}_{11} \\ \underline{x}_{12} \\ . \\ . \\ . \\ \underline{x}_{1p} \end{pmatrix}; \; g_2 = \begin{pmatrix} \underline{x}_{21} \\ \underline{x}_{22} \\ . \\ . \\ . \\ \underline{x}_{2p} \end{pmatrix}; \ldots, \; g_h = \begin{pmatrix} \underline{x}_{h1} \\ \underline{x}_{h2} \\ . \\ . \\ . \\ \underline{x}_{hp} \end{pmatrix},$$

such that $d_k \geq d_{k+1}$ and $\sum_{k=1}^{h} n_k = N$.

(3) Select an initial point nonsingular design from the h groups to make up an n point design beginning from the points in g_1, followed by g_2, and so on.

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

(5) From the above, compute standardized generalized variance function of degree $2n'$ as

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

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

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

where

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

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

(6) Compute the m-component gradient vector, $\underline{g}$, by taking partial derivatives of $g(\underline{x})$ with respect to x_i.

That is,

$$\underline{g} = \{ \frac{\partial(g(\underline{x}))}{\partial(x_i)} \}$$

$$= \begin{pmatrix} g_1(x) \\ g_2(x) \\ . \\ . \\ . \\ g_m(x) \end{pmatrix}.$$

(7) Substitute the values of the design measure in the g_i,

$$\xi_n = \begin{pmatrix} \underline{x}_1 \\ \underline{x}_2 \\ . \\ . \\ . \\ \underline{x}_n \end{pmatrix}; \quad \underline{x}_i = (x_{i1}, x_{i2}, \ldots, x_{im}).$$

(8) Compute the simple arithmetic average

$$\underline{\bar{x}}_j = \sum_{i=1}^{n} \underline{x}_i \,/\, n,$$

where n is the number of support points.

(9) Define the direction vector, $\underline{d}_j$ as

$$\underline{d}_j = \sum_{i=1}^{n} \theta_i \underline{g}_i;$$

where θ is the coefficient of convex combination; $\theta_i \in (0, 1)$;

$$\sum_{i=1}^{n} \theta_i = 1,$$

and the variance of $\underline{d}_i$ is

$$\mathrm{Var}(\underline{d}_i) = \sum_{i=1}^{n} \theta_i^2 a_i,$$

where a_i is the variance at each point.

And to optimizing the variance of $\mathrm{Var}(\underline{d}_i)$, we take a partial derivatives of $\mathrm{Var}(\underline{d}_i)$ with respect to θ_i. That is,

$$\frac{\partial(V(\underline{d}))}{\partial(\theta_i)} = 2\theta_i a_i - 2(1 - \theta_1 - \theta_2 - \ldots - \theta_{n-1})a_n = 0.$$

Thus,

$$\frac{\partial(V(\underline{d}))}{\partial(\theta_1)} = 2\theta_1 a_1 - 2(1 - \theta_1 - \theta_2 - \ldots - \theta_{n-1})a_n = 0,$$

$$\frac{\partial(V(\underline{d}))}{\partial(\theta_2)} = 2\theta_2 a_2 - 2(1 - \theta_1 - \theta_2 - \ldots - \theta_{n-1})a_n = 0,$$

$$\ldots$$

$$\ldots$$

$$\ldots$$

$$\frac{\partial(V(\underline{d}))}{\partial(\theta_{n-1})} = 2\theta_{n-1} a_{n-1} - 2(1 - \theta_1 - \theta_2 - \ldots - \theta_{n-1})a_n = 0,$$

and by the method of system of equations, we have the above equations in matrix form as

$$\begin{pmatrix} a_1 + a_n & a_n & \cdot & \cdot & \cdot & a_n \\ a_n & a_2 + a_n & \cdot & \cdot & \cdot & a_n \\ & \cdot & a_3 + a_n & & & \cdot \\ & \cdot & & \cdot & & \cdot \\ & \cdot & & & \cdot & \cdot \\ & \cdot & & & & a_{n-1} + a_n \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \\ \cdot \\ \cdot \\ \cdot \\ \theta_{n-1} \end{pmatrix} = \begin{pmatrix} a_n \\ a_n \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} \theta_1 \\ \theta_2 \\ \cdot \\ \cdot \\ \cdot \\ \theta_{n-1} \end{pmatrix} = \begin{pmatrix} a_1 + a_n & a_n & \cdot & \cdot & \cdot & a_n \\ a_n & a_2 + a_n & \cdot & \cdot & \cdot & a_n \\ & \cdot & a_3 + a_n & & & \cdot \\ & \cdot & & \cdot & & \cdot \\ & \cdot & & & \cdot & \cdot \\ & \cdot & & & & a_{n-1} + a_n \end{pmatrix}^{-1} \begin{pmatrix} a_n \\ a_n \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{pmatrix}.$$

$$\Rightarrow \begin{pmatrix} \theta_1 \\ \theta_2 \\ \cdot \\ \cdot \\ \cdot \\ \theta_{n-1} \end{pmatrix} = A^{-1} \begin{pmatrix} a_n \\ a_n \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{pmatrix} \Leftrightarrow \underline{\theta} = A^{-1} \underline{a}.$$

The value of

$$\theta_n = 1 - \sum_{i-1}^{n-1} \theta_i,$$

and normalize θ_i as

$$\theta_i^* = \theta_i \left(\sum_{i=1}^{n} \theta_i^2\right)^{-\frac{1}{2}}.$$

(10) Define the step-length ρ_j as

$$g(\rho_j) = g(\underline{\bar{x}} + \rho \underline{d}),$$

$$\therefore \frac{d[d(\rho)]}{d\rho} = \frac{d[g(\underline{\bar{x}} + \rho \underline{d})]}{d\rho},$$

and solve for ρ.

(11) Obtain a point by substituting the values of the vectors, $\underline{\hat{\bar{x}}}$, $\underline{\hat{d}}$, and $\hat{\rho}$ into

$$\underline{x}_j^* = \underline{\bar{x}} + \rho \underline{d}.$$

(12) Compute the prediction variance of each design point as $\underline{x}_i' M^{-1}(\xi_n^0) \underline{x}_i$; $i = 1, 2, \ldots, n$ 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

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

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

(13) 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.

(14) Is

$$\underline{x}_j^{*\prime} M^{-1}(\xi_n^0)\underline{x}_j^* \not> \underline{x}'_{\min} M^{-1}(\xi_n^0)\underline{x}_{\min},$$

and

$$|\det M_j(\xi_n) - \det M_{j-1}(\xi_n)| \leq \epsilon; \quad \epsilon \geq 0,$$

stop otherwise return to (3) above.

The algorithm

Step 1. Start with an initial design measure, ξ_n^0;

obtain the design matrix, $X(\xi^0)$; $M(\xi^0)$, and $M^{-1}(\xi_n^0)$; such that $|M(\xi_n^0)| > 0$.

Step 2. Generate the general variance function, $g(\underline{x}) = \underline{x}' M^{-1}(\xi_n^0)\underline{x}$; $\underline{x} \in \widetilde{X}$.

Step 3. Obtain the vectors; $\overline{\underline{x}}$, $\underline{d}$, ρ and make a move to

$$\underline{x}_j = \overline{\underline{x}} + \rho \underline{d}.$$

Step 4. Compute $\underline{x}'_i M^{-1}(\xi_n^0)\underline{x}_i$; $i = 1, 2, \ldots, n$ and select $V(\underline{x}_{\min}) = \underline{x}'_{\min} M^{-1}(\xi_n^0)\underline{x}_{\min}$.

Step 5. Exchange $\underline{x}_{\min}$ with $\underline{x}_{\max}$ if $V(\underline{x}_{\max}) > V(\underline{x}_{\min})$ and define ξ^1 thereafter.

Step 6. Stop if $V(\underline{x}_{\max}) \not> V(\underline{x}_{\min})$, such that $|\det M_j(\xi_n) - \det M_{j-1}(\xi_n)| \leq \epsilon$; $\epsilon \geq 0$;

else return to Step 1 above.

3. Numerical Examples

Example 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 [2]; Atkinson et al. [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

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

Thus, the variance function is

$$g(\underline{x}) = 2.5624 - 3.8248x^2 + 5.0624x^4.$$

The gradient function $\underline{g} = g_1$ is

$$g_1 = \frac{d[g(\underline{x})]}{dx}$$

$$= -7.65x + 20.25x^3,$$

and substituting the values of the design points in the g_1 to have the results of gradient vector. The values of the convex combination, $\underline{\theta}$, is

$$\underline{\theta} = A^{-1}\underline{a};$$

where the matrix A and vector $\underline{a}$ are given below:

$$A = \begin{pmatrix} 7.6 & 3.8 & 3.8 \\ 3.8 & 6.0 & 3.8 \\ 3.8 & 3.8 & 6.0 \end{pmatrix}; \quad \underline{a} = \begin{pmatrix} 3.8 \\ 3.8 \\ 3.8 \end{pmatrix}.$$

The table hereunder shows points of the initial design, their gradient values, their variances, and values of θ.

Table 1. The initial design points, variance at each point, the gradient values, and the θ

S/No	Point	g_1	a_i	θ_i
1	-1	-12.6	3.8	.1833
2	$-1/3$	1.8	2.2	.3167
3	$1/3$	-1.8	2.2	.3167
4	1	12.6	3.8	.1833

The direction vector is

$$\underline{d}_j = \sum_{i=1}^{n} \theta_i^* \underline{g}_1$$

$$= \underline{\theta}^{*'} \underline{g}$$

$$= -8.1166 \times 10^{-4},$$

and normalize to have

$$\underline{d}^* = -1.0000.$$

The starting point $\underline{\bar{x}}_j$ is

$$\underline{\bar{x}}_j = \sum_{i=1}^{4} \underline{x}_i \,/\, 4 = 0.0.$$

Compute the step-length ρ as

$$g(\rho) = g(\underline{\bar{x}} + \rho \underline{d}),$$

$$g(\rho) = 2.5625 - 3.825(0 - \rho)^2 + 5.0625(0 - \rho)^4.$$

Thus,

$$\frac{d[g(\underline{\bar{x}} + \rho \underline{d})]}{d\rho} = 0,$$

$$-7.65\rho + 20.25\rho^3 = 0,$$

and solving for ρ, we have

$$\rho = -.614636;\ \rho = 0.0;\ \text{or}\ \rho = .614636.$$

Make a move to have

$$\underline{x}_1 = -.6146,\ \text{or}\ \underline{x}_1 = 0.0,\ \text{or}\ \underline{x}_1 = .6146.$$

The point of maximum variance among these three points is

$$\underline{x}^* = 0.0;$$

and from Table 1 above, the variance of 2nd and 3rd points are equal, and hence the 2nd point is dropped for the new point $\underline{x}^*$ to enters the design.

The new extended design matrix is

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

$$X' X(\xi^1) = M(\xi^1) = \begin{pmatrix} 4.0000 & .3333 & 2.1111 \\ .3333 & 2.1111 & .0370 \\ 2.1111 & .0370 & 2.0123 \end{pmatrix}.$$

The variance-covariance matrix is

$$M^{-1}(\xi^1) = \begin{pmatrix} 0.5733 & -0.0800 & -0.6000 \\ -0.0800 & 0.4850 & 0.0750 \\ -0.6000 & 0.0750 & 1.1250 \end{pmatrix}; \det M(\xi^0) = 7.4074.$$

The standardized general variance function is given by

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

Thus, the variance function is

$$g(\underline{x}) = 2.2933 - .64x - 2.86x^2 + .6x^3 + 4.5x^4.$$

The process is continued to obtain a second point $\underline{x}_2^*$, that would replace another point in the design. The determinant of $(X_2'X_2)$ is

$$\mathrm{Det}(X_2'(\xi^1)X_2(\xi^1)) = 7.9252.$$

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

Table 2. 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	0	.3333	1	7.4074	.3841
2	– 1	0	– .1124	1	7.9252	.5178
3	– 1	0	.0536	1	7.9828	.0576
4	– 1	0	– .0265	1	7.9958	.0130
5	– 1	0	.0111	1	7.9993	.0035

In this table, the value of $\epsilon = 0.0035$ is considered very small, meaning that the optimal design is achieved. Therefore, the optimal design points are, $(-1, 0, .0111, 1)$.

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

In the experimental region, $\widetilde{X}$, pick the following points and group them according to their relative distance from the center:

$$g_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix}; \; g_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \\ -1 & 0 \\ 0 & 1 \end{pmatrix}; \; g_3 = \begin{pmatrix} 1/4 & 1/4 \\ 1/4 & -1/4 \\ -1/4 & -1/4 \\ -1/4 & 1/4 \end{pmatrix}; \; g_4 = (0 \;\; 0).$$

Begin with the initial design measure as

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

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

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

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

The variance-covariance matrix is

$$M^{-1}(\xi^0) = \begin{pmatrix} 1.1756 & .0667 & -.0667 & .0167 & .05 & -1.2422 \\ .0667 & .2500 & 0.0 & 0.0 & 0.0 & -.0667 \\ -.0667 & 0.0 & .25 & 0.0 & -.25 & .3167 \\ .0167 & 0.0 & 0.0 & .2500 & 0.0 & -.0167 \\ .05 & 0.0 & -.25 & 0.0 & 1.5000 & -1.3 \\ -1.2422 & -.0667 & .3167 & -.0167 & -1.3 & 2.5589 \end{pmatrix};$$

$$\mathrm{Det}M(\xi^0) = 225.0000,$$

the standardized general variance function is

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

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

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

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 standardized variance function is

$$g(\underline{x}) = 7.0536 + 0.8004x_1 + 2.1x_1^2 + 9x_1^4 - 0.8004x_2 + 0.2004x_1x_2 - 3x_1^2x_2$$

$$-13.4064x_2^2 - 0.8004x_1x_2^2 - 14.1x_1^2x_2^2 + 3.8004x_2^3 - 0.2004x_1x_2^3 + 15.3534x_2^4.$$

The gradient function $\underline{g} = \{g_1, g_2\}$ is

$$g_1 = \frac{\partial[g(\underline{x})]}{\partial x_1}$$

$$= .8004 + 4.2x_1 + 36x_1^3 + .2004x_2 - 6x_1x_2 - .8004x_2^2 - 28.2x_1x_2^2 - .2004x_2^3;$$

$$g_2 = \frac{\partial[g(\underline{x})]}{\partial x_2}$$

$$= -.8004 + .2004x_1 - 3x_1^2 - 26.8128x_2 - 1.6008x_1x_2 - 28.2x_1^2x_2 + 11.4012x_2^2$$

$$- .6012x_1x_2^2 + 61.4136x_2^3,$$

and substituting the values of the design points in the g_1 and g_2 to have the results of gradient vectors. The values of $\underline{\theta}$ is

$$\underline{\theta} = A^{-1}\underline{a};$$

where the matrix A and vector $\underline{a}$ are given below:

$$A = \begin{pmatrix} 12 & 6 & 6 & 6 & 6 \\ 6 & 12 & 6 & 6 & 6 \\ 6 & 6 & 12 & 6 & 6 \\ 6 & 6 & 6 & 12 & 6 \\ 6 & 6 & 6 & 6 & 12 \end{pmatrix}; \quad \underline{a} = \begin{pmatrix} 6 \\ 6 \\ 6 \\ 6 \\ 6 \end{pmatrix}.$$

The table hereunder shows points of the initial design, their gradient values, their variances, and values of θ.

The direction vector is

$$\underline{d}_j = \sum_{i=1}^{n} \theta_i^* \underline{g}_i$$

$$= \underline{\theta}^{*'} \underline{g}$$

$$= \begin{pmatrix} .0002 \\ .0038 \end{pmatrix},$$

and normalize to have

$$\underline{d}^* = \begin{pmatrix} .0499 \\ .9988 \end{pmatrix}.$$

Table 3. The initial design points, variance at each point, the gradient values, and the θ

S/No	Point	$\underline{g} = (g_1, g_2)$	θ	a_i
1	– 1, 1	– 6.0, 16.0032	.1667	6
2	– 1, – 1	– 18.0, 0.0	.1667	6
3	1, –1	18.0, 2.4	.1667	6
4	1, 1	6.0, 12.0	.1667	6
5	0, – 1	0.0, – 24.0	.1667	6
6	– .25, .25	.0005, – 6.4002	.1667	6

The starting point $\underline{\bar{x}}_j$ is

$$\underline{\bar{x}}_j = \sum_{i=1}^{6} \underline{x}_i / 6$$

$$= \begin{pmatrix} -.0417 \\ -.1250 \end{pmatrix}.$$

Compute the step-length ρ as

$$g(\rho) = g(\underline{\bar{x}} + \rho \underline{d}),$$

$$g(\rho) = 7.0536 + 0.8004(-.0417 + .0499\rho) + 2.1(-.0417 + .0499\rho)^2 + \ldots$$

$$+ 15.3534(-.1250 + .9988\rho)^4.$$

Thus,

$$\frac{d[g(\underline{\bar{x}} + \rho \underline{d})]}{d\rho} = 0,$$

$$2.6166 - 26.6681\rho - 11.4988\rho^2 - 60.9702\rho^3 = 0,$$

and solving for ρ, we have

$$\rho = -.623425;\ \rho = .0961631;\ \text{or}\ \rho = .715858.$$

Make a move to have

$$\underline{x}_1 = \begin{pmatrix} -.0728 \\ -.7477 \end{pmatrix};\ \underline{x}_1 = \begin{pmatrix} -.0369 \\ -.029 \end{pmatrix};\ \underline{x}_1 = \begin{pmatrix} -.0060 \\ .5900 \end{pmatrix}.$$

The point of maximum variance among these three points is

$$\underline{x}^* = \begin{pmatrix} -.0369 \\ -.02900 \end{pmatrix},$$

and from Table 3 above, the variance of all the points are equal, but the point with minimum effect on determinant is the last point and is dropped for the new point $\underline{x}^*$ to enters the design.

The new extended design matrix is

$$X_2(\xi^1) = \begin{pmatrix} 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & -1 & 0 & 0 & 1 \\ 1 & -.0369 & -.029 & .0011 & .0014 & .0008 \end{pmatrix}.$$

The process is continued to obtain a second point $\underline{x}_2^*$, that would replace another point in the design. The determinant of $(X_2'X_2)$ is

$$\text{Det}(X_2'(\xi^1)X_2(\xi^1)) = 255.5696.$$

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

Table 4. 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	– .0369, – .0290	255.5696	30.5696
2	– 1, 1	– 1, – 1	1, – 1	1, 1	0, – 1	.0248, .0057	255.9834	.4138
3	– 1, 1	– 1, – 1	1, – 1	1, 1	0, – 1	– .0108, – .0003	256.0000	.0166
4	– 1, 1	– 1, – 1	1, – 1	1, 1	0, – 1	– .0105, .0001	256.0000	.0000

The value of the $\epsilon = 0.0$ is considered very small, meaning that the optimal design is reached. Atkinson and Donev [1] used KL exchange algorithm to solve the problem of generating an exact *D*-optimal design for this regression model and obtain the same result which Box and Draper [5] obtained via a computer hill-climbing search.

Their *D*-optimal design is $n = (-1, -1), (1, -1), (-1, 1), (-.1315, -.1315)$, $(.3945, 1), (1, .3945)$.

Performance of algorithms

Generally, performance of algorithms is considered on two folds. The first one is the computer execution time (c. e. t.) of the algorithm to get to *D*-optimal design. In this work, 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 Persorio CQ56 laptop computer.

The second 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

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

The table below shows how the variance gradient-based line search compares with the KL-exchange algorithm reported by Atkinson and Donev.

Table 5. The performance of non grid line search for second order models

Design problem			Performance of non grid	Performance relative to KL exchange	Execution time
m	p	n	$\|M(\xi)\|$	D_{eff}	in seconds
1	3	4	7.9993	.9999	.011
2	6	6	256.0000	0.9924	4.310

The Table 5 above shows that variance gradient-based line search is as efficient as the result reported using KL exchange method for one and two factor quadratic polynomial models. The new method reached the optimal design points in only five and four iteration cycles in a time of .011 and 4.31 seconds, respectively.

4. Conclusion

A technique for constructing D-optimal exact designs in continuous experimental region is presented. The method is very easy without computational clumsiness. Initial design points are selected by maximum distant from the centre of the experimental region, so as to avoid running many instances of randomly generated initial designs. Exchange of points are done to remove those initial design points that are not optimally chosen and finally, it makes use of continuous search over the space of trial, $\widetilde{X}$, and therefore circumvents the problems associated with the use of large grid of points.

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