A NOTE ON CYCLIC ORTHOGONAL DESIGNS

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Abstract: Orthogonality is considered to be one of the most important features for design of experiment. In this paper, we investigate orthogonal main-effect designs with cyclic structure in order to ensure the balance among all design columns. We show that such designs exist for any number of factors (k) and moreover, they are not unique. An explicit form for D-efficiency of cyclic orthogonal designs is derived. It is shown that D-optimal cyclic design essentially involves minimizing the tightness of the experimental range. The minimum tightness D-optimal cyclic orthogonal designs are presented and tabulated for $k < 10$.

Key words and phrases: D-optimality, Plackett and Burman designs, Regular simplex designs, T-optimality.

1. Introduction

The first-order design has great value in response surface methodology at the initial stage; for example, screening input variables or estimating the direction of steepest ascent. The construction of first-order response surface designs which are optimal in some sense has received a great deal of attention in the literature (see Lin (1993) and references therein). The saturated design which investigates k variables in $n = k + 1$ runs is commonly employed. Although orthogonality is one of the most important features in selecting a design, it is in general not possible. For example, in the case of a two-level design, the Plackett and Burman type orthogonal design is only available when n is a multiple of four. On the other hand, some first-order orthogonal designs, such as regular simplex designs (Box (1952)), are presented in an asymmetric manner, which may create problems in practice (for instance, allocating factors to design columns or determining the experimental regions which suitably fit the coded variables). In this paper, we consider first-order orthogonal design with cyclic structure. The cyclic structure has been adapted to generate *symmetry* among all design columns. Here, "symmetry" refers to identical experimental range and the common structure of all design columns.

Consider the first-order polynomial model in k variables:

$$Y = \mathbf{X}\boldsymbol{\beta} + \varepsilon = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1\xi_1 + \boldsymbol{\beta}_2\xi_2 + \cdots + \boldsymbol{\beta}_k\xi_k + \varepsilon, \tag{1}$$

where Y is the response variable and ξ_i's are the independent variables. A cyclic design in k variables with first row $[x_1, x_2, \ldots, x_k]$ can be constructed by cyclically permuting the values in the first row to create $k - 1$ more rows and then adding a row of all -1's as the final row. Thus, the design matrix $\mathbf{X}$ for a cyclic design in k variables can be written in the general form as

$$X = \begin{bmatrix} 1_{kx1} & \Gamma_0 X_1 & \Gamma_{k-1} X_1 & \cdots & \Gamma_1 X_1 \\ 1 & -1 & -1 & \cdots & -1 \end{bmatrix}, \tag{2}$$

where $X_1 = [x_1, x_k, x_{k-1}, \ldots, x_2]'$, $1_{k \times 1}$ is the $k \times 1$ vector of ones and Γ_h is a circulant matrix whose first row has l in the $(h+1)$th column and zero elsewhere (see John and Williams (1995)). A first-order design is orthogonal if the inner product of any two columns of the $\mathbf{X}$ matrix equals zero. Namely, $(\Gamma_i X_1)'(\Gamma_j X_1) = -1$ for all $i, j = 0, \ldots, k - 1$ and $i \neq j$. Adding the initial condition $1'X_1 = 1$, the conditions for a cyclic orthogonal design yield a set of $(C_2^k + 1)$ equations to be solved. As we shall see, however, the total number of equations can be reduced to $[\frac{k}{2}] + 1$.

2. Cyclic Orthogonal Designs

It follows easily that $\Gamma_h \Gamma_s = \Gamma_{h+s}$, and $\Gamma_h' = \Gamma_{k-h}$, where $h + s$ is reduced mod k. Consequently, $\Gamma_{k-i}' \Gamma_{k-i-s} = \Gamma_i \Gamma_{k-i-s} = \Gamma_{k-s}$. Using the fact that these are equations in scalars, we have

$$X_1' \Gamma_{k-s} X_1 = X_1' \Gamma_s' X_1 = X_1' \Gamma_s X_1. \tag{3}$$

Thus, there are at most k different equations to be solved to obtain a cyclic orthogonal design:

$$\sum_{i=1}^{k} x_i = 1, \tag{4a}$$

$$X_1' \Gamma_s X_1 = -1, \quad s = 1, \ldots, k - 1. \tag{4b}$$

In fact, we can further reduce the total number of equations to $[\frac{k}{2}]+1$ for obtaining a cyclic orthogonal design, as shown below.

Proposition 2.1. *There are exactly $[\frac{k}{2}] + 1$ independent equations in solving a cyclic orthogonal design system* (4a, 4b).

Proof. Applying Equation (3), we have $X_1' \Gamma_s X_1 = X_1' \Gamma_{k-s} X_1$ for $s = 1, \ldots, [\frac{k}{2}]$. These equations, together with the initial independent equation (4a), imply that there are at most $[\frac{k}{2}] + 1$ independent equations. On the other hand, the first $s = 1, \ldots, [\frac{k}{2}]$ equations in (4b) involve products of all possible pairs among

$x_1, \ldots, x_k$. Each product appears in exactly one equation. Thus, by adding equation (4a), there are at least $[\frac{k}{2}] + 1$ independent equations. This completes the proof.

3. Existence Properties and Design Efficiency

A cyclic orthogonal design with the form (2) exists for any positive integer k. This can be seen by taking $z = x_1 = x_2 = \cdots = x_{k-1}$ and $w = x_k = 1 - (k-1) \cdot z$ in equation (4a); then, all of the equations in (4b) reduce to the equation $k \cdot z^2 - 2 \cdot z - 1 = 0$. The roots for such a quadratic equation are

$$(z, w) = \Big(\frac{1 \pm (k+1)^{\frac{1}{2}}}{k}, \frac{1 \mp (k-1)(k+1)^{\frac{1}{2}}}{k} \Big).$$

Besides the solution above, other solutions are also possible. (All possible solutions for $k = 2, 3$, and 4 are given in Lin and Chang (1999).) Further, optimality criteria can be imposed to choose among them.

Since cyclic orthogonal designs have $X'X = (k+1)\mathbf{I}$, the determinant of $X'X$ is always a constant, $||X'X|| = (k+1)^{k+1}$. This can be seen by noting $x_1^2 + \cdots + x_k^2 = k$ (see Appendix of Lin and Chang (1999)). For a fair comparison on design efficiency, we re-scale all values of design points into the range $[-1, 1]$. Namely, we code $x_{(k+1)}$ to 1 and $x_{(1)}$ to -1, where $x_{(k+1)}$ and $x_{(1)}$ are the maximum and minimum values, respectively, among all x_i's and -1. To standardize the design points, we let $\boldsymbol{\alpha} = (x_{(k+1)} + x_{(1)})/2$ be the center and let $\boldsymbol{\beta} = x_{(k+1)} - x_{(1)}$ be the scale; then the coded variables are $y_i = 2(x_i - \alpha)/\boldsymbol{\beta}$, $i = 1, \ldots, k, k+1$, where $x_{k+1} = -1$. The standardized cyclic orthogonal design matrix, similar to equation (2), is now

$$S = \begin{bmatrix} 1_{kx1} & \Gamma_0 Y_1 & \Gamma_{k-1} Y_1 & \cdots & \Gamma_1 Y_1 \\ 1 & \mathcal{Y}_{k+1} & \mathcal{Y}_{k+1} & \cdots & \mathcal{Y}_{k+1} \end{bmatrix}, \tag{5}$$

where $Y_1 = [\mathcal{Y}_1, \mathcal{Y}_k, \mathcal{Y}_{k-1}, \ldots, \mathcal{Y}_2]'$. It can be further shown that $||S'S|| = 4^k(k+1)^{k+1}/\boldsymbol{\beta}^{2k}$ (see Lin and Chang (1999) for the proof).

It is clear now that maximizing $||S'S||$ is equivalent to minimizing $\boldsymbol{\beta} = x_{(k+1)} - x_{(1)}$, the tightness of the experimental range. Designs satisfying equations (4a, 4b) with minimal tightness are called T-optimal cyclic orthogonal designs. For a T-optimal design, we solve the following optimization problem: minimize y subject to $[\frac{k}{2}] + 1$ independent equations (4a) and (4b); $|x_i - x_j| \le y$, for all $i \ne j \in \{1, 2, \ldots, k+1\}$.

The T-optimal designs for $k < 10$ are tabulated in Table 1. The d-efficiencies and tightness values are also provided. Here, we have used the d-efficiency defined $\frac{||S'S||^{1/n}}{n}$ as in Lin (1993). For larger values of k, the T-optimal designs can be

obtained in a similar manner. The d-efficiencies for regular simplex designs, after re-scaling to the $(-1, 1)$ range, are $(0.4204, , 0.3482, 0.2970, 0.2588, 0.2293, 0.2057, 0.1866)$ for $k = 3, \ldots, 9$ respectively. It is clear that the T-optimal designs dominate the regular simplex designs in terms of d-efficiency. Note that when the T-optimal designs are used in practice, one first looks up Table 1 to generate the X matrix in (2) and then converts the X matrix into the S matrix in (5). It is the re-scaled S matrix that is used for design of experiments.

Table 1. T-optimal designs for $k < 10$.

k	$(x_1, \ldots, x_k)$	β	d-efficiency
1	(1.000)	2.0	1.0
2	$(1.367, -0.367)$	2.3666	0.7990
3	$(-1.000, 1.000, 1.000)$	2.0	1.0
4	$(0.809, -1.427, 0.809, 0.809)$	2.2361	0.8365
5	$(-0.787, 0.202, -1.000, 1.292, 1.292)$	2.2923	0.7966
6	$(-1.061, 0.608, -1.061, -0.084, 1.299, 1.299)$	2.3595	0.7532
7	$(1.000, -1.000, -1.000, 1.000, 1.000, 1.000, -1.000)$	2.0	1.0
8	$(-1.009, 0.398, -1.009, 0.438, -0.578, -0.431, 1.596, 1.596)$	2.605	0.6251
9	$(-1.120, -0.069, -1.120, -0.069, 1.242, -1.120, 0.774, 1.242, 1.242)$	2.3621	0.7412

Acknowledgement

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