

A New Class of Cyclic Orthogonal Designs

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Abstract. A class of orthogonal main effect designs with cyclic structure is investigated by Lin and Chang (2001). The cyclic structure ensures the balance and symmetry among design columns. This paper gives a new class of cyclic orthogonal designs for main effect plans. We use a numerical method to obtain these designs and this class of designs exists for any number of factors.

1. Introduction, Cyclic Designs

Consider the first order model in k variables

$$Y = X\beta + \varepsilon = \beta_0 + \beta_1x_1 + \cdots + \beta_kx_k + \varepsilon \quad (1)$$

where Y is the response variable and $x_i; i = 1, 2, \dots, k$ are independent set of variables. A cyclic design in k variables with first row as (x_1, x_2, \dots, 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 -1 's as the final row. Thus the design matrix X for a cyclic design in k -variables for model (1) can be written in general form as

$$X = \begin{bmatrix} 1_{k \times 1} & \Gamma_0 X_1 & \Gamma_{k-1} X_1 & \cdots & \Gamma_1 X_1 \\ 1 & -1 & -1 & \cdots & -1 \end{bmatrix} \quad (2)$$

where $X_1 = (x_1, x_2, \dots, x_k)'$ is the $k \times 1$ vector, $1_{k \times 1}$ is the $k \times 1$ vector with all elements as unity and Γ_h is a Circulant matrix whose first row has 1 in the $(h + 1)^{\text{th}}$ column and zero elsewhere (John and Williams (1995)). The design X is orthogonal if the off-diagonal elements of $X'X$ are zero i.e. if the inner product of any two distinct columns of X is zero, or in other words

$$(\Gamma_i X_1)'(\Gamma_j X_1) = -1, \quad i, j \in \{1, 2, \dots, k - 1\} \text{ and } i \neq j. \quad (3)$$

Adding the initial condition $1'X_1 = 1$, the conditions for a cyclic orthogonal design yields $\binom{k}{2} + 1$ equations to be solved.

Keywords. Cyclic designs, Orthogonal designs, Plackett Burman designs.

Received: 14 March 2013; Accepted: 16 December 2013

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2. Cyclic Orthogonal Design

Lin and Chang (2001) have shown that to find Cyclic Orthogonal Design with block size k , we have to solve the following $\left(\left\lceil \frac{k}{2} \right\rceil + 1\right)$ independent equations.

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

$$X_1' \Gamma_h X_1 = -1, \quad h = 1, 2, \dots, \left\lceil \frac{k}{2} \right\rceil \tag{5}$$

We now show that to solve the above set of non-linear simultaneous equations given in (4) and (5) numerically, we require k independent equations (Jain et al. (2004, page 7)). In order to obtain these k equations we introduce a new matrix U_h satisfying $\Gamma_h = U_h + U_{k-h}'$, where U_h is a $k \times k$ matrix with elements of h^{th} diagonal as unity and all other elements as 0. Here by h^{th} diagonal we mean the h^{th} diagonal parallel to the principal diagonal starting from North East corner of the $k \times k$ matrix. In particular, when $k = 4$ we have four U_h 's corresponding to $h = 1, 2, 3, 4$ and these are

$$U_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad U_2 = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$U_3 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad U_4 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

For $h = 1, 2, \dots, \left\lceil \frac{k}{2} \right\rceil$, substituting $\Gamma_h = U_h + U_{k-h}'$ in (5) we get

$$X_1'(U_h + U_{k-h}')X_1 = -1, \tag{6}$$

which is same as

$$X_1'(U_h + U_{k-h}')X_1 = -1, \quad \text{which is satisfied by setup}$$

$$X_1'U_h X_1 = -\frac{1}{2}, \quad h = 1, 2, \dots, k-1. \tag{7}$$

We get a set of $(k-1)$ equations satisfying (5). Thus, we have following theorem

Theorem 2.1. *Cyclic Orthogonal Design can be obtained by solving the set of k equations given by (4) and (7).*

Adding all the equations in (7) we get

$$X_1' \left(\sum_{h=1}^{k-1} U_h \right) X_1 = -\frac{k-1}{2}$$

or

$$\sum_{i=1}^{k-1} \sum_{\substack{j=1 \\ j>i}}^{k-1} x_i x_j = -\frac{k-1}{2} \tag{8}$$

Subtracting twice of (8) from the square of (4) ,we have

$$\sum_{i=1}^k x_i^2 = k. \tag{9}$$

Thus, we have following theorem

Theorem 2.2. *Cyclic design can be obtained by solving any set of k independent equations represented by (4), (7) and (9).*

3. Numerical Solution for Cyclic Orthogonal Design

In order to obtain Cyclic Orthogonal Design, we first find an initial solution $x^0 = (x_1^0, x_2^0, \dots, x_k^0)$ by solving equations (4) and (9). For this we have following theorem

Theorem 3.1. *Assume*

$$x_1 + x_2 + \dots + x_{k-2} = \lambda \tag{10}$$

$$x_1^2 + x_2^2 + \dots + x_{k-2}^2 = \mu \tag{11}$$

Then a solution to equations (4) and (9) exist if $2k - 2\mu - (1 - \lambda)^2 \geq 0$.

Proof. Using (10) and (11) in equation (4) and (9) we get

$$x_{k-1} + x_k = 1 - \lambda \tag{12}$$

$$x_{k-1}^2 + x_k^2 = k - \mu \tag{13}$$

Eliminating x_{k-1} from (12) and (13) we get

$$2x_k^2 - 2(1 - \lambda)x_k + \mu - k + (1 - \lambda)^2 = 0 \tag{14}$$

Now (14) will have real roots if $2k - 2\mu - (1 - \lambda)^2 \geq 0$.

One can notice that infinite many points $x = (x_1, x_2, \dots, x_k)$ lying on a circle with centre $\left(\frac{1}{k}, \frac{1}{k}, \dots, \frac{1}{k}\right)$ and radius $\frac{\sqrt{k^2 - 1}}{k}$ in a k -dimensional space will satisfy $2k - 2\mu - (1 - \lambda)^2 \geq 0$. Among these points any point which satisfy any $(k - 2)$ equations given in (7) will form the first row of cyclic orthogonal design.

After obtaining the initial solution say $x^0 = (x_1^0, x_2^0, \dots, x_k^0)$ satisfying (4) and (9) we use Newton-Raphson method described in Jain et al. (2004, page 7) to obtain a point which satisfy any set of $(k - 2)$ equations given in (7) and this will form the first row of cyclic orthogonal design.

The numerical method is described as follows:

Method:

Let $F = (F_1, F_2, \dots, F_k)'$ denotes the column vector of functions F_i ; $i = 1, 2, \dots, k$ of (x_1, x_2, \dots, x_k) where F_i 's are defined as

$$F_i(x_1, x_2, \dots, x_k) = \begin{cases} X_1' U_i X_1 + \frac{1}{2}, & i = 1, 2, \dots, k - 1, \\ \sum_{i=1}^k x_i - 1, & i = k. \end{cases} \tag{15}$$

Starting with the initial solution $x^0 = (x_1^0, x_2^0, \dots, x_k^0)$, we obtain the sequences of iterates using Newton-Raphson method described in Jain et al. (2004, page 7) as

$$X^{(s+1)} = X^s - J^{-1}F^s \tag{16}$$

where $x^{(s)} = (x_1^{(s)}, x_2^{(s)}, \dots, x_k^{(s)})$, $F^{(s)} = (F_1^{(s)}, F_2^{(s)}, \dots, F_k^{(s)})$, $F_i^{(s)} = F_i(x_1^{(s)}, x_2^{(s)}, \dots, x_k^{(s)})$ and J is the Jacobian matrix of functions F_1, F_2, \dots, F_k at $x^{(s)}$.

Writing the Jacobian matrix J as a sum of two matrices A and B we can further simplify our calculations, where the matrices A and B are

$$A = (a_{ij}) \quad \text{where } a_{ij} = \begin{cases} x_{k-i+j}, & j \leq i \leq k-1, \\ \frac{1}{2}, & i = k, \\ 0, & \text{otherwise.} \end{cases}$$

and

$$B = (b_{ij}) \quad \text{where } b_{ij} = \begin{cases} x_{i+j-k}, & i + j \geq k, i \leq k-1, \\ \frac{1}{2}, & i = k, \\ 0, & \text{otherwise.} \end{cases}$$

We continue iterating till $(k - 2)$ equations in (7) are satisfied. To illustrate the method, we consider the case when $k = 5$.

Assuming $x_1 = 0.11, x_2 = 0.12, x_3 = 0.13$, we get $\lambda = 0.36$ and $\mu = 0.0434$ which satisfy $2k - 2\mu - (1 - \lambda)^2 = 3.0828 > 0$. Using (12) and (14) we get, $x_4 = 0.186139$ and $x_5 = -1.22139$. Thus, we have an initial solution $(0.11, 0.12, 0.13, 0.1861, -1.2214)$. The iterated values of this initial solution in the first five iterations are given below:

$X^{(1)}$	$X^{(2)}$	$X^{(3)}$	$X^{(4)}$	$X^{(5)}$
0.306726	0.284755	0.295934	0.297604	0.297611
0.685226	0.509807	0.494843	0.496308	0.496318
1.39177	0.895605	0.771291	0.764418	0.764398
0.977372	1.109082	1.123192	1.121726	1.121716
-2.36109	-1.79925	-1.68526	-1.68006	-1.68004

We obtain the vector $X_1 = (0.297611 \quad -1.680043 \quad 1.121716 \quad 0.764398 \quad 0.496318)'$ satisfying (7).

We obtain designs for different values of k ranging between $k = 1$ to $k = 11$. For this we take $x_1 = 0.11$ and $x_j = x_{j-1} + 0.01, j = 2, 3, \dots, k - 2$ and used the method described above. We obtain the points given in Table 1 as the first rows of COD's for $k = 1$ to 11.

We observe that the designs for $k = 1$ and 2 are unique but for the other values of k , we get a number of points which can be taken as the first row of Cyclic orthogonal designs, and these points depend on the initial point which in turn depend on the choice of the values of x_1, x_2, \dots, x_{k-2} .

Table 1: The first rows of cyclic orthogonal designs for different values of k

k	x_1, x_2, \dots, x_k
1	1
2	1.367, -0.367
3	0.11, -0.6933, 1.5833
4	0.3734, -1.3387, 1.2445, 0.7207
5	0.2976, -1.6800, 1.1217, 0.7643, 0.4963
6	0.2541, -1.9675, 1.0172, 0.7592, 0.5514, 0.3855
7	0.2253, -2.2186, 0.9310, 0.7360, 0.5718, 0.4343, 0.3199
8	0.2046, -2.4434, 0.8597, 0.7070, 0.5744, 0.4598, 0.36116, 0.2766
9	0.1887, -2.6485, 0.8001, 0.6770, 0.5679, 0.4713, 0.3861, 0.3113, 0.2458
10	0.1761, -2.838, 0.7496, 0.6482, 0.5567, 0.4744, 0.4005, 0.3343, 0.2752, 0.2227
11	0.1658, -3.0149, 0.7063, 0.6212, 0.5434, 0.4724, 0.4078, 0.3491, 0.2960, 0.2479, 0.2046

4. Conclusion

This paper deals with a new class of cyclic orthogonal designs for main effect plans. We use a numerical method to obtain these designs and this class of designs exists for any number of factors.

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