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Research Paper

#### Optimality of some circular balanced block designs under interference model with compound symmetry correlation

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Abstract: For the interference models, the assumption is often made that the size of the blocks (k) is not greater than the number of treatments (t). Typically, it is difficult to specify optimal block designs theoretically or algorithmically when k > t. In this article, we focus on a one-sided interference model with compound symmetry correlation for the observations and obtain universally optimal block designs for both cases  $k \leq t$  and k > t. We present some methods for constructing these optimal designs for various numbers of treatments and block sizes.

**Keywords:** Circular block design; Compound symmetry structure; Interference model; neighbor balanced design; Universal optimality. **Mathematics Subject Classification (2010):** 62K05, 62K10.

# 1 Introduction

In serological, agricultural, horticultural, and medical experiments, sometimes, interference models can occur. These models arise when the response to a treatment is affected by the other treatments in the neighbor plots. For example, in varietal trials, the yields of shorter varieties may be depressed due to shading from taller neighbor varieties (Kempton and Lockwood, 1984).

neighbor balanced designs ensure to minimize the influence of neighbor effects on treatment comparisons. Rees (1967) introduced this concept in a serological experiment, where treatments were organized in circular blocks such that each treatment have two neighboring treatments.

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A block design is called circular if each treatment in its blocks has two neighbors or in other words, the treatments within each block are circularly ordered. A set of k elements  $\{a_1, a_2, \ldots, a_k\}$  arranged in the circular order  $a_1 \rightarrow a_2 \rightarrow \cdots \rightarrow a_k \rightarrow a_1$  is said to be circularly ordered. The element  $a_{i+1}$  is said to be the right-neighbor of  $a_i$ , and  $a_i$  is said to be the left-neighbor of  $a_{i+1}$ , when i+1 is calculated in (modulo k)+1.

Let  $\mathcal{D}_{t,b,k}$  denote the class of circular block designs where t, b and k are the numbers of treatments, blocks and plots per block, respectively. For example, let

$$1$$
  $2$   $3$   $4$   $5$ 

be a block of an arbitrary circular design with t = k = 5. According to the circular structure of this block, treatment 5 is the left-neighbor of treatment 1.

A basic problem in the theory of experimental designs is to characterize optimal designs. There are various criteria for assessment of optimality of experimental designs. Kiefer (1975) introduced the definition of universally optimal designs such that they are optimal under all optimality criteria (e.g., A, D, E).

Some researchers have studied different aspects of optimality of designs in the field of interference models. For example, there are several results on optimality of circular neighbor balanced designs (CNBDs) and circular neighbor balanced designs at distances 1 and 2 (CNBD2s) defined by Druilhet (1999), under the fixed and mixed interference models, where the observations are correlated or not (Druilhet, 1999; Filipiak and Markiewicz, 2003, 2005, 2007; Bailey et al., 2017). Azaïs et al. (1993) presented construction methods and the catalog of CNBDs and CNBD2s with the size of blocks equal to t or t - 1.

The circular neighbor-balanced at distances up to  $\gamma$ ,  $\text{CNBD}(\gamma)$ , was introduced by Ai et al. (2007). Filipiak and Markiewicz (2012) defined circular weakly neighbor balanced designs (CWNBDs) and showed their universal optimality under the interference model with one-sided neighbor effects. Universal optimality of some CNBDs of the second and higher order, under the interference models with two-sided neighbor effects at distances one or more, has been proven by Ahmed et al. (2014).

Although the size of blocks may be so large, in the literature on interference models, the assumption is usually made that  $k \leq t$ .

If k > t, the universally optimal circular block designs are usually difficult to obtain. Khodsiani and Pooladsaz (2022) introduced circular equineighbored designs (CEDs) and obtained results regarding their universal optimality under the block-treatment model and circulant correlation matrix for every k and t. Fakhari and Pooladsaz (2022) considered an interference model with equal left- and right-neighbor effects for uncorrelated errors when  $k = t + 1, t + 2, \ldots, 2t - 1$ .

In this article, we consider universal optimality criterion for the general case,

$$k = ht + s,\tag{1}$$

where h and s are two non-negative integers, k > 2 and s < t.

This article is organized as follows. In Section 2, we introduce the notations and definitions that will be used throughout the paper. In Section 3, we present the universal optimality of some circular balanced block designs under the interference model with one-sided neighbor effects and correlated observations. Furthermore, we discuss some methods for constructing these optimal designs in both cases  $k \leq t$ , and k > t

with s = 0, 1 and different values of h as described in equation (1). Finally, we provide examples to illustrate the application of these methods.

#### 2 Notations and definitions

The notation d(j, i) represents the treatment assigned to plot *i* of block *j* for the design *d* in  $\mathcal{D}_{t,b,k}$ . The left-neighbor interference model can be expressed as

$$y_{ji} = \tau_{d(j,i)} + \eta_{d(j,i-1)} + \beta_j + \varepsilon_{ji}; \quad j = 1, \dots, b \text{ and } i = 1, \dots, k,$$
 (2)

where  $y_{ji}$  represents the response on plot *i* of block *j*,  $\tau_{d(j,i)}$  denotes the effect of treatment d(j,i),  $\eta_{d(j,i-1)}$  represents the left-neighbor effect of d(j,i-1),  $\beta_j$  represents the effect of block *j*, and  $\varepsilon_{ji}$  is a random error with zero mean.

Let  $\mathbf{y}' = (y_{11}, \ldots, y_{1k}, y_{21}, \ldots, y_{2k}, y_{b1}, \ldots, y_{bk})$  is the vector of observations of order n = bk. In matrix notation, the model (2) can be written as,

$$\boldsymbol{y} = \boldsymbol{X}_d \boldsymbol{\tau} + \boldsymbol{L}_d \boldsymbol{\eta} + \boldsymbol{B} \boldsymbol{\beta} + \boldsymbol{\varepsilon},\tag{3}$$

where  $\tau$ ,  $\eta$  and  $\beta$  are the vectors of treatment, left-neighbor and block effects, respectively, and  $\varepsilon$  is a vector of random errors with  $\mathbf{E}(\varepsilon) = \mathbf{0}_n$  and  $\operatorname{Cov}(\varepsilon) = \mathbf{V}$ . Also,  $\mathbf{X}_d$ ,  $\mathbf{L}_d$  and  $\mathbf{B} = \mathbf{I}_b \otimes \mathbf{1}_k$  are design matrices for treatments, left-neighbors and blocks, respectively.  $\mathbf{I}_b$  is the identity matrix of order b,  $\mathbf{0}_n$  is the *n*-vector of zeros,  $\mathbf{1}_k$  is the *k*-vector of ones, and  $\otimes$  is the Kronecker product.

There are different structures for covariance matrix V. Under interference models, it is usually assumed that the observations in different blocks are uncorrelated but that observations within blocks are correlated with the same correlation structure. In other words,  $V = \sigma^2(I_b \otimes \Lambda)$  where  $\sigma^2$  is an unknown positive constant, and  $\Lambda$  is a known symmetric positive definite correlation matrix.

The compound symmetry correlation structure is a commonly used correlation structure in the design of experiments. Several papers have discussed the implementation and application of the compound symmetry correlation structure in various fields. For example, Smith et al. (2017) examined the impact of using the compound symmetry correlation structure in longitudinal data analysis and showed its usefulness in modeling correlated data with equal correlation. Filipiak et al. (2023) studied a statistical testing methodology for assessing independence among variables in the presence of compound symmetry covariance structure. Kim et al. (2021) discussed the importance of efficient designs in studying lifetime distributions and proposed a robust approach that incorporates compound symmetry correlation.

Under compound symmetry correlation structure, there is the same correlation between each pair of plots in a block, i.e.

$$\boldsymbol{\Lambda} = \boldsymbol{I}_k + \rho(\boldsymbol{J}_k - \boldsymbol{I}_k), \tag{4}$$

where  $|\rho| < 1$  is the correlation coefficient and  $J_k = \mathbf{1}_k \mathbf{1}'_k$ . This correlation structure simplifies the analysis by reducing the number of parameters that need to be estimated compared to other correlation structures.

Under the interference model (3), Li et al. (2015) showed that the information matrix for estimating treatment effects is,

$$C_d = C_{d,11} - C_{d,12} C_{d,22}^- C_{d,21}, \tag{5}$$

with matrices  $C_{d,11} = T'_d V^* T_d$ ,  $C_{d,12} = T'_d V^* L_d$  and  $C_{d,22} = L'_d V^* L_d$  where  $C^-_{d,22}$ is a generalized inverse of  $C_{d,22}$ ,  $V^* = I_b \otimes \Lambda^*$  and

$$\mathbf{\Lambda}^* = \mathbf{\Lambda}^{-1} - (\mathbf{1}'_k \mathbf{\Lambda}^{-1} \mathbf{1}_k)^{-1} \mathbf{\Lambda}^{-1} \mathbf{1}_k \mathbf{1}'_k \mathbf{\Lambda}^{-1}.$$
 (6)

Let  $C = \{C_d : d \in D_{t,b,k}\}$  and  $\lambda(C_d) = (\lambda_1(C_d), \lambda_2(C_d), \dots, \lambda_t(C_d))$  where  $\lambda_i(C_d)$  is *i*-th largest eigenvalue of  $C_d$ . Given the function  $\Phi : C \longrightarrow \mathbf{R}$ , a design  $d^*$  in  $\mathcal{D}_{t,b,k}$  is  $\Phi$ -optimal with respect to C if  $\Phi(C_{d^*}) \leq \Phi(C_d)$  for all  $d \in D_{t,b,k}$ .

**Definition 2.1.** (Kiefer, 1975) A design  $d^*$  will be universally optimal in  $\mathcal{D}_{t,b,k}$  if  $d^*$  is  $\Phi$ -optimal w.r.t any real-valued function  $\Phi$  satisfying the following conditions: i. For two designs  $d_1$  and  $d_2$  in  $\mathcal{D}_{t,b,k}$ , if  $\lambda(C_{d_1}) \leq \lambda(C_{d_2})$  in the Schur ordering then  $\Phi(C_{d_1}) \leq \Phi(C_{d_2})$ .

ii.  $\Phi(C_d)$  is a function of the eigenvalues of  $C_d$ .

*iii.* If  $\lambda_i(\mathbf{C}_{d_1}) \geq \lambda_i(\mathbf{C}_{d_2})$  for all  $i = 1, 2, \ldots, t$  then  $\Phi(\mathbf{C}_{d_1}) \leq \Phi(\mathbf{C}_{d_2})$ .

Throughout this paper we use some properties of a balanced block design (BBD), i.e. such a design  $d \in \mathcal{D}_{t,b,k}$  for which

(i) all  $n_{d,ij} = \lfloor \frac{k}{t} \rfloor$  or  $\lfloor \frac{k}{t} \rfloor + 1$  where  $n_{d,ij}$  is the (i, j)-th entry of  $N_d = X'_d B$  and  $\lfloor x \rfloor$  is the largest integer not exceeding x,

(ii) all the replications of teatments are equal (say r) and

(iii) every pair of distinct treatments occurs together in the same number of blocks (say  $\lambda$ ).

All designs satisfying (i) are called generalized binary designs (GBDs). Note that a GBD reduces to a binary design when  $k \leq t$  and so, a BBD reduces to a balanced incomplete block design (BIBD) when  $k \leq t$ .

**Definition 2.2.** (Druilhet (1999)) A circular BIBD such that for each ordered pair of distinct treatments there exist exactly l inner plots which receive the first chosen treatment and which have the second one as right neighbor, is called circular neighbor balanced design (CNBD).

### 3 Main results

For correlation matrix (4), we have

$$\boldsymbol{\Lambda}^{-1} = \frac{1}{v_2} (v_1 \boldsymbol{I}_k + \rho \boldsymbol{J}_k),$$

where  $v_1 = (1-k)\rho - 1$  and  $v_2 = (k-1)\rho^2 - (k-2)\rho - 1$ . Note that, if  $\rho = \frac{1}{1-k}$  then  $v_1 = v_2 = 0$ . So, for correlation matrix (4),  $\rho$  can not be equal to  $\frac{1}{1-k}$ . From (6), it follows that,

$$\boldsymbol{\Lambda}^* = a(\boldsymbol{I}_k - \frac{1}{k}\boldsymbol{J}_k),$$

where  $a = \frac{v_1}{v_2}$ . Under the interference model (3) and correlation matrix (4), the information matrix for estimating treatment effects has the form (5) with matrices,

$$\boldsymbol{C}_{d,11} = \boldsymbol{C}_{d,22} = a(\boldsymbol{R}_d - \frac{1}{k}\boldsymbol{N}_d\boldsymbol{N}_d'), \tag{7}$$

$$C_{d,12} = C'_{d,21} = a(S_d - \frac{1}{k}N_dN'_d),$$
 (8)

where  $\mathbf{R}_d = \mathbf{X}_d \mathbf{X}'_d = \text{diag}(r_{d,1}, r_{d,2}, \dots, r_{d,t})$  such that  $r_{d,i}$  is the replication of treatment *i* in design *d*,  $\mathbf{S}_d = \mathbf{X}'_d(\mathbf{I}_b \otimes \mathbf{H}_k)\mathbf{X}_d$  is a  $t \times t$  left-neighboring matrix of a circular design *d* and  $\mathbf{H}_k$  denotes the  $k \times k$  left-neighbor incidence matrix, that is the matrix with the following elements

$$(\boldsymbol{H}_k)_{ij} = \begin{cases} 1, & \text{if } (i-j=1) \text{ or } (i=1 \text{ and } j=k), \\ 0, & \text{o.w.} \end{cases}$$

In fact, the *ij*-th element of  $S_d$ , denoted as  $s_{d,ij}$ , indicates the number of times that treatment *i* is the left neighbor of treatment *j* at distance 1. So, by Definition 2.2, design *d* is a CNBD if it is a circular BIBD such that  $S_d = l(J_t - I_t)$  where *l* is a positive integer.

We denote  $\mathcal{D}_{t,b,k}$  as a subclass of  $\mathcal{D}_{t,b,k}$  with no treatment preceded by itself, i.e. for every  $d \in \overline{\mathcal{D}}_{t,b,k}$ , there is no self-neighboring for the treatments.

Kiefer (1975) proved that design  $d^* \in \mathcal{D}_{t,b,k}$  is universally optimal if (i)  $C_{d^*}$  is completely symmetric, i.e. all diagonal elements of  $C_{d^*}$  are equal and all its off-diagonal elements are equal, and (ii)  $C_{d^*}$  has maximal trace over  $\mathcal{D}_{t,b,k}$ .

Kushner (1997) defined the quadratic function  $q_d : \mathbb{R} \longrightarrow \mathbb{R}$  as follows,

$$q_d(x) = c_{d,11} + 2c_{d,12}x + c_{d,22}x^2, \qquad x \in \mathbb{R},$$

where  $c_{d,ij} = \text{tr}(C_{d,ij})$ , i, j = 1; 2. The function  $q_d(x)$  has the minimum value at  $x_d = -\frac{c_{d,12}}{c_{d,22}}$  such that,

$$q_d(x) \ge q_d^*(x_d) = c_{d,11} - \frac{(c_{d,12})^2}{c_{d,22}}$$

We state the analogue of Theorem 4.4 of Kushner (1997) in the next proposition,

**Proposition 3.1.** Let  $d^* \in \mathcal{D}_{t,b,k}$  have completely symmetric  $C_{d,ij}$ , i, j = 1; 2. If  $q_d^* \leq q_{d^*}^*$  for every  $d \in \mathcal{D}_{t,b,k}$ , then  $d^*$  is universally optimal.

**Remark 3.2.** A design d is called degenerate, if  $q_d(x) = 0$  for all x. It is clear that such design cannot be optimal, therefore it is not considered here.

**Theorem 3.3.** If  $d^*$  is a circular BBD such that  $S_{d^*}$  is completely symmetric, then  $d^*$  is universally optimal over  $\overline{\mathcal{D}}_{t,b,k}$  under model (3) and compound symmetry correlation matrix (4).

*Proof.* According to Equations (7) and (8), since  $d^*$  is BBD, the matrices  $\mathbf{R}_d$ ,  $\mathbf{N}_d \mathbf{N}'_d$  and therefore  $\mathbf{C}_{d^*,ij}$ , i, j = 1, 2, are completely symmetric.

Also, under model (3) and correlation matrix (4), we have

$$q_d^* = a \left( bk - \operatorname{tr}(\frac{1}{k} N_d N_d') - \frac{(\operatorname{tr}(S_d) - \operatorname{tr}(\frac{1}{k} N_d N_d'))^2}{bk - \operatorname{tr}(\frac{1}{k} N_d N_d')} \right).$$

So, for every  $d \in \overline{\mathcal{D}}_{t,b,k}$ ,

$$q_d^* = abk \left( 1 - \left( \frac{bk}{\operatorname{tr}(\frac{1}{k} \boldsymbol{N}_d \boldsymbol{N}_d')} - 1 \right)^{-1} \right).$$
(9)

Since  $q_d^*$  in Equation (9) is a decreasing function of  $\operatorname{tr}(\frac{1}{k}N_dN'_d)$ ,  $q_d^*$  is maximized when  $\operatorname{tr}(\frac{1}{k}N_dN'_d)$  is minimum. It is known (cf. Shah and Sinha (1989)) that  $\operatorname{tr}(N_dN'_d)$  is minimal for BBD and thus, by Proposition 3.1 the proof is complete.

For obtaining design  $d^*$  of Theorem 3.3, we must construct a circular BBD with completely symmetric left-neighboring matrix without self-neighborring. There are two cases as follows:

**Case 1.** If  $k \leq t$  then there is no self-neighboring in any blocks of a BIBD and therefore  $d^*$  of Theorem 3.3 is a CNBD which can be constructed by the methods of Azaïs et al. (1993).

**Case 2.** If k > t, we present the mothods for construction of optimal design  $d^*$  by the values of s in Equation (1). Our methods are used for two cases s = 0 and s = 1.

When s is zero. Let t and k are in Equation (1) with s = 0. In this case, for constructing design  $d^*$  in Theorem 3.3, we need b = t - 1 blocks. At first, we obtain a primary design, say  $d_p$ , which is a CNBD(t, t - 1, t). Now, we repeat the treatment in *i*-th plot of block j of  $d_p$  to the plots  $i, i + t, i + 2t, \ldots, i + (h - 1)t$  of block j of  $d^*$ ,  $i = 1, 2, \ldots, t$  and  $j = 1, 2, \ldots, t - 1$ .

For example, let t = 5 and k = 15. So, h = 3, s = 0 and the primary design  $d_p$  is constructed as below,

where each row is a block. Therefore, under model (3) and correlation matrix (4) the following design is universally optimal over  $\overline{\mathcal{D}}_{5,4,15}$ 

When s is one. Let t and k are in Equation (1) with s = 1. In this case, for constructing design  $d^*$  in Theorem 3.3, we need b = t(t-1) blocks. At first, we obtain a primary design, say  $d_p$ , which is a CNBD(t, t - 1, t). Now, we repeat the treatment in *i*-th plot of block j of  $d_p$  to the plots  $i, i + t, i + 2t, \ldots, i + (h-1)t, i = 1, 2, \ldots, t$ , and put an extra replication of the 2-th plot of block j of  $d_p$  to the plot ht + 1 of block j of  $d^*, j = 1, 2, \ldots, t - 1$ .

For example, let t = 5 and k = 11. So, h = 2, s = 1 and the primary design  $d_p$  can be considered as  $d_p$  in (10). Thus, under model (3) and correlation matrix (4) the

following design is universally optimal over  $\bar{\mathcal{D}}_{5,20,13}$ 

	$\frac{1}{2} \frac{2}{3} \frac{3}{4} \frac{5}{5} \frac{1}{2} \frac{2}{3} \frac{3}{4} \frac{5}{5} \frac{1}{2} \frac{2}{3} \frac{3}{4} \frac{5}{5} \frac{1}{2} \frac{2}{3} \frac{3}{4} \frac{5}{5} \frac{1}{5} \frac{1}$	23451345124512351234	34512512342345145123	45123234515123434512	51234451233451223451	$\frac{1}{2} \frac{2}{3} \frac{4}{4} \frac{5}{5} \frac{1}{2} \frac{2}{3} \frac{4}{5} \frac{5}{1} \frac{2}{2} \frac{3}{3} \frac{4}{5} \frac{5}{1} \frac{2}{2} \frac{3}{3} \frac{4}{5} \frac{5}{5} \frac{1}{2} \frac{2}{3} \frac{4}{5} \frac{5}{5} \frac{1}{2} \frac{2}{3} \frac{4}{5} \frac{5}{5} \frac{1}{5} \frac{2}{5} \frac{1}{5} \frac{1}$	23451345124512351234	$ \frac{34512512342345145123}{2342345145123} $	45123234515123434512	51234451233451223451	23451345124512351234
$d^*$ :	4	5 1	1	2	3	4	5 1	1	2	3	5 1
	Э	T	2	3	4	Э	T	2	3	4	T
	1	- 3	5	2	4	1	- 3	5	2	4	- 3
	2	4	1	3	5	2	4	1	3	5	4
	3	5	2	4	1	3	5	2	4	1	5
	4	1	3	5	2	4	1	3	5	2	1
	5	2	4	1	3	<b>5</b>	2	4	1	3	2
	1	4	2	<b>5</b>	3	1	4	2	<b>5</b>	3	4
	2	5	3	1	4	2	5	3	1	4	5
	3	1	4	2	5	3	1	4	2	5	1
	4	2	5	3	1	4	2	5	3	1	2
	5	3	1	4	2	5	3	1	4	2	3
	1	5	4	3	2	1	5	4	3	2	5
	2	1	5	4	3	2	1	5	4	3	1
	3	2	1	5	4	3	2	1	5	4	2
	4	3	2	1	5	4	3	2	1	5	3
	5	4	3	2	1	5	4	3	2	1	4

Note that in our methods of constructing  $d^*$  in Theorem 3.3 with t treatments and block size k, we require

$$b = \begin{cases} t - 1, & \text{if } s = 0, \\ t(t - 1), & \text{if } s = 1, \end{cases}$$

blocks which does not depend on h. As a result, the value of b does not need to be excessively large, even for large k. For example, if k = 41 and t = 5 then we have h = 8 and s = 1. So, the universally optimal design can be constructed by b = 20 blocks.

#### Discussion and conclusions

In this article, we consider the left-neighbor interference model, which assumes a correlation structure of compound symmetry for the observations. Using Kushner's method, we obtain the design that maximizes the trace of the information matrix on  $\bar{\mathcal{D}}_{t,b,k}$  for each k and t as defined in Equation (1). By adding the condition that the information matrix of this design is completely symmetric, the universally optimal design is obtained. Also, the methods of constructing these designs are mentioned with examples. It is noticed that in our methods the required numbers of blocks are not excessively large, even for large k.

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