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On optimality of change-over designs balanced for first and second order residual effects

1. INTRODUCTION

Designs in which treatments are applied to experimental units in sequences over a number of periods are known as repeated measurements designs or change-over designs (CODs). These designs have been used in several fields of experimentation like dairy cow feeding trials (Patterson and Lucas, 1962), clinical trials (Cook, 1995), psychological experiments. Sometimes, due to short duration of the experimental periods or owing to nature of the response of treatments, the performance in a given period is affected not only by the treatment applied in that period but also by the residual effects of preceding treatments. If the residual effect continues for one period after the application of treatment, it is called the first order residual effect and if it persists up to second subsequent period, it is known as the second order residual effect. One of the methods of eliminating the residual effects is to insert a rest period or washout period between two treatment periods, sufficiently long enough for any effect of the earlier treatments to be dissipated. However, this practice is not always feasible or desirable. Another alternative is to include higher order residual effect parameters in the model and to use designs which allow the estimation of these effects along with adjustment for them. In

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this paper we consider the latter course and assume the presence of first and second order residual effects of treatments.

The CODs with second and higher order residual effects of treatments have been studied by Sharma (1977), John and Quenouille (1977), Bose and Mukherjee (2000) etc. Hedayat and Afsarinejad (1978), Kunert (1984), Hedayat and Zhao (1990), Mathews (1994) and others studied optimality of change-over designs permitting the estimation of first order residual effects. Here, universal optimality of a class of CODs balanced for first and second order residual effects has been established. Details of universal optimality can be found in Kiefer (1975), however, the sufficient conditions for establishing universal optimality are given below:

A design $d^* \in D$ (the class of competing designs) is universally optimal (Kiefer 1975), if its information matrix, C_{d^*} is such that

(i) C_{d^*} is completely symmetric, i.e., C_{d^*} is of the form a $I_v + b\, J_v$ where I_v is the identity matrix of order v and J_v is a square matrix of order v with all elements unity and a and b are scalars; and

(ii) trace $(C_{d^*}) >$ trace (C_d) for all d with $C_d \in \mathbf{B}_{v,0}$, the class of all symmetric, non-negative definite matrices of order v with row sums equal to zero.

A universally optimal design is necessarily A-, D-, and E-optimal.

2. Experimental setup and the model

We consider a change-over design d with v treatments using n experimental units for p periods which allows the estimation of direct, first and second order residual effects of the treatments under the additive fixed effects model

$$Y = \mu 1 + P\pi + \Delta\tau + D_1\chi_1 + D_2\chi_2 + S\psi + \varepsilon \tag{1}$$

where

$Y = np \times 1$ vector of observations,

$1 = np \times 1$ vector of unities,

$P = np \times p$ matrix of observations vs. period effects,

$\Delta = np \times v$ matrix of observations vs. direct effects of treatments,

$D_1 = np \times v$ matrix of observations vs. first residual effects of treatments,

$D_2 = np \times v$ matrix of observations vs. second residual effects of treatments,

$S = np \times n$ matrix of observations vs. experimental unit effects,

$\mu =$ general mean,

$\pi = (\pi_1, \pi_2, \ldots, \pi_p)'$, vector of p period effects,

$\tau = (\tau_1, \tau_2, \ldots, \tau_v)'$, vector of v direct effects of treatments,

$\chi_1 = (\chi_{11}, \chi_{12}, \ldots, \chi_{1v})'$, vector of v first order residual effects,

$\chi_2 = (\chi_{21}, \chi_{22}, \ldots, \chi_{2v})'$, vector of v second order residual effects,

$\psi = (\psi_1, \psi_2, \ldots, \psi_n)'$, vector of n experimental unit effects, and

ε is a random error term assumed to be $N(0, \sigma^2 I_{np})$; 0 and I_{np} being the null vector and identity matrix both of order np, respectively. Evidently, $np > 3v + p + n + 1$ for the estimation of the parameters in model (1).

Besides, we use the following notations for incidence matrices:

Notations

M_1: direct effects vs. first residual effects,

M_2: direct effects vs. second residual effects,

M_3: first residual effects vs. second residual effects,

L_1: direct effects vs. period effects,

L_2: direct effects vs. experimental unit effects,

E_1: first residual effects vs. period effects,

E_2: second residual effects vs. period effects,

N_1: first residual effects vs. experimental unit effects,

N_2: second residual effects vs. experimental unit effects.

And also, let

$R = \mathrm{diag}(r_1, r_2, \ldots, r_v)$, diagonal matrix with r_i $(i = 1, 2, \ldots, v)$ being the number of times the ith treatment appears in d,

$R_1 = \mathrm{diag}(\rho_{11}, \rho_{12}, \ldots, \rho_{1v})$, diagonal matrix with ρ_{1i} $(i = 1, 2, \ldots, v)$ being the number of times the treatments in d are immediately preceded by i^{th} treatment,

$R_2 = \text{diag}(\rho_{21}, \rho_{22}, \ldots, \rho_{2v})$, diagonal matrix; ρ_{2i} $(i = 1, 2, \ldots, v)$ is the number of times the treatments in d are preceded by two positions by the ith treatment,

$r = (r_1, r_2, \ldots, r_v)'$, column vector of r_i's,

$\rho_1 = (\rho_{11}, \rho_{12}, \ldots, \rho_{1v})'$, column vector of ρ_{1i}'s,

$\rho_2 = (\rho_{21}, \rho_{22}, \ldots, \rho_{2v})'$, column vector of ρ_{2i}'s.

In the partitioned form the model (1) can be written as

$$Y = X_1\theta_1 + X_2\theta_2 + \varepsilon \tag{2}$$

where $\theta_1[= (\tau \quad \chi_1 \quad \chi_2)']$ is the vector of parameters of interest, and $\theta_2[= (\pi \quad \psi \quad \mu)']$ is the vector of nuisance parameters that is, the parameters of least interest and $[X_1 : X_2] = [\Delta \quad D_1 \quad D_2 : P \quad S \quad 1]$.

It can be easily seen that

$$X_1'X_1 = \begin{vmatrix} R & M_1 & M_2 \\ M_1' & R_1 & M_3 \\ M_2' & M_3' & R_2 \end{vmatrix}, \qquad X_1'X_2 = \begin{vmatrix} L_1 & L_2 & r \\ E_1 & N_1 & \rho_1 \\ E_2 & N_2 & \rho_2 \end{vmatrix},$$

$$X_2'X_2 = \begin{vmatrix} nI_p & J_{p,n} & nJ_{p,1} \\ J_{n,p} & pI_n & pJ_{n,1} \\ nJ_{1,p} & pJ_{1,n} & np \end{vmatrix} \tag{3}$$

$$\text{and} \quad (X_2'X_2)^- = \begin{vmatrix} (I_p + J_{p,p}/p)/n & -J_{p.n}/np & 0 \\ -J_{n,p}/np & I_n/p & 0 \\ 0' & 0' & 0 \end{vmatrix};$$

where $(X_2'X_2)^-$ is a g-inverse of $X_2'X_2$ and $J_{p,n}$ is $p \times n$ matrix with all its elements unity.

Minimization of the residual sum of squares with respect to θ_1 and θ_2 under model (2), yields the following normal equations:

$$X_1'X_1\theta_1 + X_1'X_2\theta_2 = X_1'Y \tag{4}$$

$$X_2'X_1\theta_1 + X_2'X_2\theta_2 = X_2'Y\,. \tag{5}$$

Solution of equations (4) and (5) gives the joint information matrix for direct, first and second order residual effects as

$$C(\theta_1) = X_1'X_1 - X_1'X_2(X_2'X_2)^-X_2'X_1\,.$$

which under (3) simplifies to

$$C(\theta_1) = \begin{vmatrix} A & B & C \\ B' & D & E \\ C' & E' & F \end{vmatrix} \tag{6}$$

with

$$\begin{aligned} A &= R - n^{-1}L_1L_1' - p^{-1}L_2L_2' + (np)^{-1}rr' \\ B &= M_1 - n^{-1}L_1E_1' - p^{-1}L_2N_1' + (np)^{-1}r\rho_1' \\ C &= M_2 - n^{-1}L_1E_2' - p^{-1}L_2N_2' + (np)^{-1}r\rho_2' \\ D &= R_1 - n^{-1}E_1E_1' - p^{-1}N_1N_1' + (np)^{-1}\rho_1\rho_1' \\ E &= M_3 - n^{-1}E_1E_2' - p^{-1}N_1N_2' + (np)^{-1}\rho_1\rho_2' \\ F &= R_2 - n^{-1}E_2E_2' - p^{-1}N_2N_2' + (np)^{-1}\rho_2\rho_2' \end{aligned} \tag{7}$$

The information matrices for direct effects, first order residual effects and second order residual effects from (6) are given by

$$C_d(\tau) = A - [B \quad C] \begin{vmatrix} D & E \\ E' & F \end{vmatrix}^{-} \begin{vmatrix} B' \\ C' \end{vmatrix}, \tag{8}$$

$$C_d(\chi_1) = D - [B' \quad E] \begin{vmatrix} A & C \\ C' & F \end{vmatrix}^{-} \begin{vmatrix} B \\ E' \end{vmatrix}, \tag{9}$$

and

$$C_d(\chi_2) = F - [C' \quad E'] \begin{vmatrix} A & B \\ B' & D \end{vmatrix}^{-} \begin{vmatrix} C \\ E \end{vmatrix}, \tag{10}$$

respectively, where Z^- is a g-inverse of Z, i.e., $ZZ^-Z = Z$.

We now give some definitions that will be used in the subsequent section.

DEFINITION 1. A change-over design will be called *balanced* for the estimation of direct, first and second order residual effects, if it satisfies the following conditions:

(i) Each treatment occurs in a given period an equal number of times, say λ_1,

(ii) Every treatment occurs in a given sequence an equal number of times, say λ_2,
(iii) Each treatment is immediately preceded by every other treatment including itself equally frequently, and
(iv) Every treatment is also preceded by each other treatment as well as by itself by two positions equally often.

Evidently, for a balanced change-over design (BCOD), $p = \lambda_2 v$ and $n = \lambda_1 v$.

DEFINITION 2. A change-over design allowing the estimation of direct, first and second order residual effects with two pre-periods (observations are not recorded during pre-periods), in which the treatments in the first pre-period are exactly the same as those in the last but one period and the treatments in the second pre-period are the treatments of the last period, will be called a *circular change-over design*.

Obviously, every experimental unit in a circular design receives the first and second order residual effects of the treatments applied in the last and the last but one period, in addition to the first and second residual effects of treatments applied in the other periods.

DEFINITION 3. A design which is balanced as well as circular will be called *circular balanced change-over design* (CBCOD).

In the following Section we establish optimality of CBCODs.

3. OPTIMALITY OF CIRCULAR BALANCED CHANGE-OVER DESIGNS

We prove the following:

THEOREM. For given parameters (v, p, n), a circular balanced change-over design, whenever it exists, is universally optimal for the estimation of direct effects, first order residual and second order residual effects of treatments among all the competing designs, under the additive fixed effects model (1).

Proof: Let $D(v, p, n)$ denote the class of CBCODs with parameters (v, p, n) and let d^* be a design in $D(v, p, n)$. We first establish that d^*, whenever it exists, is universally optimal for the estimation of direct effects.

To do this, following Kiefer (1975), we show that $C(\tau)$ for d^* is completely symmetric and has maximum trace in the class of considered designs. It may be seen that for any design $d^* \in D(v, p, n)$,

$$\begin{aligned}
&L_1 = \lambda_1 J_{v,p} && L_2 = \lambda_2 J_{v,n} \\
&E_1 = E_2 = \lambda_1 J_{v,p} && N_1 = N_2 = \lambda_2 J_{v,n} \\
&R = (np/v) I_v = p\lambda_1 I_v && R_1 = R_2 = (np/v) I_v = n\lambda_2 I_v \\
&r = (np/v) 1_v = p\lambda_1 1_v && \rho_1 = \rho_2 = (np/v) 1_v = n\lambda_2 1_v \\
&M_1 = M_2 = M_3 = \lambda J_{v,v}
\end{aligned} \tag{11}$$

where $\lambda = (np)/v^2 = \lambda_1\lambda_2$; $\lambda_1 = n/v$ and $\lambda_2 = p/v$.

In view of (11), B and C given at (7) reduce to the null matrices and the information matrix for direct effects from d^*, $C_{d^*}(\tau)$ simplifies to

$$C_{d^*}(\tau) = A = aI_v + bJ_{v,v} \tag{12}$$

where $a = p\lambda_1$ and $b = -\lambda_1\lambda_2$. Thus, $C_{d^*}(\tau)$ is completely symmetric.

Now to prove that the trace(A) is maximum, let $L_1 = ((m_{ih}))$ and $L_2 = ((n_{il}))$; $(i = 1, \ldots, v; h = 1, \ldots, p; l = 1, \ldots, n)$. Evidently, $\sum_i m_{ih} = n$ (for each h), $\sum_i n_{il} = p$ (for each l) and $\sum_l n_{il} = r_i$ (for each i). From (7),

$$\begin{aligned}
\text{trace}(A) = \sum_i A_{ii} &= \\
&= np - (1/n)\sum_h \sum_i m_{ih}^2 - (1/p)\sum_l \sum_i n_{il}^2 + (1/np)\sum_i r_i^2 ,
\end{aligned}$$

so that

$$np\left(np - \sum_i A_{ii}\right) = p\sum_h \sum_i m_{ih}^2 + \left(n\sum_l \sum_i n_{il}^2 - \sum_i r_i^2\right) . \tag{13}$$

The second term on the right hand side of (13), that is

$$\begin{aligned}
n\sum_l \sum_i n_{il}^2 - \sum_i r_i^2 &= n\sum_i \left[\sum_l n_{il}^2 - r_i^2/n\right] = \\
&= n\sum_i \left[\sum_l \left(n_{il} - n^{-1}\sum_l n_{il}\right)^2\right] \geq 0 .
\end{aligned} \tag{14}$$

Equality in (14) holds when

$$\sum_l \sum_i n_{il}^2 = \sum_i r_i^2/n\,. \tag{15}$$

Eq. (15) is satisfied when $r_i = np/v$ and $n_{il} = p/v$. Clearly, each design $d^* \in D(v, p, n)$ satisfies these conditions. Now, maximization of the trace(A) implies minimization of $\sum_h \sum_i m_{ih}^2$. It can be seen that the minimum value of $\sum_i m_{ih}^2$ subject to $\sum_i m_{ih} = n$ is attained when $m_{ih} = \lambda_1$. Thus

$$\sum_h \sum_i m_{ih}^2 \geq pv\lambda_1^2 \tag{16}$$

with equality holding for d^*. Since both the terms on the right hand side of (13) attains the lower bounds, the trace(A) is maximum for d^* among all the designs. This establishes universal optimality of CBCOD d^* for the estimation of direct effects.

Likewise, it can be proved that d^* is universally optimal for the estimation of first and second order residual effects. Hence the theorem.

A class of CBCODs with parameters $(v, p = 3v, n = v^2)$ can be obtained by adding two pre-periods, to the designs given in Sharma (1977). In view of the theorem, this class of designs is universally optimal for the estimation of direct, first and second order residual effects under the model (1).

We give below an illustration of obtaining universally optimal circular balanced change-over design from the design given in Sharma (1977).

ILLUSTRATION. Let $v = 4$. Represent the treatments by the elements of mod (4), viz. $0, 1, 2, 3$. Construct an orthogonal array of size $4^2(= 16)$, 3 constraints, level 4, strength 2 and index 1 (Vajda, 1967) and call it, the basic array [shown in Fig.1 by boldface, rows (periods)1-3]. Now add $i(= 1, 2, 3)$ to each element of this basic array and reduce, if necessary, the resulting total mod(4). Thus we get an arrangement of 3×4 $(= 12)$ rows of $4^2(= 16)$ elements each, including the rows in the basic array. This arrangement is shown in Fig.1 split under the 4 sets corresponding to the 4 elements of the module which forms a balanced change-over design with rows representing periods and columns, the experimental units. The universally optimal CBCOD with parameters $v = 4$, $p = 12$, $n = 16$ is then obtained by

		Experimental Units															
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Pre-	0_1	3	3	3	3	0	0	0	0	1	1	1	1	2	2	2	2
Periods	0_2	3	0	1	2	0	1	2	3	1	2	3	0	2	3	0	1
	1	**0**	**1**	**2**	**3**	**0**	**1**	**2**	**3**	**0**	**1**	**2**	**3**	**0**	**1**	**2**	**3**
	2	**0**	**0**	**0**	**0**	**1**	**1**	**1**	**1**	**2**	**2**	**2**	**2**	**3**	**3**	**3**	**3**
	3	**0**	**1**	**2**	**3**	**1**	**2**	**3**	**0**	**2**	**3**	**0**	**1**	**3**	**0**	**1**	**2**
	4	1	2	3	0	1	2	3	0	1	2	3	0	1	2	3	0
	5	1	1	1	1	2	2	2	2	3	3	3	3	0	0	0	0
	6	1	2	3	0	2	3	0	1	3	0	1	2	0	1	2	3
Periods	7	2	3	0	1	2	3	0	1	2	3	0	1	2	3	0	1
	8	2	2	2	2	3	3	3	3	0	0	0	0	1	1	1	1
	9	2	3	0	1	3	0	1	2	0	1	2	3	1	2	3	0
	10	3	0	1	2	3	0	1	2	3	0	1	2	3	0	1	2
	11	3	3	3	3	0	0	0	0	1	1	1	1	2	2	2	2
	12	3	0	1	2	0	1	2	3	1	2	3	0	2	3	0	1

Fig. 1. A universally optimal circular balanced change-over design for 4 treatments.

repeating the treatments of the 11th period in the first zero-th period (0_1) and that of the 12th period in the second zero-th period (0_2).

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SUMMARY

Here, universal optimality of circular balanced change-over designs allowing the estimation of first and second order residual effects of treatments has been established under an additive fixed effects model. A class of circular balanced change-over designs with parameters $(v, p = 3v, n = v^2)$ has been shown to be universally optimal for the estimation of direct, first order as well as second order residual effects.

Sull'ottimalità dei disegni bilanciati per effetti residui del primo e secondo ordine

RIASSUNTO

In questo lavoro viene dimostrata l'ottimalità dei disegni bilanciati circolarmente nella stima degli effetti residui di trattamento per un modello additivo ad effetti fissi. Si dimostra che una classe di disegni bilanciati circolarmente con parametri $(v, p = 3v, n = v^2)$ è universalmente ottimale per la stima di effetti residui del primo e del secondo ordine.

KEY WORDS

Circular change-over designs; Pre-periods; Balanced change-over designs; Direct effects; Residual effects; Universal optimality.

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