Chapter 2
OCDs in Completely Randomized Design Set-Up

2.1 Introduction

We consider in this chapter the one-way linear model with v treatments, c covariates and a total of n experimental units. We work under the linear model

$$y_{ij} = \tau_i + \sum_{t=1}^{c} \gamma_t z_{ij}^{(t)} + e_{ij}, \quad 1 \leq j \leq n_i, \ 1 \leq i \leq v. \tag{2.1.1}$$

where $n_i (> 1)$ is the number of times the ith treatment is replicated; clearly

$$\sum_{i=1}^{v} n_i = n. \tag{2.1.2}$$

For $1 \leq j \leq n_i, 1 \leq i \leq v$, here y_{ij} is the observation arising from the jth replication of the ith treatment, τ_i effect due to the ith treatment.

In matrix notation the above model can be represented as

$$\left(\mathbf{Y}, \ \mathbf{X}\boldsymbol{\tau} + \mathbf{Z}\gamma, \ \sigma^2 \mathbf{I}_n\right), \tag{2.1.3}$$

where, $\mathbf{Y}$ is an observation vector and $\mathbf{X}$ is the design matrix corresponding to vector of treatment effects $\boldsymbol{\tau}^{v\times 1}$ and $\mathbf{Z} = ((z_{ij}^{(t)}))$ is the design matrix corresponding to vector of covariate effects $\boldsymbol{\gamma}^{c\times 1} = (\gamma_1, \ \gamma_2, \ldots, \gamma_c)'$. This is referred to as *one-way model with covariates* (*without the general mean*).

Troya Lopes (1982a, b) studied the nature of optimal allocation of treatments and covariates in the above set-up for simultaneous estimation of the (fixed) treatment effects (in the absence of the general effect) and the covariate effects with maximum efficiency in the sense of minimum generalized variance. This is to note that the information matrix with respect to model (2.1.3) is given by $\sigma^{-2}\mathbf{I}(\boldsymbol{\eta})$, where

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$$\mathbf{I}(\boldsymbol{\eta}) = \begin{pmatrix} \mathbf{X}'\mathbf{X} & \mathbf{X}'\mathbf{Z} \\ \mathbf{Z}'\mathbf{X} & \mathbf{Z}'\mathbf{Z} \end{pmatrix} \tag{2.1.4}$$

and $\boldsymbol{\eta}' = \left(\boldsymbol{\tau}', \boldsymbol{\gamma}'\right)$.

The problem is to suggest an optimal allocation scheme (for given design parameters $n,\ v,\ c$) for efficient estimation of the treatment effects as well as the covariate effects by ascertaining the values of the covariates for each one of them, assuming that each one is controllable and quantitative within a stipulated finite closed interval.

The information matrix of $\boldsymbol{\gamma}$ is given by

$$\sigma^{-2} I(\gamma) = \mathbf{Z}'\mathbf{Z} \ - \ \mathbf{Z}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Z} \tag{2.1.5}$$

where $(\mathbf{X}'\mathbf{X})^{-}$ is a generalised inverse of $\mathbf{X}'\mathbf{X}$ satisfying

$$\mathbf{X}'\mathbf{X}\left(\mathbf{X}'\mathbf{X}\right)^{-}\mathbf{X}'\mathbf{X} = \mathbf{X}'\mathbf{X}$$

(cf. Rao 1973, p. 24). It is evident that $\mathbf{Z}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{Z}$ is a positive semi-definite matrix. So from (2.1.5), it follows that

$$\sigma^{-2} I(\gamma) \leq \mathbf{Z}'\mathbf{Z} \tag{2.1.6}$$

in the Loewner order sense (vide Pukelsheim 1993) where for two non-negative definite matrices $\mathbf{A}$ and $\mathbf{B}$, $\mathbf{A}$ is said to dominate $\mathbf{B}$ in the Lowener order sense if $\mathbf{A} - \mathbf{B}$ is a non-negative definite matrix.

Equality in (2.1.6) is attained whenever

$$\mathbf{X}'\mathbf{Z} = \mathbf{0}. \tag{2.1.7}$$

If $\mathbf{Z}$ satisfies (2.1.7), then treatment effects and covariate effects are orthogonally estimated. Again under condition (2.1.7), the information matrix $\mathbf{I}(\gamma)$ reduces to $\mathbf{I}(\gamma) = \mathbf{Z}'\mathbf{Z}$. The z-values are so chosen that $\mathbf{Z}'\mathbf{Z}$ is positive definite so that from (2.1.6)

$$Var(\widehat{\gamma_t}) \geq \frac{\sigma^2}{\sum_{i=1}^{v}\sum_{j=1}^{n_i} z_{ij}^{(t)2}} \geq \frac{\sigma^2}{n} \tag{2.1.8}$$

as $z_{ij}^{(t)} \in [-1, 1];\quad \forall\, i, j, t.$

Now equality in (2.1.8) holds for all i if and only if the $\mathbf{Z}$-matrix is such that

$$\mathbf{z}^{(s)\prime}\mathbf{z}^{(t)} = 0 \ \forall\, s \neq t. \tag{2.1.9}$$

and

$$z_{ij}^{(t)} = \pm 1 \tag{2.1.10}$$

Condition (2.1.7) implies that the estimators of ANOVA effects parameters or parametric contrasts do not interfere with those of the covariate effects and conditions (2.1.9) and (2.1.10) imply that the estimators of each of the covariate effects are such that these are pairwise uncorrelated, attaining the minimum possible variance.

Thus the covariate effects are estimated with the maximum efficiency if and only if

$$\mathbf{Z}'\mathbf{Z} = n\mathbf{I}_c \tag{2.1.11}$$

along with (2.1.7). The designs allowing the estimators with the minimum variance are called *globally optimal designs* (cf. Shah and Sinha 1989, p. 143). Henceforth, we shall only be concerned with such optimal estimation of regression parameters and by optimal covariate design, *to be abbreviated as OCD hereafter*, we shall only mean *globally optimal design*, unless otherwise mentioned.

It is clear that conditions (2.1.7) and (2.1.11) hold simultaneously if and only if z_{ij}'s are necessarily +1 or –1 and that condition (2.1.7) is satisfied.

It is difficult to visualize the **Z**-matrix satisfying conditions (2.1.7) and (2.1.11). In the set-up of the model (2.1.3), it transpires from Troya Lopes (1982a) that optimal estimation of the treatment effects and the covariates effects is possible when the treatment replications are all necessarily equal, assuming that n is a multiple of v, the number of treatments. We set $n = bv$, where b is the common replication of treatments, henceforth. Das et al. (2003) had represented each column of the **Z**-matrix by a $v \times b$ matrix **W** with elements of ± 1, where the rows of **W** correspond to the v treatments and the columns of **W** correspond to different replication numbers. Condition (2.1.7) implies that the sum of each row of **W** should vanish. Again, condition (2.1.11) implies that the sum of products of the corresponding elements, i.e. the Hadamard product of $\mathbf{W}^{(s)}$ and $\mathbf{W}^{(t)}$, defined in (2.1.13) should also vanish, $1 \le s < t \le c$. The above two facts can be represented in the following schematic forms through the row totals and Hadamard product.

Row Totals:

$$\mathbf{W}^{(s)} = \begin{array}{c|ccc|c} \text{Tr.} & \multicolumn{3}{c}{\text{Repl. no.} \rightarrow} & \text{Row} \\ \downarrow & 1 \;\; 2 & \ldots & b & \text{Totals} \\ 1 & & & & 0 \\ 2 & & & & 0 \\ \vdots & & (\pm 1) & & \vdots \\ v & & & & 0 \end{array} \tag{2.1.12}$$

Hadamard product of $\mathbf{W}^{(s)}$ and $\mathbf{W}^{(t)}$ (cf. Rao 1973, p. 30):

$$\mathbf{W}^{(s)} * \mathbf{W}^{(t)} = \begin{array}{c|ccc|} \text{Tr.} & \multicolumn{3}{c}{\text{Repl. no.} \rightarrow} \\ \downarrow & 1 \;\; 2 & \ldots & b \\ 1 & & & \\ 2 & & & \\ \vdots & & (w_{ij}^{(s)} w_{ij}^{(t)}) & \\ v & & & \end{array} \tag{2.1.13}$$

where '*' denotes Hadamard product. For orthogonality of sth and tth columns of $\mathbf{Z}$, it is required that $\sum_{i=1}^{v}\sum_{j=1}^{b} w_{ij}^{(s)} w_{ij}^{(t)} = 0$.

The schematic representation (2.1.12), (2.1.13) of Das et al. (2003) is a breakthrough in the sense that handling of $\mathbf{Z}$-matrix has been made much easier and it has been followed throughout the monograph.

Troya Lopes (1982a) first studied the nature of optimal allocation of treatments and covariates in the above set-up when $\frac{n}{v}$ is an integer. It may be noted that whenever condition (2.1.7) is ensured, presence of the covariates in model (2.1.3) does not pose any threat to the usual "optimal treatment allocation" problem. In Sect. 2.2, following Troya Lopes, we intend to discuss about the availability of $\mathbf{Z}$-matrices satisfying (2.1.7) and (2.1.11) when the treatment allocation matrix $\mathbf{X}$ corresponds to equal allocation number, i.e. in situations where n is a multiple of v. We will write $n = vb$ so that b is the common allocation number of the v treatments under investigation. The situations where (2.1.7), (2.1.11) and $b = \frac{n}{v}$ = integer are satisfied, are identified as *regular* cases. Otherwise it is called a *non-regular* case. If the situation is non-regular, then it is not possible to allocate simultaneously the treatments and covariates optimally. For non-regular situation, efficient allocation of treatments and covariates simultaneously can be done by using other specific optimality criteria. Dey and Mukerjee (2006) and Dutta et al. (2014) considered this problem in non-regular situations and found D-optimal designs in this context. Details are presented in Sect. 2.3.

It has been seen that Hadamard matrix plays a key role for constructing OCDs. Definition of Hadamard matrix (cf. Hedayat et al. 1999, p. 145) is given below:

Definition 2.1.1 A Hadamard matrix $\mathbf{H}_t$ of order t is a $t \times t$ matrix with elements ± 1 satisfying

$$\mathbf{H}_t \mathbf{H}_t' = t\mathbf{I}_t.$$

2.2 Covariate Designs Under Regular Cases

Consider the case when n is a multiple of v, that is $n = vb$ where b is such that $\mathbf{H}_b$, Hadamard matrix of order b, exists. We shall also consider some cases where b is even. Then ANOVA parameters as well as the covariate effect-parameters can be estimated orthgonally and/or most efficiently. This holds simultaneously for c covariates and one can deduce maximum possible value of c for this to happen. As already mentioned, the most efficient estimation of γ-components is possible when (2.1.7) and (2.1.11) are simultaneously satisfied and these conditions reduce, in terms of $\mathbf{W}$-matrices defined in above, to C_1, C_2 where

$$\left.\begin{array}{ll} C_1. & \text{Each of the } c \ \mathbf{W}\text{-matrices has all row-sums equal to zero;} \\ C_2. & \text{The grand total of all the entries in the Hadamard product} \\ & \text{of any two distinct } \mathbf{W}\text{-matrices reduces to zero.} \end{array}\right\} \quad (2.2.1)$$

Now we define optimum **W**-matrices for covariate designs in CRD set-up.

Definition 2.2.1 With respect to model (2.1.3), the c **W**-matrices corresponding to the c covariates are said to be optimum if they satisfy conditions C_1 and C_2 of (2.2.1).

In this context, the following results were deduced in Troya Lopes (1982a).

Theorem 2.2.1 *Let c^* be the maximum number of covariates that can be optimally accommodated. Then a lower bound to c^* is given by*

(a) *b–1 when v = odd, $\mathbf{H}_b$ exists*;
(b) *2(b–1) when $v \equiv 2 \pmod 4$, $\mathbf{H}_b$ exists*;
(c) *4(b–1) when $v \equiv 0 \pmod 4$, $\mathbf{H}_b$ exists*;
(d) *$3v$ when $b \equiv 0 \pmod 4$, $\mathbf{H}_v$ exists*;
(e) *v when $b \equiv 2 \pmod 4$, $\mathbf{H}_v$ exists.*

Proof Hadamard matrix $\mathbf{H}_b$ is given to exist and we write it as

$$\mathbf{H}_b = (\mathbf{h}_1,\ \mathbf{h}_2, \ldots, \mathbf{h}_{b-1}, \mathbf{1})\,. \quad (2.2.2)$$

The choice of optimum **W**-matrices is indicated below one by one. The verification of (2.2.1) is immediate and we leave it to the reader. The Kronecker product of two matrices is formally defined in Chap. 5 (Definition 5.1.1) and it is used in the constructions below.

(a)

$$\mathbf{W}^{(j)\ v\times b} = \mathbf{1}_v \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1; \quad (2.2.3)$$

(b)

$$\left.\begin{array}{rl} \mathbf{W}^{(j)\ v\times b} &= (1,\ \ 1)' \otimes \mathbf{1}_{\frac{v}{2}} \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1; \\ \mathbf{W}^{(b-1+j)\ v\times b} &= (1,\ \ -1)' \otimes \mathbf{1}_{\frac{v}{2}} \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1. \end{array}\right\} \quad (2.2.4)$$

(c)

$$\left.\begin{array}{rl} \mathbf{W}^{(j)\ v\times b} &= (1,\ \ 1,\ \ 1,\ \ 1)' \otimes \mathbf{1}_{\frac{v}{4}} \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1; \\ \mathbf{W}^{(b-1+j)\ v\times b} &= (1,\ \ -1,\ \ 1,\ \ -1)' \otimes \mathbf{1}_{\frac{v}{4}} \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1; \\ \mathbf{W}^{(2(b-1)+j)\ v\times b} &= (1,\ \ -1,\ \ -1,\ \ 1)' \otimes \mathbf{1}_{\frac{v}{4}} \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1; \\ \mathbf{W}^{(3(b-1)+j)\ v\times b} &= (1,\ \ 1,\ \ -1,\ \ -1)' \otimes \mathbf{1}_{\frac{v}{4}} \otimes \mathbf{h}'_j, \quad 1 \le j \le b-1. \end{array}\right\} \quad (2.2.5)$$

(d) Let us represent a Hadamard matrix $\mathbf{H}_v$ of order v as

$$\mathbf{H}_v = \left(\mathbf{h}^*_1,\ \mathbf{h}^*_2, \ldots, \mathbf{h}^*_v\right). \quad (2.2.6)$$

$$\left.\begin{aligned} \mathbf{W}^{(j)\ v\times b} &= (1,\ \ -1,\ \ 1,\ \ -1)\otimes \mathbf{1}'_{\frac{b}{4}}\otimes \mathbf{h}^*_j,\ \ 1\le j\le v;\\ \mathbf{W}^{(v+j)\ v\times b} &= (1,\ \ -1,\ \ -1,\ \ 1)\otimes \mathbf{1}'_{\frac{b}{4}}\otimes \mathbf{h}^*_j,\ \ 1\le j\le v;\\ \mathbf{W}^{(2v+j)\ v\times b} &= (1,\ \ 1,\ \ -1,\ \ -1)\otimes \mathbf{1}'_{\frac{b}{4}}\otimes \mathbf{h}^*_j,\ \ 1\le j\le v. \end{aligned}\right\} \tag{2.2.7}$$

(e)

$$\mathbf{W}^{(j)\ v\times b} = (1,\ \ -1)\otimes \mathbf{1}'_{\frac{b}{2}}\otimes \mathbf{h}^*_j,\ \ 1\le j\le v. \tag{2.2.8}$$

□

Remark 2.2.1 In case (c), we can assume existence of $\mathbf{H}_v$ for all practical purposes as $v \equiv 0 \pmod 4$. So in this case, an optimal design for maximum possible $v(b-1)$ optimum **W**-matrices can easily be constructed as

$$\mathbf{W}^{((b-1)(i-1)+j)} = \mathbf{h}^*_i \otimes \mathbf{h}'_j,\ \ i = 1, 2, \ldots, v,\ \ j = 1, 2, \ldots, b-1. \tag{2.2.9}$$

This was obtained in (Rao et al. 2003) where it was observed that OCDs in CRD and RBD have one to one correspondences with mixed orthogonal array (MOA) (definition given in Chap. 3). This fact will be discussed in Sect. 3.3 of Chap. 3 in some further details.

2.3 Covariate Designs Under Non-regular Cases

Now we examine the situations where at least any one of the conditions (2.1.7), (2.1.11) and $b = \frac{n}{v}$ = integer is violated. In that case, it is not possible to estimate simultaneously ANOVA parameters and $\boldsymbol{\gamma}$-parameters orthogonally and/or most efficiently. Thus we consider D-optimality criterion to give an efficient allocation of treatments and covariates in Set-up (2.1.1). Dey and Mukerjee (2006) and Dutta et al. (2014) have considered this situation and found D-optimal design. Here we discuss their contributions in this direction in details.

The vector of parameters $\boldsymbol{\theta}$, where

$$\boldsymbol{\theta} = (\mu_1,\ \mu_2, \ldots, \mu_v, \gamma_1, \ldots, \gamma_c)' \tag{2.3.1}$$

is assumed to be estimable.

The information matrix for $\boldsymbol{\theta}$ is given by $\sigma^{-2}\mathbf{I}(\boldsymbol{\theta})$, where

$$\mathbf{I}(\boldsymbol{\theta}) = \begin{pmatrix} \mathbf{N} & \mathbf{T} \\ \mathbf{T}' & \mathbf{Z}'\mathbf{Z} \end{pmatrix}, \tag{2.3.2}$$

$$\mathbf{N} = \mathrm{Diag}(n_1, n_2, \ldots, n_v), \tag{2.3.3}$$

$$\mathbf{T} = (\mathbf{T}'_1, \mathbf{T}'_2, \ldots, \mathbf{T}'_v)',\ \ \mathbf{T}_i = \mathbf{1}'_{n_i}\mathbf{Z}_i, \tag{2.3.4}$$

$$\mathbf{Z}^{n\times c} = (\mathbf{Z}_1', \mathbf{Z}_2', \ldots, \mathbf{Z}_v')' \tag{2.3.5}$$

and

$$\mathbf{Z}_i^{n_i\times c} = \begin{pmatrix} z_{i1}^{(1)} & z_{i1}^{(2)} & \ldots & z_{i1}^{(c)} \\ z_{i2}^{(1)} & z_{i2}^{(2)} & \ldots & z_{i2}^{(c)} \\ \vdots & \vdots & \ddots & \vdots \\ z_{in_i}^{(1)} & z_{in_i}^{(2)} & \ldots & z_{in_i}^{(c)} \end{pmatrix}. \tag{2.3.6}$$

For D-optimality, we have to maximize the determinant of $\mathbf{I}(\boldsymbol{\theta})$, denoted as $\det(\mathbf{I}(\boldsymbol{\theta}))$, with respect to the design variables $\{z_{ij}^{(t)}\}$ satisfying $z_{ij}^{(t)} \in [-1, 1], \quad 1 \le j \le n_i, \ 1 \le i \le v$ and n_i's satisfying (2.1.2).

From (2.3.2) it is easy to see that

$$\begin{aligned} \det(\mathbf{I}(\boldsymbol{\theta})) &= \left(\prod_{i=1}^{v} n_i\right)\det(\mathbf{Z}'\mathbf{Z} - \mathbf{T}'\mathbf{N}^{-1}\mathbf{T}) \\ &= \left(\prod_{i=1}^{v} n_i\right)\det(\mathbf{Z}'\mathbf{Z} - \sum_i n_i^{-1}\mathbf{T}_i'\mathbf{T}_i) \\ &= \det(\mathbf{N})\det(\mathbf{C}), \end{aligned} \tag{2.3.7}$$

where

$$\mathbf{C} = \mathbf{Z}'\mathbf{Z} - \sum_i n_i^{-1}\mathbf{T}_i'\mathbf{T}_i. \tag{2.3.8}$$

Note that $\mathbf{C}$ is the information matrix for the regression coefficients $\gamma_1, \gamma_2, \ldots, \gamma_c$. The maximization of $\det(\mathbf{I}(\boldsymbol{\theta}))$ is done in two stages. In the first stage, the maximization is done for varying z-values for fixed n_i's. This leads to an upper bound for $\det(\mathbf{I}(\boldsymbol{\theta}))$ obtained through completely symmetric $\mathbf{C}$-matrices. At the second stage, maximization is done for varying n_i's subject to $\sum_i n_i = n$, and this leads to a sufficiently small class $\mathcal{N}$ of contending $\mathbf{n} = (n_1, n_2, \ldots, n_v)$'s wherein the overall upper bound to $\det(\mathbf{I}(\boldsymbol{\theta}))$ belongs.

2.3.1 First Stage of Maximization

Maximisation of $\mathbf{I}(\boldsymbol{\theta})$ with respect to $z_{ij}^{(t)} \in [-1, 1]$ is based on the following lemma.

Lemma 2.3.1 *A necessary condition for maximization of det(*$\mathbf{C}$*) of* (2.3.8) *with respect to* $z_{ij}^{(t)} \in [-1, 1]$*, for fixed* n_i*'s is that* $z_{ij}^{(t)} = \pm 1 \ \forall i, j$ *and* t*.*

Proof From (2.3.8), $\mathbf{C}$ can be expressed as

$$\mathbf{C} = \mathbf{Z}'\mathbf{M}\mathbf{Z} = \mathbf{Z}^{*\prime}\mathbf{Z}^{*} \tag{2.3.9}$$

where

$$\mathbf{Z}^{*} = \mathbf{M}\mathbf{Z}, \quad \mathbf{M} = \text{diag}(\mathbf{M}_1, \mathbf{M}_2, \ldots, \mathbf{M}_v), \quad \mathbf{M}_i = (\mathbf{I}_{n_i} - n_i^{-1}\mathbf{1}_{n_i}\mathbf{1}'_{n_i}). \tag{2.3.10}$$

It is known that (cf. Galil and Kiefer 1980; Wojtas 1964), det$(\mathbf{Z}^{*\prime}\mathbf{Z}^{*})$ is maximum at the extreme entries of $\mathbf{Z}^{*}$. Again, as $z_{ij}^{(t)*}$'s are linear in $z_{ij}^{(t)}$'s, the determinant is maximum at the extreme values of $z_{ij}^{(t)}$'s for all i, j and t. Hence the lemma follows. □

Theorem 2.3.1 *For fixed* $\{n_i\}$*'s satisfying* (2.1.2)*,*

$$det(\mathbf{I}(\boldsymbol{\theta})) \le \left(\prod_{i=1}^{v} n_i\right)\{a + (c-1)b\}(a-b)^{c-1} \tag{2.3.11}$$

where

$$a = n - \delta, \quad b = |\xi - \delta| \tag{2.3.12}$$

$$\delta = \sum_{i=1}^{v} n_i^{-1}\delta_i, \quad \delta_i = 1(0) \text{ if } n_i = \text{odd(even)} \tag{2.3.13}$$

$$\xi = \xi(n, \delta) = \begin{cases} \lfloor\delta\rfloor & \text{if both of } n,\ \lfloor\delta\rfloor \text{ are odd or even} \\ \lfloor\delta\rfloor + 1 & \text{if } n = \text{odd},\ \lfloor\delta\rfloor = \text{even or n=even}, \lfloor\delta\rfloor = \text{odd} \end{cases} \tag{2.3.14}$$

$\lfloor\delta\rfloor$ = *greatest integer less than equal to* δ.

Proof Because of Lemma 2.3.1, we restrict $z_{ij}^{(t)}$ to the class $\boldsymbol{\chi} = \{z_{ij}^{(t)} : z_{ij}^{(t)} = \pm 1\}$. From the Eq. (2.3.8), we note that, $c_{t,t'}$, the $(t, t')^{\text{th}}$ element of the $\mathbf{C}$-matrix is given by

$$c_{t,t'} = \sum_i \left\{ \sum_j z_{ij}^{(t)} z_{ij}^{(t')} - \frac{\left(\sum_j z_{ij}^{(t)}\right)\left(\sum_j z_{ij}^{(t')}\right)}{n_i} \right\}, \quad 1 \le t, t' \le c. \tag{2.3.15}$$

It follows from Wojtas (1964) that det$(\mathbf{C})$ is maximum when $\mathbf{C}$ is completely symmetric with all the diagonal elements equal to a and all off-diagonal elements equal to b where a and b are given by $\max\limits_{1\le t\le c} c_{tt}$ and $\min\limits_{1\le t\ne t'\le c} |c_{tt'}|$ respectively. Again as

$z_{ij}^{(t)} = \pm 1 \; \forall i$, j and t, for fixed n_i's, it can be deduced that

$$\max_{1 \le t \le c} c_{tt} = n - \delta = a, \quad \min_{1 \le t \ne t' \le c} |c_{tt'}| = |\xi - \delta| = b \tag{2.3.16}$$

where δ and ξ are given in (2.3.13) and (2.3.14) respectively. Therefore the theorem follows. □

2.3.2 Second Stage of Maximization

In view of Theorem 2.3.1, we now consider the problem of maximizing

$$g(\mathbf{n}) = g(n_1,\ n_2, \ldots, n_v) = \left(\prod_{i=1}^{v} n_i\right)\{a + (c-1)b\}(a-b)^{c-1} \tag{2.3.17}$$

with respect to n_i's subject to $\sum_{i=1}^{v} n_i = n$, where a and b are given by (2.3.12)–(2.3.14), so as to find the overall upper bound of $\det(\mathbf{I}(\boldsymbol{\theta}))$. The following lemma helps to reduce the class $\mathcal{N}$ of $\mathbf{n}$'s where $\mathbf{n} = (n_1,\ n_2, \ldots, n_v)$, satisfying (2.1.2), to a subclass in which maximum of $g(\mathbf{n})$ lies.

Lemma 2.3.2 *Let* $\mathbf{n}^* = \left(n_1^*,\ n_2^*, \ldots, n_v^*\right)$ *be a maximizer of* $g(\mathbf{n})$ *of* (2.3.17) *subject to the condition* (2.1.2). *Then* $\mathbf{n}^*$ *cannot have*

(i) *two unequal odd elements*;
(ii) *two even elements that differ by more than 2*;
(iii) *an even and an odd element that differ by more than 1.* □

Proof (i) Without loss of generality it is assumed that n_1^* and n_2^* be odd and $n_1^* \le n_2^* - 2$. Define $\widetilde{\mathbf{n}} = (\widetilde{n}_1,\ \widetilde{n}_2, \ldots, \widetilde{n}_v)$, where $\widetilde{n}_1 = n_1^* + 1$, $\widetilde{n}_2 = n_2^* - 1$ and $\widetilde{n}_i = n_i^* \; \forall i \ne 1, 2$. Note that $\widetilde{n}_i$'s satisfy condition (2.1.2). Then by Eq. (2.3.17),

$$\begin{aligned}\frac{g(\widetilde{\mathbf{n}})}{g(\mathbf{n}^*)} &= \left(\prod_{i=1}^{v} \widetilde{n}_i\right) \Big/ \left(\prod_{i=1}^{v} n_i^*\right)\left(\frac{\{\widetilde{a}+(c-1)\widetilde{b}\}(\widetilde{a}-\widetilde{b})^{c-1}}{\{a^*+(c-1)b^*\}(a^*-b^*)^{c-1}}\right) \\ &= \frac{(n_1^*+1)(n_2^*-1)}{n_1^* n_2^*}\,\frac{\{\widetilde{a}+(c-1)\widetilde{b}\}(\widetilde{a}-\widetilde{b})^{c-1}}{\{a^*+(c-1)b^*\}(a^*-b^*)^{c-1}},\end{aligned} \tag{2.3.18}$$

where,

$$\widetilde{a} = n - \sum_{i=1}^{v} \widetilde{n}_i^{-1}\widetilde{\delta}_i = n - \sum_{i=1}^{v} n_i^{*-1}\delta_i^* + \frac{1}{n_1^*} + \frac{1}{n_2^*} = a^* + \frac{1}{n_1^*} + \frac{1}{n_2^*} \tag{2.3.19}$$

Again,

$$\widetilde{b} = \left| \widetilde{\xi} - \sum_{i=1}^{v} \widetilde{n}_i^{-1} \widetilde{\delta}_i \right| \leq \left| \xi^* - \sum_{i=1}^{v} n_i^{*-1} \delta_i^* + \left(\frac{1}{n_1^*} + \frac{1}{n_2^*} \right) \right| \leq b^* + \left(\frac{1}{n_1^*} + \frac{1}{n_2^*} \right). \quad (2.3.20)$$

We consider the two cases $\widetilde{b} \leq b^*$ and $\widetilde{b} > b^*$ separately.
(a) Let $\widetilde{b} \leq b^*$. Then, as by (2.3.19), $\widetilde{a} > a^*$, it follows that $g(\widetilde{\mathbf{n}}) > g(\mathbf{n}^*)$, which is impossible.
(b) Let $\widetilde{b} > b^*$ and let $\widetilde{b}$ assume the highest possible value given in (2.3.20). Then from (2.3.18)–(2.3.20), it is seen that

$$\frac{g(\widetilde{\mathbf{n}})}{g(\mathbf{n}^*)} > \frac{(n_1^* + 1)(n_2^* - 1)}{n_1^* n_2^*} > 1 \quad (2.3.21)$$

which is again a contradiction. As the inequality (2.3.21) is true for the highest value of $\widetilde{b}$, it will be true for all values of $\widetilde{b}$ in $[b^*,\ b^* + \frac{1}{n_1^*} + \frac{1}{n_2^*}]$ as $\widetilde{a} > a^*$.
(ii) If possible, let $\mathbf{n}^*$ have two even elements, say $n_1^* < n_2^*$ which differ by more than 2. Then as in (i) above, we reach at a contradiction by increasing n_1^* by two and decreasing n_2^* by two.
(iii) If possible, let $\mathbf{n}^*$ have an even element n_1^* and an odd element n_2^* which differ by more than 1.

Case A: Let $n_1^* > n_2^*$. Satisfying (2.1.2), define $\widetilde{\mathbf{n}} = (\widetilde{n}_1,\ \widetilde{n}_2, \ldots, \widetilde{n}_v)$, where $\widetilde{n}_1 = n_1^* - 2,\ \widetilde{n}_2 = n_2^* + 2$ and $\widetilde{n}_i = n_i^*\ \forall i \neq 1, 2$. Then by Eq. (2.3.17), we have

$$\frac{g(\widetilde{\mathbf{n}})}{g(\mathbf{n}^*)} = \frac{(n_1^* - 2)(n_2^* + 2)\{\widetilde{a} + (c-1)\widetilde{b}\}(\widetilde{a} - \widetilde{b})^{c-1}}{(n_1^* n_2^*)\{a^* + (c-1)b^*\}(a^* - b^*)^{c-1}} \quad (2.3.22)$$

where,

$$\widetilde{a} = n - \sum_i \widetilde{n}_i^{-1} \widetilde{\delta}_i = \left(n - \sum_i n_i^{*-1} \delta_i^* \right) + \left(\frac{1}{n_2^*} - \frac{1}{n_2^* + 2} \right) = a^* + \left(\frac{1}{n_2^*} - \frac{1}{n_2^* + 2} \right) \quad (2.3.23)$$

$$\widetilde{b} = |\widetilde{\xi} - \widetilde{\delta}| \leq |(\xi^* - \delta^*) + \left(\frac{1}{n_2^*} - \frac{1}{n_2^* - 2} \right)| \leq b^* + \left(\frac{1}{n_2^*} - \frac{1}{n_2^* - 2} \right). \quad (2.3.24)$$

We consider two cases when $\widetilde{b} \leq b^*$ and $\widetilde{b} > b^*$. For $\widetilde{b} \leq b^*$, it follows, from (2.3.22) that $g(\widetilde{\mathbf{n}}) > g(\mathbf{n}^*)$ as $\widetilde{a} > a^*$. Again, for $\widetilde{b} > b^*$, we assume its highest value viz. $b^* + (\frac{1}{n_2^*} - \frac{1}{n_2^* - 2})$ from (2.3.24) and use it in (2.3.22). It is seen that $g(\widetilde{\mathbf{n}}) > g(\mathbf{n}^*)$, which obviously holds for all other values of $\widetilde{b} > b^*$ as $\widetilde{a} > a^*$.

So we reach at a contradiction that $\mathbf{n}^*$ is a maximizer of $g(\mathbf{n})$.

Case B: Let $n_1^* < n_2^*$ (i.e. $n_1^* \leq n_2^* - 3$), then we have the following two cases:

(a) n_2^* is not the only odd element of $\mathbf{n}^*$.
(b) n_2^* is the only odd element of $\mathbf{n}^*$.

For (a), let $\mathbf{n}^*$ have another odd element n_3^*. Then by part (i) of this lemma, n_2^*=n_3^*. Define $\widetilde{\mathbf{n}} = (\widetilde{n}_1, \widetilde{n}_2, \ldots, \widetilde{n}_v)$, where $\widetilde{n}_1 = n_1^* + 2$, $\widetilde{n}_2 = \widetilde{n}_3 = n_2^* - 1$ and $\widetilde{n}_i = n_i^*\ \forall\, i \neq 1, 2, 3$. Then by (2.3.17)

$$\frac{g(\widetilde{\mathbf{n}})}{g(\mathbf{n}^*)} = \frac{(n_1^*+2)(n_2^*-1)^2}{(n_1^* n_2^* n_3^*)} \frac{\{\widetilde{a} + (c-1)\widetilde{b}\}(\widetilde{a} - \widetilde{b})^{c-1}}{\{a^* + (c-1)b^*\}(a^* - b^*)^{c-1}}. \tag{2.3.25}$$

where,

$$\widetilde{a} = n - \sum_i \widetilde{n}_i^{-1} \widetilde{\delta}_i = \left(n - \sum_i n_i^{*-1} \delta_i\right) + \frac{2}{n_2^*} = a^* + \frac{2}{n_2^*} \tag{2.3.26}$$

$$\widetilde{b} = |\widetilde{\xi} - \widetilde{\delta}| \leq |(\xi^* - \delta^*) + \frac{2}{n_2^*}| \leq b^* + \frac{2}{n_2^*}. \tag{2.3.27}$$

If $\widetilde{b} \leq b^*$, then from (2.3.25) and (2.3.26) $g(\widetilde{\mathbf{n}}) > g(\mathbf{n}^*)$ which is a contradiction.

If $\widetilde{b} > b^*$, the above contradiction also holds by the same reasons as given in Case A.

For (b), let us define $\widetilde{\mathbf{n}} = (\widetilde{n}_1, \widetilde{n}_2, \ldots, \widetilde{n}_v)$ satisfying (1.2) where $\widetilde{n}_1 = n_1^* + 2$, $\widetilde{n}_2 = n_2^* - 2$ and $\widetilde{n}_i = n_i^*\ \forall\, i \neq 1, 2$. Proceeding as before, it can be proved that

$$\widetilde{a} = a^* + \left(\frac{1}{n_2^*} - \frac{1}{n_2^* - 2}\right), \quad \widetilde{b} = \left(1 - \frac{1}{n_2^* - 2}\right). \tag{2.3.28}$$

Using (2.3.28) in (2.3.17), it is seen that

$$\frac{g(\widetilde{\mathbf{n}})}{g(\mathbf{n}^*)} = \frac{(n_1^*+2)(n_2^*-2)}{n_1^* n_2^*} \frac{\left(n + c - 1 - \frac{c}{n_2^*-2}\right)}{\left(n + c - 1 - \frac{c}{n_2^*}\right)} > 1 \quad \text{as } (n_2^* - n_1^*) \geq 3.$$

This is again a contradiction. Therefore the lemma follows. □

From Lemma 2.3.2, we get the following theorem whose proof is immediate.

Theorem 2.3.2 *Let $\overline{o}$ be an odd integer, where $\overline{o} = \lfloor \frac{n}{v} \rfloor$ or $\lfloor \frac{n}{v} \rfloor + 1$ according as $\lfloor \frac{n}{v} \rfloor$ is odd or even and $\mathbf{n}^* = \left(n_1^*, n_2^*, \ldots, n_v^*\right)$ be a maximizer of $g(\mathbf{n})$ of (2.3.17) subject to $\sum_i n_i = n$. Then $n_i^* \in \{\overline{o} - 1, \overline{o}, \overline{o} + 1\}$.*

Lemma 2.3.3 *If f, f^- and f^+ be the frequencies of $\overline{o}$, $\overline{o}-1$ and $\overline{o}+1$ respectively, then the following relations*

$$f + f^- + f^+ = v; \quad \overline{o} f + (\overline{o} - 1) f^- + (\overline{o} + 1) f^+ = n, \tag{2.3.29}$$

minimize considerably the search for optimum $\mathbf{n}$*, for which* $g(\mathbf{n})$ *is a maximum.*

Let $\mathcal{N}^*$ ($\subset \mathcal{N}$) denote the class of $\mathbf{n}$'s satisfying Theorem 2.3.2 and Lemma 2.3.2.

Remark 2.3.1 For given n, v and c, let $g(\mathbf{n}^*)$ be the maximum of $g(\mathbf{n})$ of (2.3.17) over $\mathbf{n} = (n_1, n_2, \ldots, n_v)$ subject to $\sum_i n_i = n$. Then by Theorem 2.3.1

$$\det(\mathbf{I}(\boldsymbol{\theta}) \leq g(\mathbf{n}^*). \tag{2.3.30}$$

If a choice of $\{z_{ij}^{(t)}\}$ exists corresponding to $\mathbf{n}^*$, such that equality in (2.3.30) holds, then $\mathbf{n}^*$ together with $\{z_{ij}^{(t)}\}$ gives a D-optimal design.

Remark 2.3.2 If all n_i's are even, so that all the $\mathbf{T}_i$'s of (2.3.4) may be made equal to zero, then it is possible to estimate the regression parameters $\boldsymbol{\gamma}$'s orthogonally to the μ_i's. In that case, $\boldsymbol{\gamma}$'s are estimated most efficiently with the minimum possible variance when $\mathbf{Z}'\mathbf{Z} = n\mathbf{I}_c$.

Remark 2.3.3 If $n_i = \frac{n}{v}$ = an even integer for all i, the situation reduces to regular case and then Remark 2.3.1 is in full agreement with Troya Lopes (1982a) and in that case $\boldsymbol{\gamma}$'s can be estimated most efficiently so that each estimator has minimum possible variance when $\mathbf{Z}'\mathbf{Z} = n\mathbf{I}_c$.

Remark 2.3.4 If the v levels of the single factor set-up are assumed to be the v level combinations of m factors $\mathrm{F}_1, \ldots, \mathrm{F}_m$ having $s_1, \ldots, s_m$ levels, respectively ($v = \prod s_i$), then the optimum design for the single factor set-up is also optimum for the estimation of $\boldsymbol{\gamma}$ and all effects up to m-factor interactions which can be obtained through an orthogonal transformation of $\boldsymbol{\gamma}$ and the mean vector $\boldsymbol{\mu}$ corresponding to the v level combinations.

2.3.3 Examples

Now we consider following examples to illustrate the above method.

Example 2.3.1 Let us consider the one-way set-up with $n = 12$, $v = 4$. It follows that $\mathcal{N}^* = \{(3, 3, 3, 3), (2, 3, 3, 4), (2, 2, 4, 4)\} \equiv \{(3^4), \ (2, 3^2, 4), \ (2^2, 4^2)\}$.

(a) For $c = 1$, $\mathbf{n}^* = (3^4)$ is the unique maximizer of $g(\mathbf{n})$ and this $\mathbf{n}^*$ together with $\mathbf{Z}_1' = (1,\ 1,\ -1)$, $\mathbf{Z}_2' = (1,\ 1,\ -1)$, $\mathbf{Z}_3' = (1,\ 1,\ -1)$, $\mathbf{Z}_4' = (1,\ 1,\ -1)$ gives a D-optimal design.
(b) For $c = 2$ both $\mathbf{n}^* = (2, 3^2, 4)$ and $(2^2, 4^2)$ are maximizers of $g(\mathbf{n})$.
(i) $\mathbf{n}^* = (2^2, 4^2)$ and

$$\mathbf{Z}_1 = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \mathbf{Z}_2 = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \mathbf{Z}_3 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & 1 \\ -1 & -1 \end{pmatrix}, \mathbf{Z}_4 = \begin{pmatrix} -1 & 1 \\ -1 & -1 \\ 1 & 1 \\ 1 & -1 \end{pmatrix},$$

give a D-optimal design.
(ii) $\mathbf{n}^* = (2, 3^2, 4)$ and

$$\mathbf{Z}_1 = \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}, \mathbf{Z}_2 = \begin{pmatrix} -1 & 1 \\ 1 & -1 \\ 1 & 1 \end{pmatrix}, \mathbf{Z}_3 = \begin{pmatrix} 1 & -1 \\ -1 & 1 \\ -1 & -1 \end{pmatrix}, \mathbf{Z}_4 = \begin{pmatrix} -1 & 1 \\ -1 & -1 \\ 1 & 1 \\ 1 & -1 \end{pmatrix}, \text{ also}$$

give a D-optimal design.
(c) For $c = 3,\ 4$, $\mathbf{n}^* = (2^2, 4^2)$ is the unique maximizer of $g(\mathbf{n})$.

Example 2.3.2 In one-way set-up with $n = 9,\ v = 3,\ c = 3$, D-optimal design should be searched within the set $\{(2, 3, 4),\ (3^3)\}$ of $\mathbf{n}$. It is seen that for $\mathbf{n} = (3^3)$ and

$$\mathrm{D}_1: \quad \mathbf{Z}^{(1)} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}, \ \mathbf{Z}^{(2)} = \begin{pmatrix} -1 & + & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix} \text{ and } \mathbf{Z}^{(3)} = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix},$$

$\mathbf{C} = \text{diag}(8, 8, 8)$ and $g(\mathbf{n}) = 3^3.8^3$. But for $\mathbf{n} = (2, 3, 4)$, and

$$\mathrm{D}_2: \quad \mathbf{Z}^{(1)} = \begin{pmatrix} 1 & 1 & 1 \\ -1 & -1 & -1 \end{pmatrix}, \ \mathbf{Z}^{(2)} = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix} \text{ and } \mathbf{Z}^{(3)} = \begin{pmatrix} 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & 1 \end{pmatrix}$$

It can be seen that $\mathbf{C} = 8\mathbf{I}_3 + \frac{2}{3}\mathbf{J}_3$, where $\mathbf{J}_3$ is a 3×3 matrix containing elements one only. Also $g(2, 3, 4)$ which is equal to 15360, attains the upper bound in (2.3.14) and $g(2, 3, 4) > g(3, 3, 3)$ implying that D_2 is D-optimal.

Again for $n = 9$, $v = 3$, $c = 4$, it is noted that $\mathbf{n}^* = (2, 3, 4)$ together with

$$\mathrm{D}_3: \quad \mathbf{Z}^{(1)} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 \end{pmatrix}, \ \mathbf{Z}^{(2)} = \begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

and $$\mathbf{Z}^{(3)} = \begin{pmatrix} 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \end{pmatrix}$$

maximizes $g(\mathbf{n})$ of (2.3.17) and hence gives a D-optimal design.

Remark 2.3.5 It is seen from the examples that the choice of optimum **n** depends on the number of the covariates used apart from the number of cells v in the set-up. Again it is noted from (2.3.7) that $\det(\mathbf{I}(\boldsymbol{\theta}))$ depends on two factors viz. $\det(\mathbf{N})(=\prod_i n_i)$ and $\det(\mathbf{C})$. Determinant of $\mathbf{N}$ increases as the homogeneity between the n_i's increases subject to $\sum_i n_i = n$. On the other hand $\det(\mathbf{C})$ increases, apart from c, with the largeness of a and the smallness of b, which again are achieved by inclusion of maximum number of even n_i's closed to $\lfloor \frac{n}{v} \rfloor$. The number of odd n_i's subject to $\sum_i n_i = n$, in between the even ones with proper homogeneity, actually strikes a balance between $\det(\mathbf{N})$ and $\det(\mathbf{C})$. It is also seen that, when c is small, $\det(\mathbf{N})$ is the dominant factor, while, if c is large $\det(\mathbf{C})$ becomes the dominant factor.

Incidentally, the above analysis is based on the work in Dutta et al. (2014) and it improves over what was achieved in Dey and Mukerjee (2006).

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