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A New Class of Optimal Designs in the Presence of a Quantitative Covariate

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Abstract

We propose to discuss at length the problem of placement of one controllable covariate in the context of an experiment involving several 'treatments'. We do this while extracting maximum information on the unknown parameter attached to the covariate's values in the mean model for the observations. The experimental set-up is a bit different, and this calls for an interesting non-trivial study on optimality in the context of a single-covariate linear regression model.

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1 Introduction

There are two parallel developments in the construction, analysis and optimality of varietal designs. One of these is associated with the Analysis of Variance (ANOVA) set-up and in particular, the block design set-up. The pioneering work is due to Bose and his co-authors on the construction and analysis of Balanced Incomplete Block Designs (BIBDs) and other families of designs, and many authors contributed in this area. In this connection one may refer to Raghavarao (1971) for detailed references on initial development towards constructions of designs.

The optimality problems have been formulated in various ANOVA models arising in experimental designs. For an exhaustive review of the work done in the area prior to 90's, one is to referred to the monograph by Shah and Sinha (1989). The other development is associated with the analysis and optimality of regression designs where the response depends on the levels of a number of controllable quantitative factors, called covariates. Again, excellent text books are available in this area of research viz. Fedorov (1972), Silvey (1980) and Pukelsheim (1993). A relatively recent monograph on this topic is by Liski et al (2002).

In the analysis of covariance models where both qualitative and quantitative factors are present, the problem of inference on varietal contrasts corresponding to qualitative factors were studied by Harville (1975), Wu (1981) and Nachtsheim (1989). The problem of determining optimum designs for the estimation of regression parameters corresponding to controllable covariates was first considered by Lopes Troya (1982a, 1982b). She restricted investigations in the set-up of Completely Randomized Designs (CRDs). Das et al. (2003) extended it to the block design set-up viz. Randomised Block Designs (RBDs) and some series of Balanced Incomplete Block Designs (BIBDs) and constructed Optimum Covariate Designs (OCDs) for optimal and simultaneous estimation of covariates' parameters.

The literature on optimum designs is so vast and is developing so fast in different directions that it would be impossible to cover the area comprehensibly in such a short article. In the above we have tried to cite only those references which have direct link with one or other aspect of the problem to be considered here.

In this paper, an attempt has been made to construct OCDs for the estimation of the covariate parameter in a specific experimental design set-up. The model formulation closely follows the usual covariates model as in Lopes Troya and others. But, it is not quite the same. We will consider two formulations of the specific experimental set-up (and, consequently, of the underlying allocation design). In both the cases, we will search for optimal design(s) for most efficient estimation of the covariate parameter.

2 Formulation I

There is a non-stochastic feature, quantified as X, associated with every experimental unit in a finite population of n experimental units (eu's). Assume X lies in the closed interval $[-1, 1]$ and that there are altogether $t(> 1)$ distinct values of X covering all the n units according to the following scheme :

$$[(x_i, f_i); 1 \leq i \leq t; \sum_i f_i = n; -1 \leq x_1 < \ldots < x_t \leq 1]$$

There are v experimental 'treatments' to be allocated, one to each of these eu's and with τ_j as the effect of the j^{th} treatment; $j = 1, 2, \ldots, v$. The following Incidence Matrix describes the layout of the design:

$X - values$	*Treatment Allocations*						*Totals*
x_1	f_{11}	f_{12}	$\cdots$	f_{1j}	$\cdots$	f_{1v}	f_1
x_2	f_{21}	f_{22}	$\cdots$	f_{2j}	$\cdots$	f_{2v}	f_2
x_3	f_{31}	f_{32}	$\cdots$	f_{3j}	$\cdots$	f_{3v}	f_3
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$
x_i	f_{i1}	f_{i2}	$\cdots$	f_{ij}	$\cdots$	f_{iv}	f_i
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$	f_{1v}	$\ldots$
x_t	f_{t1}	f_{t2}	$\cdots$	f_{tj}	$\cdots$	f_{tv}	f_t
Totals	r_1	r_2	$\cdots$	r_j	$\cdots$	r_v	n

Clearly, $F = ((f_{ij}))$ is the treatment allocation matrix with $f_{ij} \geq 0$ and it is arbitrary subject to the pre-assigned row totals f_i's and with arbitrary column totals r_j's except that each $r_j > 0$. We contemplate a fixed effects additive model given by

$$Y_{iju} = \mu + \beta x_i + \tau_j + e_{iju}$$

whenever $f_{ij} > 0$, for $u = 1, 2, \ldots, f_{ij}; 1 \leq j \leq v; 1 \leq i \leq t$. Usual assumptions on the error distributions apply. The given design parameters are n and v. The quantities to be ascertained are

$$(i)\ t > 1; (ii)\ -1 \leq x_1 < x_2 < \ldots < x_t \leq 1; (iii)\ f_i's,$$

and hence $((f_{ij}))$'s and r_j's such that information on β parameter is maximized, subject to estimability of the τ-contrasts.

Joint Information Matrix for the τ-vector and the β-parameter for the above design layout is given by

$$\left[\begin{array}{ccccc|c} r_1 & 0 & 0 & \cdots & 0 & \sum_i x_i f_{i1} = S_1, say \\ 0 & r_2 & 0 & \cdots & 0 & \sum_i x_i f_{i2} = S_2, say \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & r_v & \sum_i x_i f_{iv} = S_v, say \\ \hline S_1 & S_2 & S_3 & \cdots & S_v & \sum_i x_i^2 f_i = SS, say \end{array}\right]$$

Note that $\sum\sum_{ij} x_i f_{ij} = \sum_i x_i f_i = \sum_j S_j; S_j = \sum_i x_i f_{ij}$.

Let $I(\beta) = SS - \sum_j S_j^2/r_j; SS = \sum\sum_{ij} x_i^2 f_{ij} = \sum_i x_i^2 f_i$.

Our purpose is to maximize $I(\beta)$ for variations in (t, x_i, f_i, r_j)'s, finally leading to the $((f_{ij}))$ matrix. This formulation is quite easy to sort out. We re-write $I(\beta)$ as $\sum_j[\sum_i x_i^2 f_{ij} - S_j^2/r_j] = \sum_j[Q_j]$, say.

Lemma 1. For fixed $r_j, Q_j \leq r_j - I(odd)/r_j$, where $I(odd) = 1$ if r_j is odd; $= 0$ if r_j is even.

Proof. Easy since $-1 \leq x_i \leq 1$ for each i.

Therefore, $I(\beta) = \sum_j Q_j \leq n - \sum_j[I(odd)/r_j] \leq n$. Henceforth, we assume n to be even and choose r_j's also to be even integers so that $I(\beta)$ may attain the upper bound n. In order to attain the bound, we set $t = 2, x_1 = -1$ and $x_2 = +1$ and further, each r_j as an even integer. One choice is : $n = 2b = 2(v-1) + 2(b-v+1); r_1 = \ldots = r_{(v-1)} = 2; r_v = 2(b-v+1)$.

However, as is well known, this allocation design will stay away from a treatment-optimal design which calls for equal or nearly equal treatment replications. Hence, we consider the representation $n = vr + s$ where $0 < s < v$. In that case, the treatment allocations are : r (with replication $(v-s)$) and $r+1$ (with replication s). At this stage, maximization rests on whether r is odd or even. It follows that $I(\beta) = n - (v-s)I(r\ odd)/r - sI(r\ even)/(r+1)$. For $r = 2q$, $I(\beta) = n - s/(r+1)$ while $n = 2qv + s$ and for $r = 2q+1, I(\beta) = n - (v-s)/r$ while $n = v(2q+1) + s$. Further, all treatment contrasts are estimable. With the formulation given above, β-parameter is estimated with maximum precision for the above allocations, though there are many choices of the underlying designs.

3 Formulation II

We now confine to a situation wherein the observations are 'generated in pairs' - based on pairs of distinct treatments chosen from the set of all v treatments. Thus, as before, we have $t > 1$ distinct choices of x-values inside $[-1, +1]$ and for each x_i, there are pairs of treatments chosen and utilized to produce pairs of observations. We assume that in the process we generate all $b = \binom{v}{2}$ pairs of observations so that $n = 2 \times \binom{v}{2} = v(v-1)$. Naturally, the choice of a design corresponds to a partition of b pairs into t classes. Note that this formulation trivially leads to estimability of all treatment effects contrasts. Our purpose is to characterize an optimal design for most efficient estimation of the β-parameter underlying the same model as stipulated above.

It may be noted that this formulation is a bit different from usual linear regression set-up involving a number of treatments. Herein we are contemplating a situation involving a production process. Every run of the experiment using any covariate value utilizes enough input material to accommodate two distinct treatments which constitute a block, so to say. An immediate generalization would call for accommodating triplets of treatments and so on. We will discuss this aspect later. We start with a very general design specification, with k_i treatment pairs generated from the i^{th} block; $i = 1, 2, , ., t$, as outlined in Table 1.

Table 1

$Blocks$	$x - values$	$Treatment\ Pairs$	$Treatment\ Replications$	$Total$
1	x_1	$[\{1i_p, 1i_q\}; 1 <= p < q <= v;]$	$f_{11}\ \ f_{12}\ \ \cdots\ \ f_{1v}$	$2k_1$
2	x_2	$[\{2i_p, 2i_q\}; 1 <= p < q <= v;]$	$f_{21}\ \ f_{22}\ \ \cdots\ \ f_{2v}$	$2k_2$
$\cdots$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
t	x_t	$[\{ti_p, ti_q\}; 1 <= p < q <= v;]$	$f_{t1}\ \ f_{t2}\ \ \cdots\ \ f_{tv}$	$2k_t$

In the above, it is understood that all allocations (of pairs of treatments) within and across different blocks are distinct. Naturally, the above allocation parameters satisfy

$$(i) \sum_j f_{ij} = 2k_i; (ii) \sum_i k_i = b.$$

Further, we assume, without loss of generality, $-1 \le x_1 < x_2 < .. < x_t \le 1$. Define F as the block $\times$ treatment incidence matrix as indicated above. That is, $F = ((f_{ij})); 1 \le i \le t; 1 \le j \le v$. It follows that

$$I(\beta) = \mathbf{x}'Q\mathbf{x}/(v-1)$$

where $\mathbf{x} = (x_1, x_2, \dots, x_t)'$ and
$Q_{ii} = 2(v-1)k_i - \sum_j f_{ij}^2; Q_{ii'} = -\sum_j f_{ij} f_{i'j}$. In other words,

$$Q = 2(v-1)Diag.(k_i) - FF'$$

The 'decision variables' are : $t(> 1)$, distinct x-values, k-values subject to (ii) and elements of the matrix F subject to (i) above. The problem is that of maximization of $I(\beta)$. Note that the treatment pairs can be listed according to the dictionary style, viz., $[(1, 2), \dots, (1, v); (2, 3), \dots, (2, v); \dots; (v-1, v)]$. For any given specification of the decision variables listed above, starting with the vector $\mathbf{x}$ of order $t \times 1$, let us naturally extend it to a vector $\mathbf{x}^*$ of order $b \times 1$, by repeating x_i in exactly k_i positions as per the specification of the treatment pairs in the above allocation matrix and the dictionary style representation. Note that (ii) ensures $\sum_i k_i = b$. Further to this, it also follows that $\mathbf{x}'Diag.(k_i)\mathbf{x} = \mathbf{x}^{*'}\mathbf{x}^*$. Likewise, let us 'convert' the F-matrix of order $t \times v$ to an 'Incidence' matrix N' of order $b \times v$ in an obvious manner so that $F'\mathbf{x} = N\mathbf{x}^*$ is a vector of order $v \times 1$.

With these two suggested conversions, $I(\beta) = \mathbf{x}^{*'}[2(v-1)I - N'N]\mathbf{x}^*$ where $\mathbf{x}^*$ is a vector of b components $(x_1^*, x_2^*, \dots, x_b^*)$ with elements not necessarily all distinct.

Naturally, the class of choices of the design parameters encompasses all choices of $\mathbf{x}^*$ subject to $-1 \le x^*_{min} < x^*_{max} \le 1$. Here, N is the treatment $\times$ block incidence matrix involving elements 0 and 1 where the b blocks are arranged in dictionary style. Note that since $b = \binom{v}{2}$, each treatment is replicated exactly $(v-1)$ times in the entire design. The problem is thus to make an 'optimal' choice of the $\mathbf{x}^*$-vector with elements not necessarily distinct. We have resolved this problem - rather non-trivially. We do not know if a simpler approach exists.

For the rest of the paper, we will revert back to the notation of x from x^* so that x-values are not necessarily distinct and there are $b = v_{c_2}$ pairs of treatments attached to the x-values. Not to obscure the essential steps of reasoning, we will go through the following steps. Essentially, we claim that for every $v > 2$, there is an optimal choice of the x-values across all the b pairs of treatments, and that these are located at the extreme points, viz., -1 and 1. The specific allocations depend on the nature of v and we distinguish among

Case 1. $v = 4t$
Case 2. $v = 4t+1$
Case 3. $v = 4t+2$
Case 4. $v = 4t+3$.

First note that for $t = 2$, $I(\beta)$ reduces to $Q(\mathbf{x})/r$ where $Q(\mathbf{x}) = [\mathbf{x}'(2rI - N'N)\mathbf{x}]$ and $r = v - 1$. Towards maximization of $I(\beta)$, we may and will ignore the divisor r and work only with $Q(\mathbf{x})$. The following lemmas are easy to establish and we defer the proofs to Appendix A.

Lemma 2. Let $Q(\mathbf{x}) = \mathbf{x}'(kI - N'N)\mathbf{x}$ be a quadratic form where k is a positive constant and all the diagonal elements of the matrix $N'N$ are equal to a constant $d \le k$. Then maximum of $Q(\mathbf{x})$ with restriction on elements x_i, that $-1 \le x_i \le 1$, is attained at a vector $\mathbf{x}_0$ with each element ± 1.

Lemma 3. For any vector $\mathbf{x}$ with elements ± 1, $Q(\mathbf{x})$ is a multiple of 8.

Lemma 4. Let v be even. Then for every vector $\mathbf{x}$ with each element ± 1, the value of $\mathbf{x}'N'N\mathbf{x} \ge v$.

In view of Lemma 2, there exists a vector $\mathbf{x}_0$ having each element ± 1 that maximizes $Q(\mathbf{x})$. Therefore $Q(\mathbf{x}_0) = 2rb - \mathbf{x}_0'N'N\mathbf{x}_0 = PRU - \mathbf{x}_0'N'N\mathbf{x}_0$, where $PRU = 2rb$. Notice that $Q(\mathbf{x}_0) \le PRU$ and equality occurs if and only if $\mathbf{x}_0'N'N\mathbf{x}_0 = 0$. In view of Lemma 4, when v is even $\mathbf{x}_0'N'N\mathbf{x}_0 \ge v$. Therefore, in this case $Q(\mathbf{x}_0) \le PRU - v$. And in view of Lemma 3, when v is of the form $4t + 3$, PRU is not a multiple of 8 but a multiple of 4. Therefore, in this case $Q(\mathbf{x}_0) \le PRU - 4$. Thus we have,

Theorem 1. $Q(\mathbf{x}_0) \le PRU - v$ for the even values of v and $Q(\mathbf{x}_0) \le PRU - 4$ for the values of v of the form $4t + 3$. Further, $Q(\mathbf{x}_0) \le PRU$, for the values of v of the form $4t + 1$.

It is shown below by construction, that for each value of $v \geq 4$ there exists a vector $\mathbf{x}_0$ such that equality holds in the above theorem. This vector is constructed in two stages. First we get an eigen vector $\mathbf{x}$ corresponding to the eigenvalue $2r$ of the matrix $(2rI - N'N)$ that may contain some zero elements in addition to $+1$ and -1. Then we replace the zero elements of $\mathbf{x}$ with $+1$ or -1 to get $\mathbf{x}_0$. Towards this, note that $Q(\mathbf{x})$ being a quadratic form its maximum value is $M(\mathbf{x}'\mathbf{x})$ where M is maximum eigenvalue of $(2rI - N'N)$ and $\mathbf{x}$ is an eigen vector (with the restriction) corresponding to M such that $(\mathbf{x}'\mathbf{x})$ is maximum. As $N'N$ is positive semi-definite matrix its minimum eigenvalue is zero and hence maximum eigenvalue of $(2rI - N'N)$ is $2r$. That is, $M = 2r$. It is easy to show that there is always an eigen vector corresponding to M with elements in the set $-1, 0, 1$. Clearly, the maximum of $Q(\mathbf{x})$ is $2rb = v(v-1)^2$, attained when $\mathbf{x}'\mathbf{x} = b$, that is, each element of $\mathbf{x}$ is ± 1 and $\mathbf{x}'N'N\mathbf{x} = 0$. This maximum value $v(v-1)^2$ is denoted by PRU. In general, there may not be any such eigen vector $\mathbf{x}$ with each element as ± 1, in which case, PRU is not attained.

Notice that $\mathbf{x}$ is an eigen vector of $(2rI - N'N)$ corresponding to $2r$ if and only if $N\mathbf{x}$ is null vector and this implies $\mathbf{e}'\mathbf{x} = 0$. Now, let $\mathbf{x}$ be the eigen vector of $(2rI - N'N)$ corresponding to $2r$. Construction of a vector $\mathbf{x}$ such that $N\mathbf{x} = \phi$ for the values of v of the form $4t, 4t+2, 4t+1$ and $4t+3$ is given below.

Theorem 2. Let $N_{v \times b}$ be as above. There exists a vector $\mathbf{x}_{b \times 1}$ such that $N\mathbf{x} = \phi$, that is, $\mathbf{x}$ is an eigen vector of $(2rI - N'N)$ corresponding to the eigenvalue $2r$ such that

1. when v is even, that is of the form $4t$ or $4t+2$, the vector $\mathbf{x}$ has $v/2$ zero elements.

2. when v is of the form $4t+1$, the vector $\mathbf{x}$ has no zero elements.

3. when v is of the form $4t+3$, the vector $\mathbf{x}$ has 3 zero elements.

Proof. We construct a vector $\mathbf{x}$ of b elements as follows. Consider $\mathbf{x}$ as a vector of $v-1$ partitioned 'blocks' of sizes $v-1, v-2, \cdots, 2, 1$ such that the i^{th} partitioned block contains i elements in the natural order, following dictionary style.

Block No. and size	$v-1$	$v-2$	$\cdots$	2	1
$x' =$			$\cdots$		

Case 1. When v is even, that is, v is of the form $4t$ or $4t+2$.
Step 1: For each odd sized block, put zero as the first element and -1 and $+1$ alternately till the end of block. Notice that there are $v/2$ odd sized blocks.
Step 2: For each even sized block, put $+1$ and -1 alternately till the end of block.

Example 1. Let $v = 8$. Then $b = 28$. So $\mathbf{x}'$ is written as 7 blocks.

Block No.	7	6	$\cdots$	2	1
$x' =$	0 -1 +1 -1 +1 -1 +1	+1 -1 +1 -1 +1 -1	$\cdots$	+1 -1	0

Example 2. Let $v = 6$. Then $b = 15$. So $\mathbf{x}'$ is written as 5 blocks.

Block No.	5	4	3	2	1
$x' =$	0 -1 +1 -1 +1	+1 -1 +1 -1	0 -1 +1	+1 -1	0

Case 2. When v is of the form $4t + 1$.

In this case $v-1$ is even and $(v-1)/2$ is also even. Let $\mathbf{x}$ be the vector constructed as above for the even case of $4t$. Starting from block 1 replace each zero element of $\mathbf{x}$ alternately with $+1$ and -1. Let the resulting vector be $\mathbf{y}$ which is of order $4t \times 1$. Construct the new vector $\mathbf{x}$ as $\mathbf{x}' = (-\mathbf{y}'N' : \mathbf{y}')$ where N is the incidence matrix corresponding to the case of $v = 4t$.

Example 3. Let $v = 9$, that is of the form $4t + 1$. Then $b = 36$. So $\mathbf{x}'$ is written as 8 blocks. Here we use the vector constructed in example 1.

Block No.	8	7	$\cdots$	2	1
$x' =$	+1 +1 -1 -1 +1 +1 -1 -1	-1 -1 +1 -1 +1 -1 +1	$\cdots$	+1 -1	1

Case 3. When v is of the form $4t + 3$.
In this case $v - 1$ is even and $(v - 1)/2$ is odd. Let $\mathbf{x}$ be the vector constructed as above for the case of $4t + 2$. Starting from block 1 replace each zero element of $\mathbf{x}$ alternately with $+1$ and -1 except the $(v-1)^{th}$ block. Let the resulting vector be $\mathbf{y}$. Construct the new vector $\mathbf{x}$ as $\mathbf{x}' = (-\mathbf{y}'N' : \mathbf{y}')$. It is easy to check that 3 elements (first, second and v^{th} elements) of $\mathbf{x}$ are zeros and the rest of the elements are ± 1.

Example 4. Let $v = 7$, that is of the form $4t + 3$. Then $b = 21$. So $\mathbf{x}'$ is written as 6 blocks. Here we use the vector constructed in example 2.

Block No.	6	5	4	3	2	1
$x' =$	0 0 +1 +1 -1 -1	0 -1 +1 -1 +1	+1 -1 +1 -1	-1 -1 +1	+1 -1	1

In all the above cases it is easy to check that $N\mathbf{x} = \phi$. For these constructed vectors the following table gives the values of $Q(\mathbf{x})$.

Table 2

v	$x'x$	$Q(x)$	
$4t$	$b - v/2$	$2(v-1)(b-v/2)$	$PRU - v(v-1)$
$4t+1$	b	$2(v-1)b$	PRU
$4t+2$	$b - v/2$	$2(v-1)(b-v/2)$	$PRU - v(v-1)$
$4t+3$	$b - 3$	$2(v-1)(b-3)$	$PRU - 6(v-1)$

It is readily seen that only in the case of $v = 4t + 1$, the constructed $\mathbf{x}$-vector has all elements ± 1. Except for this case, in all other cases, we will suggest appropriate conversion of $\mathbf{x}$ by suitably replacing 0's by ± 1's. For the case $v = 4t + 3$ we take the vector $\mathbf{x}$ constructed above, replace the 3 zero elements (first, second and v^{th} elements) of $\mathbf{x}$, with $+1$, $+1$ and -1. Denoting the resulting vector by $\mathbf{x}_0$, it is easy to see that only the first element of $N\mathbf{x}_0$ is 2 and the rest of the elements are zeros. Hence $\mathbf{x}_0'N'N\mathbf{x}_0 = 4$. When v is even, starting from block 1 replace all the $v/2$ zero elements of $\mathbf{x}$ with $+1$ and -1 alternately. Denoting the resulting vector by $\mathbf{x}_0$, it is easy to check that each element of $N\mathbf{x}_0$ is ± 1. Hence $\mathbf{x}_0'N'N\mathbf{x}_0 = v$. Therefore, we have established that

$Q(\mathbf{x}_0) = PRU - v$, if v is even, that is, v is of the form $4t$ or $4t+2$.
$Q(\mathbf{x}_0) = PRU$, if v is of the form $4t+1$.
$Q(\mathbf{x}_0) = PRU - 4$, if v is of the form $4t+3$.
As per Theorem 1, $\mathbf{x}_0$ constructed above depending on the value of v, maximizes $Q(\mathbf{x})$.

A Table showing the values of $Q(\mathbf{x}_0)$ covering $v = 4$ *to* 17 is given later. Explicit solutions to the optimal allocation designs for the cases of $v = 6, 7, 8, 9$ are given Appendix B.

4 Generalization

In this section we consider the same problem but with distinct triplets of treatments instead of pairs of treatments. We write $p = \binom{v-1}{2}$ and $c = \binom{v}{3}$. Further we denote by N_v the incidence matrix of order $v \times \binom{v}{2}$ for the case of pairs of treatments considered in Section 2 and denote by M_v the incidence matrix of order $v \times \binom{v}{2}$ for the case of triplets of treatments. Similarly, we denote by $\mathbf{x}_v$ the vector constructed in Section 2 that maximizes $Q(\mathbf{x})$ of Section 2. It is easy to verify the function to be maximized in the case of triplets is $T(\mathbf{y}_v) = \mathbf{y}_v'(3pI - M_v'M_v)\mathbf{y}_v$, where $\mathbf{y}_v$ denotes the vector of order $c \times 1$ of covariate levels with each element in the interval $[-1, 1]$. Notice that the maximum value $T(\mathbf{y}_v)$ can attain is $3pc$, attained if and only if $M_v\mathbf{y}_v = \phi$. The following table gives the values of the scalar $\mathbf{e}_v'\mathbf{x}_v$ and the vector $N_v\mathbf{x}_v$ of order $v \times 1$ for different values of v.

Table 3

v	$\mathbf{e}_v'\mathbf{x}_v$	$(N_v\mathbf{x}_v)'$	Description
$4t$	0	$(-\mathbf{e}_2' : \mathbf{e}_2' : -\mathbf{e}_2' : \cdots : \mathbf{e}_2')$	$-\mathbf{e}_2'$ and $\mathbf{e}_2'$ occur alternately
$4t+1$	0	$(\ 0 : \ 0 : \ 0 : \cdots : \ 0)$	All elements are zero
$4t+2$	1	$(\ \mathbf{e}_2' : -\mathbf{e}_2' : \mathbf{e}_2' : \cdots : \mathbf{e}_2')$	$\mathbf{e}_2'$ and $-\mathbf{e}_2'$ occur alternately
$4t+3$	1	$(\ 2 : \ 0 : \ 0 : \cdots : \ 0)$	All elements are zero except the first which is 2

The proofs of the following two lemmas are on the same lines of proofs of Lemma 2 and Lemma 4.

Lemma 5. Maximum of $T(\mathbf{y})$ is attained at a vector $\mathbf{y}$ with each element ± 1.

Lemma 6. Let p be odd, that is, $v = 4t$ or $4t+3$. Then for every vector $\mathbf{y}_v$ with each element ± 1, the value of $\mathbf{y}'M'M\mathbf{y} \geq v$.

Now we are ready to state the main result of this section.

Theorem 3. For $v > 4$, the vector that maximizes $T(\mathbf{y}_v)$ is given by

$$\mathbf{y}_v = (\mathbf{x}'_{v-1} : \mathbf{y}'_{v-1})' \text{ when } v = 4t+3 \text{ and } \mathbf{y}_v = (-\mathbf{x}'_{v-1} : \mathbf{y}'_{v-1})' \text{ in other cases}$$

with $\mathbf{y}_4 = (1 \;\; 1 \;\; -1 \;\; -1)'$.

Proof. Notice that M_v and hence $M_v\mathbf{y}_v$ are given by

$$M_v = \begin{bmatrix} \mathbf{e}'_{v-1} & \phi' \\ N_{v-1} & M_{v-1)} \end{bmatrix} \;\; and \;\; M_v\mathbf{y}_v = \begin{bmatrix} \pm\mathbf{e}'_{v-1}\mathbf{x}_{v-1} \\ \pm N_{v-1}\mathbf{x}_{v-1} + M_{v-1}\mathbf{y}'_{v-1} \end{bmatrix}$$

Using the above expression, it is easy to check that the values of $M_v\mathbf{y}_v$ are as in the following table.

Table 4

v	$(M_v\mathbf{y}_v)'$	*description*
$4t$	$(-\mathbf{e}'_2 : \mathbf{e}'_2 : -\mathbf{e}'_2 : \cdots : \mathbf{e}'_2)$	$-\mathbf{e}'_2$ *and* $\mathbf{e}'_2$ *occur alternately*
$4t+1$	$(\;0 : \;\; 0 : \;\; 0 \; : \cdots : \;\; 0)$	*All elements are zero*
$4t+2$	$(\;0 : \;\; 0 : \;\; 0 \; : \cdots : \;\; 0)$	*All elements are zero*
$4t+3$	$(1 : \; \mathbf{e}'_2 : -\mathbf{e}'_2 : \mathbf{e}'_2 : \cdots : \mathbf{e}'_2)$	*First element is* 1*and then* $\mathbf{e}'_2$ *and* $-\mathbf{e}'_2$ *alternate*

This results in $\mathbf{y}'_vM'_vM_v\mathbf{y}_v = 0$ in case of $v = 4t+1$ or $4t+2$ and $\mathbf{y}'_vM'_vM_v\mathbf{y}_v = v$ in case of $v = 4t$ or $4t+3$. Hence $\text{Max}T(\mathbf{y}) = 3pc$, for $t = 4t+1$ or $4t+2$ and $\text{Max}T(\mathbf{y}) = 3pc - v$ for $t = 4t$ or $4t+3$ at the above constructed $\mathbf{y}_v$.

Remark. In general the vector x_v that maximizes $Q(x)$ of section 2 is not unique and so in the construction of vector y_v only x_v constructed should be used.

The following table gives the maximum values of $Q(\mathbf{x}_v)$ and $T(\mathbf{y}_v)$ for the values of $v = 4$ *to* 17. Herein PRU2 and PRU3 refer to the maximum possible values of $Q(\mathbf{x})$ and $T(\mathbf{y})$ respectively.

Table 5

v	r	b	$2rb = (PRU2)$	Max$Q(\mathbf{x}_v)$	p	c	$3pc = (PRU3)$	Max$T(\mathbf{y}_v)$
4	3	6	36	32	3	4	36	32
5	4	10	80	80	6	10	180	180
6	5	15	150	144	10	20	600	600
7	6	21	252	248	15	35	1575	1568
8	7	28	392	384	21	56	3528	3520
9	8	36	576	576	28	84	7056	7056
10	9	45	810	800	36	120	12960	12960
11	10	55	1100	1096	45	165	22275	22264
12	11	66	1452	1440	55	220	36300	36288
13	12	78	1872	1872	66	286	56628	56628
14	13	91	2366	2352	78	364	85176	85176
15	14	105	2940	2936	91	455	124215	124200
16	15	120	3600	3584	105	560	176400	176384
17	16	136	4352	4352	120	680	244800	244800

5 Concluding Observations

The formulation of the problem considered here is a bit different from that usually adopted in covariates studies involving treatment designs. Usually, the experimenter has the flexibility of choice of the quantitative covariate X for every single application of any of the v treatments under consideration. That gives rise to $[(y_{ij}; x_{ij})]$ type of data. This seems to raise a concern for increase in the cost of experimentation since the labeling of the covariate-values may undergo constant and uncontrolled changes over the entire operation of the treatment-replicated experiments! In order to avoid such scenarios, the experimenter is constrained to 'generate' observations in pairs as far as possible. We also considered briefly the generalization in the sense of generating data in 'triplets' of the treatments under consideration.

Even in the context of paired treatment scenario, consider a related problem. As before, we start with v treatments but there is a restriction of generating paired data only on a subset of $\binom{v}{2}$ treatment pairs. Given the subset, what would be the optimal allocation of x-values for most efficient estimation of the β-parameter? And, further to this, what would be the optimal subset selection and related optimal allocation of x-values for a given number of distinct treatment pairs to be covered in the experiment? These seem to be difficult issues. We believe Lemma 2 has the potential for necessary generalization to address such issues.

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Appendix A. Proofs of Lemmas 2–4

Proof of Lemma 2. Writing $\mathbf{x}$ as $(\mathbf{y} + x_i\mathbf{e}_i)$ and $N'N$ as $(dI + M)$ where d is the common diagonal element of $N'N$, we have

$$\begin{aligned} Q(\mathbf{x}) &= \mathbf{x}'(kI - N'N)\mathbf{x} \\ &= (\mathbf{y} + x_i\mathbf{e}_i)'(kI - N'N)(\mathbf{y} + x_i\mathbf{e}_i) \\ &= \mathbf{y}'(kI - N'N)\mathbf{y} + x_i^2(k-d) - 2x_i(\mathbf{y}'N'N\mathbf{e}_i) \\ &= \mathbf{y}'(kI - N'N)\mathbf{y} + x_i^2(k-d) - 2x_i(\mathbf{y}'(dI + M)\mathbf{e}_i) \\ &= \mathbf{y}'(kI - N'N)\mathbf{y} + x_i^2(k-d) - 2x_i(\mathbf{y}'M\mathbf{e}_i) \\ &= \mathbf{y}'(kI - N'N)\mathbf{y} + x_i^2(k-d) - 2x_i((\mathbf{x} - \mathbf{e_i x_i})'M\mathbf{e}_i) \\ &= \mathbf{y}'(kI - N'N)\mathbf{y} + x_i^2(k-d) - 2x_i(\mathbf{x}'M\mathbf{e}_i) \\ &= \mathbf{y}'(kI - N'N)\mathbf{y} + [x_i^2(k-d) - 2x_i(M\mathbf{x})_i] \end{aligned}$$

Now, the first term is independent of x_i and it is easy to see that the value of the second term will increase if we choose x_i as ± 1 with the sign opposite to that of $(M\mathbf{x})_i$. It must be noted that $(M\mathbf{x})_i$ dependents on other x_j's and is indeed independent of x_i. Hence the claim.

Proof of Lemma 3. As each element of $\mathbf{x}$ is ± 1, permute it so that all $+1$ elements are at the top and denote the transpose of this vector as $(\mathbf{e}'_u : -\mathbf{e}'_w)$, where u is the number of positive elements and w is the number of negative elements. Permute and partition $N'N$ accordingly as $\begin{pmatrix} N_1 & N_3 \\ N'_3 & N2 \end{pmatrix}$ so that

$$\mathbf{x}'N'N\mathbf{x} = (\mathbf{e}'_u : -\mathbf{e}'_w)\begin{pmatrix} N_1 & N_3 \\ N'_3 & N2 \end{pmatrix}\begin{pmatrix} \mathbf{e}_u \\ -\mathbf{e}_w \end{pmatrix} = \mathbf{e}'_u N_1 \mathbf{e}_u + \mathbf{e}'_w N_2 \mathbf{e}_w - 2\mathbf{e}'_u N_3 \mathbf{e}_w$$

$$= t_1 + t_2 - 2t_3, say.$$

Also note that $t_1 + t_2 + 2t_3 = 2rb$. Therefore, from the above corollary, we have, $Q(\mathbf{x}) = \mathbf{x}'(2rI - N'N)\mathbf{x} = 2r(\mathbf{x}'\mathbf{x}) - \mathbf{x}'N'N\mathbf{x} = 2rb - \mathbf{x}'N'N\mathbf{x} = 4t_3$. Further, we also have, $t_1 + t_3 = 2(v-1)u$ which is even. Since t_1 is even, this implies t_3 is even. Thus $Q(\mathbf{x})$ is a multiple of 8.

Proof of Lemma 4. Let $\mathbf{y} = N\mathbf{x}$. Then $\mathbf{x}'N'N\mathbf{x} = \sum y_i^2$. So minimum of $\mathbf{x}'N'N\mathbf{x}$ is attained when each y_i^2 is minimum. Notice that when v is even, every y_i effectively reduces to an odd $(v-1)$ combination of $+1$s and -1s. Therefore minimum of $y_i^2 = 1$ and hence of $\mathbf{x}'N'N\mathbf{x} \geq v$.

Appendix B. Explicit solutions for Optimal Allocations Designs

The following two tables give the vectors $\mathbf{x}_v$ for $v = 4$ *to* 9 for the case of pairs of treatments and $\mathbf{y}_v$ for $v = 5$ *to* 8 for the case of triplets of treatments.

Table 6. $\mathbf{x}_v$ for $v = 4$ to 9 for the case of pairs of treatments

v=4	$\mathbf{x}_4$	v=5	$\mathbf{x}_5$	v=6	$\mathbf{x}_6$	v=7	$\mathbf{x}_7$	v=8	$\mathbf{x}_8$	v=9	$\mathbf{x}_9$
										12	-1
										13	-1
										14	1
										15	1
										16	-1
										17	-1
										18	1
										19	1
								12	-1	23	1
								13	-1	24	-1
								14	1	25	1
								15	-1	26	-1
								16	1	27	1
								17	-1	28	-1
								18	1	29	1
						12	1	23	1	34	1
						13	1	24	-1	35	-1
						14	-1	25	1	36	1
						15	-1	26	-1	37	-1
						16	1	27	1	38	1
						17	1	28	-1	39	-1
				12	1	23	-1	34	1	45	-1
				13	-1	24	-1	35	-1	46	-1
				14	1	25	1	36	1	47	1
				15	-1	26	-1	37	-1	48	-1
				16	1	27	1	38	1	49	1
		12	1	23	1	34	1	45	1	56	1
		13	1	24	-1	35	-1	46	-1	57	-1
		14	-1	25	1	36	1	47	1	58	1
		15	-1	26	-1	37	-1	48	-1	59	-1
12	-1	23	-1	34	-1	45	1	56	-1	67	1
13	-1	24	-1	35	-1	46	-1	57	-1	68	-1
14	1	25	1	36	1	47	1	58	1	69	1
23	1	34	1	45	1	56	1	67	1	78	1
24	-1	35	-1	46	-1	57	-1	68	-1	79	-1
34	1	45	1	56	1	67	-1	78	1	89	-1

Table 7. $\mathbf{y}_v$ for $v = 5$ to 8 for the case of triplets of treatments

v=5	$\mathbf{y}_5$	v=6	$\mathbf{y}_6$	v=7	$\mathbf{y}_7$	v=8	$\mathbf{y}_8$
						123	-1
						124	-1
						125	1
						126	1
						127	-1
						128	-1
						134	1
						135	1
						136	-1
						137	1
						138	-1
						145	-1
						146	1
						147	-1
						148	1
						156	-1
						157	1
						158	-1
						167	-1
						168	1
						178	1
				123	1	234	1
				124	-1	235	-1
				125	1	236	1
				126	-1	237	-1
				127	1	238	1
				134	1	245	1
				135	-1	246	-1
				136	1	247	1
				137	-1	248	-1
				145	-1	256	-1
				146	-1	257	-1
				147	1	258	1
				156	1	267	1
				157	-1	268	-1
				167	1	278	1
		123	-1	234	-1	345	-1
		124	-1	235	-1	346	-1
		125	1	236	1	347	1
		126	1	237	1	348	1
		134	1	245	1	356	1
		135	1	246	1	357	1
		136	-1	247	-1	358	-1
		145	-1	256	-1	367	-1
		146	1	257	1	368	1
		156	-1	267	-1	378	-1
123	1	234	1	345	1	456	1
124	1	235	1	346	1	457	1
125	-1	236	-1	347	-1	458	-1
134	-1	245	-1	356	-1	467	-1
135	1	246	1	357	1	468	1
145	-1	256	-1	367	-1	478	-1
234	-1	345	-1	456	-1	567	-1
235	-1	346	-1	457	-1	568	-1
245	1	356	1	467	1	578	1
345	1	456	1	567	1	678	1

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