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Some Aspects of Optimal Covariate Designs in Factorial Experiments

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Abstract

Following Sinha *et al.* (2014), we initiate a study in the context of 2^n -factorial experiments involving the question of optimal allocation of covariate values. There is one controllable quantitative covariate and it is assumed to 'cover' two experimental units at a time. Earlier we dealt with block design set-up [Sinha *et al.* (2014)]. Here we take up 2^n -factorial set-up and address the question of optimal allocation of the covariate values. Results are illustrated for 2^2 - or 2^3 -factorial experiments.

Key words: Factorial experiments; Models with covariates; Optimal placement of covariate values.

1. Introduction

The key reference to this article is Sinha *et al.* (2014) dealing with a varietal design set-up. Here we start with a factorial experiment with the level-combinations having standard representations such as [(0,0), (0,1), (1,0), (1,1)] for a 2^2 experiment. There is a controllable covariate xattached to every experimental unit and x assumes values in the closed interval [-1,1]. However, every attempt towards choice and application of x necessarily 'covers' a pair of experimental units each time. Thus, for example, we may choose 2 units and apply the level combinations (0,0)and (0,1) and attach a value $x = x_1$ to each of these two units. The mean responses for the two underlying outputs $Y[(0,0); x_1]$ and $Y[(0,1); x_1]$ are assumed to be of the form $\tau(00) + \beta x_1$ and $\tau(01) + \beta x_1$ respectively. Naturally, the contrast $\tau(01) - \tau(00)$ is readily estimated.

Based on the $2^2 = 4$ level combinations, we may form 6 pairs of the above form and make use of $6 \times 2 = 12$ experimental units in pairs and thereby use 6 covariate values. All 'levelcombination contrasts' are trivially estimated and hence Main Effects and the 2-factor Interaction are unbiasedly estimated. We wish to provide unbiased estimate of the β -coefficient with utmost precision by suitable choice of the covariate values x's.

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Likewise, we may take up the case of 2^3 -factorial experiment and study similar optimality problem involving 28 *x*-values, all in the closed interval[-1, 1].

While we will develop the theory of optimization for the general case of 2^n -factorial experiment involving $2^{(n-1)}(2^n - 1)$ covariate-values, the cases of n = 2, 3 will serve as illustrative examples.

2. Optimal Choice of Covariate Values for 2ⁿ-factorial Design Set-up

For *n* factors, each at 2-levels, let $N = 2^n$ denote the total number of level combinations. Since the allocation of covariate-values is assumed to 'cover' a pair of experimental units each time, we let $c = \binom{N}{2}$ denote the number of covariates $x_i, i = 1, 2, \dots, c$ and X denote the $(c \times 1)$ vector $(x_1x_2\cdots x_c)'$. Now, it follows that $I(\beta)$ is a quadratic form in X and we denote it by a constant times Q(X).

Construction of the matrix of quadratic form:

 $I(\beta) = 2X'IX - [(c'_1X)^2 + \dots + (c'_NX)^2]/(N-1)$ = $(1/(N-1))X'\{2(N-1)I - [(c_1c'_1 + \dots + c_Nc'_N)]\}X = (1/(N-1))Q(X)$, where c_i is the coefficient vector of order $(c \times 1)$ of i^{th} constraint having (N-1) elements equal to 1 and the rest equal to 0.

Therefore each $c_i c'_i$ is a symmetric matrix of order $(c \times c)$ with only (N - 1) nonnull rows (columns) with each nonnull row (column) having (N - 1) elements equal to 1 and the rest of (c - N + 1) elements equal to 0.

Thus Q(X) = X'[2(N-1)I - M]X where $M = \sum c_i c'_i$.

Notice that M is a symmetric matrix of order $(c \times c)$ wherein each row (column) has diagonal element equal to 2, 2(N-2) elements equal to 1 and the rest of (c-2N+3) elements equal to 0.

In order to maximize Q(X) for optimal choice of X i.e., of the x_i 's, we argue, as in Sinha *et al.* (2014), that Q(X) is maximized only when the x's are each at the extremes i.e., +/-1. We skip the proof in general terms. However, we provide all the technical details below for the cases of n = 2, 3.

3. Optimal Choice of Covariate Values for 2^2 Factorial Design Set-up

We start with the following Table 1 of x-values :

Standard representation in the form $[Y, A\theta, \sigma^2 I]$ with

$$\theta = (\tau(00), \tau(01), \tau(10), \tau(11), \beta)'$$

suggests a form of the matrix A of order 12×5 and we partition it as usual to derive an expression for Information on β i.e., $I(\beta)$. For simplicity, we drop the multiplier σ^{-2} . It follows that

$$I(\beta) = 2\left(\sum x_i^2\right) - \left[(x_1 + x_2 + x_3)^2 + (x_1 + x_4 + x_5)^2 + (x_2 + x_4 + x_6)^2 + (x_3 + x_5 + x_6)^2\right]/3.$$

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x-values	level - combination(1)	level - combination(2)
x_1	(0,0)	(0,1)
x_2	(0, 0)	(1, 0)
x_3	(0,0)	(1, 1)
x_4	(0, 1)	(1, 0)
x_5	(0,1)	(1, 1)
x_6	(1,0)	(1,1)

Table 1

Optimality problem centers around optimal choice of the x's so as to maximize $I(\beta)$ when $-1 \le x_i, i = 1, 2, 3, 4, 5, 6 \le 1$.

It follows that $I(\beta)$ can be expressed as a constant times a quadratic form Q(X). $I(\beta) = X'[6I - M]X/3 = Q(X)/3$ where the matrix M with i^{th} column m_i is given in an explicit form as

	(m_1)	m_2	m_3	m_4	m_5	m_6
	2	1	1	m_4 1	1	0
	1	2	1	1	0	1
$M = \Sigma c_i c'_i =$	1	$\frac{2}{1}$	2	0	1	1
	1	1	0	2	1	1
	1	0	1	1	2	1
	0	1	1	1	1	2)

It turns out that a choice of the X's subject to the value of each of the expressions $(x_1 + x_2 + x_3)$, $(x_1 + x_4 + x_5)$, $(x_2 + x_4 + x_6)$, $(x_3 + x_5 + x_6)$ is +/-1; $x_i = +/-1$ serves the purpose and we achieve $I(\beta) = 32/3$. Specifically, one choice is

 $x_1 = -1, x_2 = +1, x_3 = -1, x_4 = -1, x_5 = +1, x_6 = +1$ which yields, for the partial sums, $(x_1 + x_2 + x_3) = -1, (x_1 + x_4 + x_5) = -1, (x_2 + x_4 + x_6) = +1, (x_3 + x_5 + x_6) = +1.$

We give a proof of the above claim below.

Lemma 1 : Let $X_0 = (x_1 x_2 \cdots x_c)'$ be the vector with elements in the interval [-1, +1] which maximizes Q(X) = X'(tI - M)X, where $t \ge max(m_{ii})$ is a positive constant. Then each component x_i of X_0 is +/-1.

Proof: Write $X_0 = U_i + x_i e_i$ where e_i is the i^{th} column of I. Then $Q(X_0) = (U_i + x_i e_i)'(tI - M)(U_i + x_i e_i) = U'_i(tI - M)U_i + x_i^2(t - m_{ii}) + 2x_iU'_i(tI - M)e_i$ $= U'_i(tI - M)U_i + x_i^2(t - m_{ii}) + 2x_iU'_i(-M)e_i = p_i + (t - m_{ii})x_i^2 + 2x_iq_i$, where $p_i = U'_i(tI - M)U_i$ and $q_i = -U'_iMe_i = -U'_im_i$ do not involve x_i . Now it is clear that for $Q(X_0)$ to be maximum the value of x_i should be +/-1 with sign as that of the constant q_i . In case $q_i = 0$, x_i can be given any of +1 or -1.

Algorithm: Start with $U_0 = \phi$. For $i = 1, 2, \dots, c$, in i^{th} step, calculate $q_i = -U'_{i-1}m_i$. Replace *ith* element of U_{i-1} with +/-1, the sign being that of q_i and denote this new vector by U_i . If $q_i = 0$ then any sign can be chosen. Add $|q_i|$ to q_i . Increase i by 1 and repeat.

After c steps, check the vector $X = U_c$ is a vector which maximizes Q(X) or not.

The following lemma is useful for checking whether the vector computed using above algorithm maximizes Q(X) or not.

Lemma 2 : Starting with $U_0 = \phi$, the final vector U_c obtained after c steps of above algorithm maximizes Q(X) if and only if $2q=2\Sigma|q_i|=\Sigma m_{ii}-N$.

Proof: Let Q_i denote $Q(U_i)$, for $i = 1, 2, \dots, c$. Notice that at i^{th} step $Q_i = Q_{i-1} + (t - m_{ii})x_i^2 + 2x_iq_i$. Hence the increment at i^{th} step is $(t - m_{ii})x_i^2 + 2x_iq_i$. Thus $Q_c = \sum ((t - m_{ii})x_i^2 + 2x_iq_i) = t \times c - \sum m_{ii} + 2 \times \sum |q_i|$. Comparing this with the maximum value $t \times c - N$ of Q(X), we get the required result.

For n = 2, N = 4, c = 6, t = 6, each $m_{ii} = 2$ and $\Sigma |q_i| = 4$ (from the table). Therefore, $2\Sigma |q_i| = 8 = \Sigma m_{ii} - N$. Hence $Q(U_c)$ maximizes Q(X).

In order to achieve the solution, it is now a matter of verification of the conditions

 $(u_1 + u_2 + u_3) = (u_1 + u_4 + u_5) = (u_2 + u_4 + u_6) = (u_3 + u_5 + u_6) = +/-1; x_i = +/-1.$

Example: For the case n = 2, the successive U vectors along with k_2 values are as follows:

q_i	0	-1	0	0	-1	2
U_0	U_1	U_2	U_3	U_4	U_5	U_6
0	1	1	1	1	1	1
0	0	-1	-1	-1	-1	-1
0	0	0	1	1	1	1
0	0	0	0	-1	-1	-1
0	0	0	0	0	-1	-1
0	0	0	0	0	0	1

The first row gives the values of $q_i = -U'_{i-1}m_i$, for $i = 1, 2, \dots, c$, and the last column displays the optimum choice of U since the conditions are readily verified to hold. For the first step when $q_1 = 0$, we chose the value +1 for the first element of U_1 . Next step $q_2 = -1$

and we take the second element of $U_2 = -1$. For the third step, $q_3 = 0$ and we choose the third element of $U_3 = 1$ and so on. The solution is not unique though. For example, another choice of the final vector is (1 - 1 1 1 - 1 1) which also maximizes Q(x).

4. Optimal Choice of Covariate Values in A 2³ Factorial Experiment

We now discuss similar result for the case of 2^3 factorial experiment. A version of Table 1 would be Table 2 as shown below. This time the matrix A is of order 28×9 and $I(\beta)$ is given by the expression [again ignoring σ^{-2}]

$$I(\beta) = 2\sum_{i} x_{i}^{2} - [(x_{1} + x_{2} + \dots + x_{7})^{2} + \dots + (x_{7} + x_{13} + x_{18} + x_{22} + x_{25} + x_{27} + x_{28})^{2}]/7$$

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It turns out that $I(\beta)$ attains its maximum value of 56 - 8/7 = 384/7 for a choice of the x's at the extreme values +/-1 subject to

One such (optimal) choice is given in the same Table 2.

The realized values of various partial sums of the x's corresponding to the above solution to the x's are given below.

5. Proof of Claim for 2^3 **Case**

The expression for Q(x) given for 2^2 factorial set-up generalizes itself naturally to the case of 2^3 factorial set-up and is given by $I(\beta) = X'[14I - M]X/7 = Q(X)/7$ where all the diagonal elements of the matrix M are each equal to 2 while its off-diagonal elements are a known combination of 0s and 1s. The Lemma 1 and the algorithm stated above both work in this set-up as well. In the above, we have given one solution and there are other solutions too.

Table 3 gives the matrix M along with the final vector U_c (obtained using the above algorithm with initial vector as null vector), the values of q_i and $|q_i|$. Q(X) attains maximum at X = U.

For n = 3, N = 8, c = 6, t = 14, each $m_{ii} = 2$ and $\Sigma |q_i| = 24$ (from the table). Therefore, $2\Sigma |q_i| = 48 = \Sigma m_{ii} - N$. Hence U_c maximizes Q(X).

For the choice vector displayed above, various partial sums, as realized, are shown below.

· 7		1 1 1 (2)	
generic $x - values$		level - combination(2)	optimal x - values
x_1	(0,0,0)	(0, 0, 1)	-1
x_2	(0, 0, 0)	(0,1,0)	-1
x_3	(0, 0, 0)	(0,1,1)	-1
x_4	(0,0,0)	(1, 0, 0)	-1
x_5	(0, 0, 0)	(1, 0, 1)	1
x_6	(0, 0, 0)	(1, 1, 0)	1
x_7	(0, 0, 0)	(1, 1, 1)	1
x_8	(0, 0, 1)	(0, 1, 0)	1
x_9	(0, 0, 1)	(0,1,1)	1
x_{10}	(0, 0, 1)	(1,0,0)	1
x_{11}	(0, 0, 1)	(1, 0, 1)	1
x_{12}	(0, 0, 1)	(1, 1, 0)	-1
x_{13}	(0, 0, 1)	(1, 1, 1)	-1
x_{14}	(0, 1, 0)	(0,1,1)	-1
x_{15}	(0, 1, 0)	(1, 0, 0)	-1
x_{16}	(0, 1, 0)	(1, 0, 1)	-1
x_{17}	(0, 1, 0)	(1, 1, 0)	1
x_{18}	(0, 1, 0)	(1, 1, 1)	1
x_{19}	(0, 1, 1)	(1, 0, 0)	1
x_{20}	(0, 1, 1)	(1, 0, 1)	1
x_{21}	(0, 1, 1)	(1, 1, 0)	1
x_{22}	(0, 1, 1)	(1, 1, 1)	-1
x_{23}	(1, 0, 0)	(1, 0, 1)	-1
x_{24}	(1, 0, 0)	(1, 1, 0)	-1
x_{25}	(1, 0, 0)	(1, 1, 1)	1
x_{26}	(1, 0, 1)	(1, 1, 0)	-1
x_{27}	(1, 0, 1)	(1, 1, 1)	1
x_{28}	(1, 1, 0)	(1, 1, 1)	-1

Table 2

(000):	$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 =$	1,
(001):	$x_1 + x_8 + x_9 + x_{10} + x_{11} + x_{12} + x_{13} =$	1,
(010):	$x_2 + x_8 + x_{14} + x_{15} + x_{16} + x_{17} + x_{18} =$	1,
(011):	$x_3 + x_9 + x_{14} + x_{19} + x_{20} + x_{21} + x_{22} =$	1,
(100):	$x_4 + x_{10} + x_{15} + x_{19} + x_{23} + x_{24} + x_{25} =$	1,
(101):	$x_5 + x_{11} + x_{16} + x_{20} + x_{23} + x_{26} + x_{27} =$	1,
(110):	$x_6 + x_{12} + x_{17} + x_{21} + x_{24} + x_{26} + x_{28} =$	1,
(111):	$x_7 + x_{13} + x_{18} + x_{22} + x_{25} + x_{27} + x_{28} =$	

It may be seen that this solution is different from the one shown earlier.

Table 3

/	
$ q_i $	0 - 0 - 0 - 0 0 m 0 m 0 m 0 - 0 - 0 0 m 0 m
q_i	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
U_c	
28	000000000000000000000000000000000000000
27	000000000000000000000000000000000000000
26	
25	
24	0 0 1 0 1 0 0 0 1 0 1 0 1 0 1 0 1 0 1 0
23	0 0 1 1 1 7 0 0 0 1 1 0 0 0 1 1 0 0 0 0
22	
21	
20	0
19	0 0 0 1 1 1 1 1 7 0 0 0 1 1 0 0 0 0 1 1 0 0 0 0
18	0 - 0 0 0 0 0 0
17	
16	0 0 0 - 0 0 - 0 0 0 0 -
15	0 - 0 0 0 0 - 0
14	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
13	
12	- 0 - 0 - 0 0 0 - 0
11	
10	
6	- 0 - 0 0 0 0 - 7 0 0 0
∞	
7	
6	
5	
4	
ŝ	
5	
1	000000000000000000000000000000000000000
	28 2 2 5 2 5 2 5 1 5 1 5 1 5 1 5 1 5 1 5 1

x-values	level - combination(1)	level - combination(2)	level - combination(3)
x_1	(0, 0)	(0, 1)	(1,0)
x_2	(0,0)	(0, 1)	(1,1)
x_3	(0,0)	(1, 0)	(1,1)
x_4	(0, 1)	(1,0)	(1,1)

Table 4

6. Generalization to 'triplets'

We now contemplate a situation when every single application of the covariate value x encompasses three experimental units i.e., 'covers the eu's in triplets'. What would be the optimal choice of covariate values for most efficient estimation of the β co-efficient ? We study the cases of 2^2 and 2^3 factorials in this section.

(A) The case of 2^2 factorial

It follows that we need 4 covariate-values x_1, x_2, x_3, x_4 as are indicated in the Table 4 below.

It transpires that $I(\beta)$ has the representation

$$I(\beta) = 3\sum_{i} x_{i}^{2} - [(T - x_{1})^{2} + (T - x_{2})^{2} + (T - x_{3})^{2} + (T - x_{4})^{2}]/3, T = \sum_{i} x_{i}^{2}$$

We readily find that $I(\beta) = [8 \sum x_i^2 - 2T^2]/3 \le 32/3$ with "=" if and only if T = 0; $x_i = +/-1$; i = 1, 2, 3, 4. Any contrast of order 4×1 involving +/-1's such as (1, 1, -1, -1) gives a solution.

(B) The case of 2^3 factorial

It follows that we need 56 covariate-values x_1, x_2, \ldots, x_{56} associated with the triplets of the level-combinations as are partially indicated in the Table 5 below.

In the above, we have displayed the first set of 21 x-values corresponding to the triplets starting with (0,0,0). Note that the second set of 15 x-values $[x_{22} - x_{36}]$ correspond to triplets starting with (0,0,1). Likewise, third set of 10 $[X_{37} - x_{46}]$ start with (0,1,0); fourth set of 6 $[x_{47} - x_{52}]$ start with (0,1,1); fifth set of 3 $[x_{53} - x_{55}]$ start with (1,0,0) and the last [sixth] set of a singleton starts with (1,0,1).

Next note that each triplet generates three observations and hence we have a total of $56 \times 3 = 168$ observations in the vector representation Y. Moreover, every x-value will have three replications. It transpires that $I(\beta)$ has the representation

$$I(\beta) = 3\sum x_i^2 - [T_1^2 + T_2^2 + \ldots + T_8^2]/21.$$

x-values	level - combination(1)	level - combination(2)	level - combination(3)
x_1	(0, 0, 0)	(0,0,1)	(0, 1, 0)
x_2	(0,0,0)	(0,0,1)	(0, 1, 1)
—	_	_	_
x_6	(0,0,0)	(0,0,1)	(1, 1, 1)
x_7	(0,0,0)	(0,1,0)	(0, 1, 1)
—	_	_	_
x_{11}	(0,0,0)	(0,1,0)	(1, 1, 1)
x_{12}	(0,0,0)	(0,1,1)	(1, 0, 0)
—	_	—	_
x_{15}	(0,0,0)	(0,1,1)	(1, 1, 1)
x_{16}	(0,0,0)	(1,0,0)	(1, 0, 1)
x_{17}	(0,0,0)	(1,0,0)	(1, 1, 0)
x_{18}	(0,0,0)	(1,0,0)	(1, 1, 1)
x_{19}	(0,0,0)	(1,0,1)	(1, 1, 0)
x_{20}	(0,0,0)	(1,0,1)	(1, 1, 1)
x_{21}	(0,0,0)	(1, 1, 0)	(1, 1, 1)

Table 5

There are eight level-combinations and therefore, eight T_i 's. Every T_i contains 21 terms and we demand it to assume the value +/-1. In the above expression, each T_i is a linear combination of x_i s. The Lemma holds true once again. Each x_i has to be necessarily +/-1. Now writing $T_i = c'_i x$ for $i = 1, 2, \dots, 8$, the following table gives the 8 these coefficient vectors c_i , along with a solution vector X.

References

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Table 6

									17
1	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	X
1	1	1	1	0	0	0	0	0	1
2	1	1	0	1	0	0	0	0	-1
3	1	1	0	0	1	0	0	0	1
4	1	1	0	0	0	1	0	0	-1
$\frac{5}{6}$	1 1	1 1	0	0	$\begin{array}{c} 0 \\ 0 \end{array}$	$\begin{array}{c} 0 \\ 0 \end{array}$	1	0	$1 \\ -1$
0 7	1	$1 \\ 0$	$\begin{array}{c} 0 \\ 1 \end{array}$	$\begin{array}{c} 0 \\ 1 \end{array}$	0	0	$\begin{array}{c} 0 \\ 0 \end{array}$	$\begin{array}{c} 1 \\ 0 \end{array}$	-1 1
8	1	0	1		1	0	0	0	-1
9	1	0	1	0	0	1	0	0	-1
3 10	1	0	1	0	0	0	1	0	-1
10	1	0	1	0	0	0	0	1	1
12	1	0	0	1	1	0	0	0	-1
$12 \\ 13$	1	0	0	1	0	1	0	0	1
14	1	0	0	1	0	0	1	0	-1
15	1	0	0	1	0	0	0	1	1
16	1	0	0	0	1	1	0	0	-1
17	1	0	0	0	1	0	1	0	1
18	1	0	0	0	1	0	0	1	-1
19	1	0	0	0	0	1	1	0	1
20	1	0	0	0	0	1	0	1	-1
21	1	0	0	0	0	0	1	1	1
22	0	1	1	1	0	0	0	0	-1
23	0	1	1	0	1	0	0	0	1
24	0	1	1	0	0	1	0	0	-1
25	0	1	1	0	0	0	1	0	1
26	0	1	1	0	0	0	0	1	-1
27	0	1	0	1	1	0	0	0	1
28	0	1	0	1	0	1	0	0	-1
29	0	1	0	1	0	0	1	0	1
30	0	1	0	1	0	0	0	1	-1
31	0	1	0	0	1	1	0	0	1
32	0	1	0	0	1	0	1	0	-1
33	0	1	0	0	1	0	0	1	1
34	0	1	0	0	0	1	1	0	-1
35	0	1	0	0	0	1	0	1	1
36	0	1	0	0	0	0	1	1	-1
37	0	0	1	1	1	0	0	0	1
38	0	0	1	1	0	1	0	0	-1
39	0	0	1	1	0	0	1	0	1
40	0	0	1	1	0	0	0	1	-1
41	0	0	1	0	1	1	0	0	1
42	0	0	1	0	1	0	1	0	-1
43	0	0	1	0	1	0	0	1	1
44	0	0	1	0	0	1	1	0	-1
45 46	0	0	1	0	0	1	0	1	1
$\frac{46}{47}$	$\begin{array}{c} 0 \\ 0 \end{array}$	0	1	0	0	$\begin{array}{c} 0 \\ 1 \end{array}$	1	$\begin{array}{c} 1 \\ 0 \end{array}$	$-1 \\ -1$
48	0	0 0	0 0	1 1	1 1	$1 \\ 0$	$\begin{array}{c} 0 \\ 1 \end{array}$	0	-1
$40 \\ 49$	0	0	0	1	1	0	$1 \\ 0$	1	-1
$\frac{49}{50}$	0	0	0	1	$1 \\ 0$	1	1	$1 \\ 0$	-1 1
50	0	0	0	1	0	1	$1 \\ 0$	1	-1
$51 \\ 52$	0	0	0	1	0	0	1	1	-1
$\frac{52}{53}$	0	0	0	0	1	1	1	0	-1
$55 \\ 54$	0	0	0	0	1	1	0	1	1
55	0	0	0	0	1	0	1	1	-1
56	0	0	0	0	0	1	1	1	1
	v	~	~	~	~	-	-	-	-