

SMALL RESPONSE SURFACE DESIGNS

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ABSTRACT

Three level factorial designs are discussed that are suitable for small second order designs. The best choice of potential design points is discussed under the criterion of minimizing the generalized variance of the parameters in the model. Two methods are illustrated that yield designs with different resolution for the main effects and two factor interactions. Both methods involve the use of Partially Balanced Arrays. The Extended Partially Balanced Array is defined as a generalization of the Partially Balanced array.

Keywords: Response Surface Design; D-optimal Design; Saturated Design; Irregular Fractional Factorial Design; Partially Balanced Array

1. INTRODUCTION

We introduce relatively small subsets of the cubic region as the support sets for 3, 4, 5, 6, 7, 8, 9 and 10 factors. We also present some new designs that have higher D-efficiency than the ones previously published; they consist of PB1-arrays on 2^m augmented on the specified support sets. Furthermore, we define the Extended Partially Balanced Array (EPBA) as a generalization of PB1-array.

Throughout this paper, the quadratic response surface model (1.1) is of interest:

$$E(y) = \beta_0 + \sum \beta_i x_i + \sum \sum \beta_{ij} x_i x_j + \sum \beta_{ii} x_i^2 + e, \quad (1.1)$$

where $i = 1, \dots, m$, $j = 1, \dots, m$, $i > j$ and $p = 1 + 2m + m(m-1)/2$ is the number of parameters in the model.

As a criterion for good designs we used D-efficiency.

D-efficiency = $100 (|T' T|^{1/p} / N)$, where T is the design matrix.

It is the relative number of runs (in %) required by a possibly non-existent orthogonal design to achieve the same $|T' T|$.

Note that for a full quadratic saturated model $|T| = |T' T|^{1/2}$, where $T' T$ is the information matrix of order p .

Our objective was to identify:

- a) the support of the *saturated* D-optimal design. A saturated design has exactly as many runs (N) as the parameters (p) in the model ($N = p$).
- b) a class of designs that can be useful in constructing designs that are good under the D-optimal criterion, for any number of factors m .

Based on a theorem proved by Pesotchinsky (1975), we considered the partition of 3^m into $m + 1$ sets E_j , $j = 0, \dots, m$, such that E_j consists of all $2^j m! / (j! (m-j)!)$ points with j nonzero coordinates. We identified subsets $E_m \cup E_{j_1} \cup E_{j_2}$ ($j_2, j_3 \neq m$) of 3^m that support the saturated D-optimal design for $m = 3, 4, 5, 6, 7, 8$ and 9 and 10 factors (see Tables II, IV, V and VI).

As a summary, we concluded the following:

- D-optimal designs are supported on a subset $E_{j_1} \cup E_{j_2} \cup E_{j_3}$ of 3^m with $m \in \{j_1, j_2, j_3\}$. Using these set as support the search for a D-optimal design becomes more feasible.
- One can improve the D-efficiency of a design supported on $E_m \cup E_{j_2} \cup E_{j_3}$ ($j_2, j_3 \neq m$) by considering *less than n* design points from E_m .
- For $m = 3, 4, 5, 6, 7$, PB1-arrays, augmented on specified subsets $E_{j_1} \cup E_{j_2}$ ($j_1, j_2 \neq m$) of 3^m , yield good designs. These PB1-arrays are irregular fractions of 2^m factorial but their index has a predictable pattern. Thus, for any m , the class of PB1-arrays (supported on E_m), can be used to construct arrays that yield designs that are good under the D-optimal criterion.
- Designs with 'balanced' structure (Partially Balanced arrays, PB1-arrays) on E_m yielded designs with higher D-efficiency. PB1-arrays though do not exist for all N (runs) and m (factors). For $m > 7$ one can consider the following generalization of the PB1-array.

Definition 1.1 A $(0, 1)$ matrix $[T^{(1)}; T^{(2)}; \dots; T^{(q)}]$ of size $N \times (m_1 + m_2 + \dots + m_q)$, in which $T^{(k)}$ ($k = 1, 2, \dots, q$) are of size $N \times m_k$, is called an EPBA (Extended Partially Balanced Array) of strength $(t_1 + t_2 + \dots + t_q)$, size N , $m_1 + m_2 + \dots + m_q$ constraints, 2 levels and index set $\{\mu(i_1, i_2, \dots, i_q) \mid 0 \leq i_k \leq t_k, k = 1, 2, \dots, q\}$, written EPB1 $(N, m_1 + m_2 + \dots + m_q, 2, t_1 + t_2 + \dots + t_q, \{\mu(i_1, i_2, \dots, i_q)\})$, if for fixed values of $t_k (\leq m_k)$, every submatrix $[T_0^{(1)}; T_0^{(2)}; \dots; T_0^{(q)}]$ of size $N \times (t_1 + t_2 + \dots + t_q)$ is such that every $(0, 1)$ vector with weight i_k in $T_0^{(k)}$ occurs exactly $\mu(i_1, i_2, \dots, i_q)$ times as a row of $[T_0^{(1)}; T_0^{(2)}; \dots; T_0^{(q)}]$ where $T_0^{(k)}$ ($k = 1, 2, \dots, q$) are of size $N \times t_k$ and consist of t_k columns of $T^{(k)}$.

All computer algorithms were written in SAS[®] programming language. PROC FACTEX and PROC OPTEX were used as implemented in SAS/QC[®]. In particular, PROC FACTEX was used to generate the set of points of 3^m and Fedorov's algorithm in PROC OPTEX was used to identify saturated D-optimal designs. SAS/QC[®] software is a trademark of SAS Institute Inc.

2. METHODOLOGY

Farrell, Kiefer and Walbran (1967) described a method for obtaining *symmetric* optimum designs for each m on the union of three E_j sets. Symmetric designs have odd moments equal to zero. For large m such designs are quite unsatisfactory and one should consider asymmetric designs. The designs discussed here are not symmetric. In fact, the design points from E_m consist of an irregular fraction of 2^m .

We considered two approaches to identify a support set $E_{j1} \cup E_{j2} \cup E_{j3}$ of the D-optimal saturated design and the structure of such design. The first approach is more useful if unbiased estimation of all main effects and two factor interactions is of interest. However, the second approach yielded designs with improved D-efficiency.

2.1 First approach

Consider only designs with $n = 1 + m + m(m-1)/2$ points from E_m and the model (2.1) with main effects and two-way interactions only:

$$E(y) = \beta_0 + \sum \beta_i x_i + \sum \sum \beta_{ij} x_i x_j + e, \quad (2.1)$$

where $i = 1, \dots, m$, $j = 1, \dots, m$ and $i > j$. Note that the number of parameters in model (2.1) is equal to n .

The results from our computer analysis about the support sets are summarized in Table II for $m = 3, 4, 5, 6, 7$ and Table V for $m = 8, 9, 10$.

Having determined a set of candidate points $E_m \cup E_{j2} \cup E_{j3}$, next we obtained a 'good' design on E_m for $m = 3, 4, 5, 6, 7, 8, 9, 10$ first (using model 2.1). Then we augmented these designs on the specified support ($E_{j2} \cup E_{j3}$).

In general, the best designs found by this computer analysis were not unique. However, we focused on Partially Balanced arrays, since for $m = 3, 4$ and 5 , one design, among the best five computer generated designs, was consisting of a Partially Balanced array on E_m (Their parameters N, m, t and the index $\{\mu_i\}$ are given in Table I).

Chakravarti (1956) introduced the concept of Partially Balanced (or simply Balanced) array. Nishii

(1981) extended the concept of Partially Balanced array to Asymmetrical Balanced array. Kuwada and Kuriki (1986) studied a special case of the Asymmetrical Balanced array, the PB1-array.

Next, we observed that, if these arrays ($m = 3, 4, 5$) are viewed as Partially Balanced arrays of strength $t = 2$ and index $\{\mu_0, \mu_1, \mu_2\}$, there is a pattern in their index. It can be written in the following way:

Pattern 2.1

Let $[(n-2(m-1))/2] = c$, where $[a]$: integer part of a .

m = 3 {2, 2, 1}: { $c+1, m-1, c$ },

m = 4 {2, 3, 3}: { $c, m-1, c+1$ } or equivalently { $c+1, m-1, c$ } by interchanging 0 and 1.

m = 5 {4, 4, 4}: special case, { $c, m-1, c$ }, $c = m-1$ here.

We extended this pattern for $m = 6$ and 7 , excluding any singular arrays. We also considered Srivastava's (1971, 1975) optimal 2^m Partially Balanced arrays of resolution V for $m = 6, 7$. The following arrays performed better than the Partially Balanced arrays given by Srivastava (Srivastava's arrays are A-optimal).

m = 6 {5, 5, 7}: { $c-1, m-1, c+1$ } or equivalently { $c+1, m-1, c-1$ }.

m = 7 {8, 6, 9}: { $c, m-1, c+1$ } or equivalently { $c+1, m-1, c$ }.

For $m=6$, the parameters n, m, t and $\{\mu_i\}$ are given in Table I. As before, this array was augmented on the specified subset of 3^m (see Table II).

For $m = 7$, using Srivastava's existence conditions it can be shown that a Balanced array of strength $t = 2$ and index {8, 6, 9} does not exist for more than 5 factors. However, we constructed a PB1-array $[T^{(1)}; T^{(2)}]$, with $T^{(1)}$ having our 'predicted' pattern, in the following way. First, we constructed a Partially Balanced array $T^{(1)}$ with $N = 36$ runs, $m = 5$ factors, strength $t = 2$ and index {8, 6, 9}. $T^{(1)}$ is also a Partially Balanced array of strength $t = 4$ and index {3, 2, 1, 2, 4}. Next, we augmented to $T^{(1)}$ a Partially Balanced array $T^{(2)}$ with $N = 36$ runs, $m = 2$ factors, strength $t = 2$ and index {6, 6, 11}. The 'combined' array $T = [T^{(1)}; T^{(2)}]$ is a PB1-array with $N = 36$ runs, $m_1 = 5, m_2 = 2, t_1 = 4, t_2 = 2$ and two symbols. Its index $\{\mu(i_1, i_2)\}$ is given in Table I. As previously, T was augmented on a specified subset of 3^m (Table II).

Note that for $m=6, 7$ the best designs obtained by the computer procedure did not involve neither Partially Balanced nor PB1-arrays. However, the designs obtained by the above method had the same D-efficiency as the best computer generated design on the same support. The D-efficiency and support set for $m = 3, 4, 5, 6, 7$ factors are given in Table II. Note also that for $m=7$ a Partially Balanced array exists for $N= 29$ but it yields a design with lower D-efficiency.

2.2 Second Approach

Consider now model (1.1), the partition of 3^m into its subsets E_j and $m!/((3! (m-3)!)$ subsets of the form $E_{j_1} \cup E_{j_2} \cup E_{j_3}$.

In this approach, our computer search revealed that one should include a certain number of points from E_m , since the D-efficiency of the 'best' designs supported on $E_{j_1} \cup E_{j_2} \cup E_{j_3}$ with $m \notin \{j_1, j_2, j_3\}$ was always less than those supported on $E_{j_1} \cup E_{j_2} \cup E_{j_3}$ with $m \in \{j_1, j_2, j_3\}$. The results from this approach are summarized in Table IV ($m = 3, 4, 5, 6, 7$) and Table VI ($m = 8, 9$).

This computer analysis also revealed that higher D-efficiency can be achieved when less than n points are selected from E_m (see v in Table IV).

Note that the best designs, found by the above procedure, were not unique in general. Nevertheless, for $m = 3, 4$ and 5 , one among the best computer generated designs was consisting of the following arrays on E_m .

m = 3: PB1-array $T = [T^{(1)}; T^{(2)}]$ with $N = 6, m_1 = 2, m_2 = 1, t_1 = 2, t_2 = 1$, two symbols and index: $\{\mu(0, 0), \mu(1, 0), \mu(2, 0), \mu(0, 1), \mu(1, 1), \mu(2, 1)\} = \{1, 1, 0, 1, 1, 0\}$.

m = 4: Partially Balanced array of strength $t = 2$ and index $\{1, 2, 2\}$.

m = 5: Partially Balanced array of strength $t = 4$ and index $\{1, 1, 1, 1, 1\}$. This is a special case of an orthogonal array. Note that the same array, as in the first approach, worked here too.

Similarly, there is a pattern in the index of the above arrays that can be written in the following way:

Pattern 2.2

Let $[(N - 2(m-1))/2] = d$,
 $[(N - 2(m-2))/2] = f$, where $[a]$: integer part of a .

m=4 $\{1, 2, 2\}$: $\{f-1, m-2, f+1\}$ or equivalently

$\{f+1, m-2, f-1\}$ by interchanging 0 and 1.

m=5 $\{4, 4, 4\}$: special case, $\{d, m-1, d\}$,
 $d = m-1$ here.

We extended this pattern for $m=6$ and 7 as follows:

m=6 $\{7, 5, 4\}$: $\{d+2, m-1, d-1\}$ and

m=7 $\{9, 5, 5\}$: $\{f+2, m-2, f-2\}$.

For $m=6$, using Srivastava's existence conditions, it can be verified that such an array does not exist for more than 5 factors. However, we constructed a PB1-array $T = [T^{(1)}; T^{(2)}]$ with $T^{(1)}$ having the 'predicted' index $\{7, 5, 4\}$, in the following way. First, we constructed $T^{(1)}$ as a Partially Balanced array with $N = 21$ runs, $m = 5$ factors, strength $t = 2$ and index $\{7, 5, 4\}$. $T^{(1)}$ is also a Partially Balanced array with $N = 21$ runs, $m = 5$ factors, strength $t = 4$ and index $\{2, 2, 1, 1, 1\}$. Next, we augmented to $T^{(1)}$ an array $T^{(2)}$ with $N = 21, m = 1$. Here, $T^{(2)}$ is an $N \times 1$ vector, so trivially is of strength $t = 1$. $T = [T^{(1)}; T^{(2)}]$ is a PB1-array with the following parameters:

m=6: PB1-array with $N = 21, m_1 = 5, m_2 = 1, t_1 = 4, t_2 = 1$ and two symbols. Its index $\{\mu(i_1, i_2)\}$ is $\{\mu(0, 0), \mu(1, 0), \mu(2, 0), \mu(3, 0), \mu(4, 0), \mu(0, 1), \mu(1, 1), \mu(2, 1), \mu(3, 1), \mu(4, 1)\} = \{1, 1, 0, 1, 1, 1, 1, 1, 0, 0\}$. As before, the above T was augmented on the specified subset of 3^m (see Table IV).

For $m=7$, using again Srivastava's existence conditions, it can be shown that an array with $N = 24$ and index $\{9, 5, 5\}$ does not exist for more than 5 factors. Using the same method as before, we constructed a PB1-array. First, we constructed a Partially Balanced array $T^{(1)}$ with $N = 24$ runs, $m = 5$ factors, strength $t = 2$ and index $\{9, 5, 5\}$. $T^{(1)}$ is also a Partially Balanced array with index $\{4, 2, 1, 1, 2\}$ and strength $t = 4$. Next, we augmented to $T^{(1)}$ a $T^{(2)}$ array with $N = 24$ runs, $m = 2$ factors, strength $t = 2$ and index $\{1, 6, 11\}$. $T = [T^{(1)}; T^{(2)}]$ is a PB1-array with the following parameters:

m = 7: PB1-array with $N = 24, m_1 = 5, m_2 = 2, t_1 = 4, t_2 = 2$ and two symbols. Its index $\{\mu(i_1, i_2)\}$ is: $\{\mu(0, 0), \mu(1, 0), \mu(2, 0), \mu(3, 0), \mu(4, 0), \mu(0, 1), \mu(1, 1), \mu(2, 1), \mu(3, 1), \mu(4, 1), \mu(0, 2), \mu(1, 2), \mu(2, 2), \mu(3, 2), \mu(4, 2)\} = \{1, 0, 0, 0, 0, 1, 1, 0, 0, 1, 1, 0, 1, 1, 0\}$.

Again, this array was augmented on a specified subset of 3^m (see Table IV). Note that for $m=6, 7$ the best designs generated by the computer procedure did

not involve neither Partially Balanced nor PB1-arrays. However, the designs obtained by the above method had the same D-efficiency as the best computer generated design on the same support. The D-efficiency and the support set of the designs obtained from this approach are given in Table IV. The number of points from E_m is denoted by v (n and p are as before). Note that for $m=6$ a Partially Balanced array exists for $N=21$ but it yields a design with lower D-efficiency. For $m=7$ the choice of $N=24$ design points was the result of identifying an array with the 'predicted' index and 'adjusting' it to include less than 29 points while yielding higher D-efficiency than the first approach. Another choice of N , but the same pattern, might result in a small 'improvement' in terms of D-efficiency.

3. RESULTS

The results from the first approach are summarized in Tables I, II.

TABLE I

n	Type of Array	Index	t
7	Balanced	{2, 2, 1}	2
11	Balanced	{0, 1, 1, 0, 1}	4
16	Balanced	{1, 1, 1, 1, 1}	4
22	Balanced	{2, 1, 1, 2, 2}	4
29	PB1	{1, 1, 0, 0, 1, 1, 0, 0, 1, 1, 0, 1, 1, 0, 1}* (4,2)	

*{ $\mu(0, 0)$, $\mu(1, 0)$, $\mu(2, 0)$, $\mu(3, 0)$, $\mu(4, 0)$, $\mu(0, 1)$, $\mu(1, 1)$, $\mu(2, 1)$, $\mu(3, 1)$, $\mu(4, 1)$, $\mu(0, 2)$, $\mu(1, 2)$, $\mu(2, 2)$, $\mu(3, 2)$, $\mu(4, 2)$ }

TABLE II

m	D-eff.	Support
3	40.00	$E_m E_{m-2}$
4	39.25	$E_m E_{m-3}$
5	45.90	$E_m E_{m-2} \cup E_{m-3}$
6	44.62	$E_m E_{m-3} \cup E_{m-4}$
7	44.78	$E_m E_{m-3} \cup E_{m-4}$, $E_m E_{m-4} \cup E_{m-5}$ $E_m E_{m-4} \cup E_{m-6}$

The D-efficiencies of other small second order designs that have been published, are given in the following Table III (Draper and Lin (1990)).

TABLE III

m	Recht-Lucas Box			Notz	Mitchel	Draper
	Shaff.		Draper		Bayne	Lin
	1967	1974	1974	1982	1976	1988
3	40.0	15.2	42.3	40.0	41.0	30.3
4	39.2	9.6	42.3	39.2	42.5	30.8
5	45.0	6.6	37.4	45.9	45.6	24.1
6	42.8	4.8	31.7	44.6	-	26.3
7	38.3	3.6	22.7	-	--	19.6
8	33.6	2.8	19.3	-	-	32.1
9	29.3	2.3	16.7	-	-	20.0
10	25.5	1.8	14.6	-	-	16.5

Table IV summarizes the results from the second approach.

TABLE IV

m	D-eff.	Support	v	n	p
3	40.95	$E_m \cup E_{m-1} \cup E_{m-2}$	6	7	10
4	42.50	$E_m \cup E_{m-1} \cup E_{m-3}$	7	11	15
5	45.89	$E_m \cup E_{m-2} \cup E_{m-3}$	16	16	21
6	45.98	$E_m \cup E_{m-3} \cup E_{m-4}$	21	22	28
7	45.10	$E_m \cup E_{m-1} \cup E_{m-3}$	24	29	36

For $m = 8, 9$ and 10 the support sets $E_m | E_{j1} \cup E_{j2}$ using the first approach are given in Table V:

TABLE V

m	D-eff.	Support
8	43.37	$E_m E_{m-4} \cup E_{m-5}$, $E_m E_{m-4} \cup E_{m-7}$
9	42.91	$E_m E_{m-5} \cup E_{m-7}$
10	43.15	$E_m E_{m-5} \cup E_{m-6}$, $E_m E_{m-6} \cup E_{m-7}$

Further results for $m = 8, 9$ and 10 from the second approach are given in Table VI below:

TABLE VI

m	D-eff.	Support	v	n	p
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8	44.56	$E_m \cup E_{m-2} \cup E_{m-3}$	26	37	45
9	44.96	$E_m \cup E_{m-1} \cup E_{m-4}$	24	46	54
10	-	-	-	56	66

4. DISCUSSION

I. In the first approach, the Partially Balanced arrays that have been obtained for $m < 7$ have the same index as the designs studied by W. Notz. However, the set of design points used to estimate the quadratic terms (x_i^2) is different.

II. The PB1-arrays that have been obtained in both approaches (first approach: $m = 7$, second approach $m = 3, 6, 7$) have the following properties:

a) Let $X = [X_1 | X_2]$, $X_1 = [x_1 \ x_2 \ \dots \ x_{m1}]$ and $X_2 = [x_{m1+1} \ \dots \ x_m]$, $M = X'X$ and $M_{11} = X_1'X_1$. Define $D_{m2} = |M| / |M_{11}|$. Then D_{m2} is 'maximum' under the restriction that X_1 has a specified index.

This is analogous to Ds-optimality for the second set of parameters (in X_2) under the restriction that X_1 is 'fixed'.

b) $M = X'X$ has the following form:

$$M = \begin{array}{ccc|cc} N & \dots & a & b & b \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ a & \dots & N & b & b \\ \hline b & \dots & b & N & c \\ b & \dots & b & c & N \end{array}$$

A geometric interpretation of the above form is the following:

the angle φ ($0 \leq \varphi \leq \pi$, $\cos \varphi = \langle x_i, x_j \rangle / |x_i| |x_j|$) between vectors x_{m1+1}, x_m and the linear space spanned by vectors $\{x_1, x_2, \dots, x_{m1}\}$ is the same (b is not necessarily 0).

III. In the first approach, the Partially Balanced and PB1 arrays that have been discussed are resolution V designs. Thus, if the assumption that interactions with three or more factors are negligible is valid, they allow unbiased estimation of all main effects and two factor interactions.

An association between a Partially Balanced array of strength $t = 2$ (l is a positive integer) and a Balanced fractional 2^m factorial design of resolution $2l + 1$ is given in Theorem 4.1 below. It was presented by Srivastava (1970) for $l = 2$, and by Yamamoto, Shirakura and Kuwada (1975) for $2l \leq m$.

Theorem 4.1 A necessary and sufficient condition for a fractional 2^m factorial design of resolution $2l + 1$ to be balanced is that T is a balanced array of strength $t = 2l$ with index set $\{\mu_i \mid i = 0, 1, \dots, 2l\}$ provided the information matrix M of the design T is non-singular.

For $m = 4, 5$ and 6 the corresponding Partially Balanced arrays are non-singular and of strength $t = 4$ (see Table I). According to Theorem 4.1 they are resolution V designs. Also, according to Proposition 4.1 below, the PB1-array corresponding to $m=7$ is also of resolution V. Proposition 4.1 is useful for determining the resolution of a PB1-array for certain cases (see Nishii (1981) and Kuwada (1988)). It is a special case of Theorems 4.2 and 5.4 of Nishii (1981).

Suppose that $t_k = m_k$ if $m_k = 2, 3, 4$ and $t_k = 4$ if $m_k > 4$ (4.1).

Proposition 4.1 If T is a PB1 ($N, m_1 + m_2, 2, t_1 + t_2; \{\mu(i_1, i_2)\}$) with t_1 and t_2 satisfying condition (4.1), and the information matrix is non-singular, then T is a design of resolution V. The converse is not always true.

In general, the PB1-arrays obtained by the second approach can be at least of strength $t = 2$. Therefore they can be designs of at least of resolution III, as long as they are non-singular (Theorem 4.1). Note that the arrays here cannot be of resolution IV, since they are not arrays of strength $t = 3$. Hartley (1959) stated that the 'cube portion' of the design (here E_m) need not be of resolution V; it can be as low as resolution III as long as the two factor interactions are not alliaised with each other. Hartley studied second order composite designs that are minimal (saturated) or near minimal.

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