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A Catalog of Orthogonally Blocked 3-Level Second-Order Designs with Run Sizes ≤ 100

Nam-Ky Nguyen and Aloke Dey

Indian Statistical Institute, Delhi Centre
7, SJSS Marg, New Delhi–110 016, India

A CATALOG OF ORTHOGONALLY BLOCKED 3-LEVEL SECOND-ORDER DESIGNS WITH RUN SIZES ≤ 100

Nam-Ky Nguyen
International School, Vietnam National University, Hanoi, Vietnam
email: namnk@isvnu.vn
and
Aloke Dey
Indian Statistical Institute, New Delhi 110 016, India
e-mail: aloke.dey@gmail.com

Abstract

Box-Behnken designs (Box and Behnken, 1958, 1960) form a very popular class of 3-level second-order designs when the number of factors is small, typically, seven or less. For larger number of factors these designs are not so popular because then, these designs require a large number of runs. This paper provides a catalog of 3-level second-order designs for 5-11 factors with run sizes ≤ 100. All the designs reported can be orthogonally blocked and are seen to have high D-efficiencies.

Keywords: D-efficiency; Response surface designs; Regular graph designs; Resolvable incomplete block designs; Rotatability measure Q^*.

1 Introduction

Box and Behnken (1958, 1960) introduced a class of 3-level second-order designs, known as Box-Behnken designs (hereafter called BBDs) for fitting a second-order response surface model. BBDs and the central composite designs (CCDs) of Box and Wilson (1951) subject to the appropriate choice of factor levels satisfy several *goodness* properties judged as essential for a second order design, such as requiring a minimum number of levels for each of the factors, being rotatable or near-rotatable, being able to be orthogonally blocked, ensuring simplicity of calculation leading to simplicity in the interpretation of the results (see Box and Draper, 2007). As such BBDs, particularly those with 3–7 factors are very popular second order designs. BBDs with eight or more factors are less popular as these designs require an excessive number of runs (128–324 runs without center runs for 8–16 factors). Smaller orthogonally blocked 3-level second order designs have been proposed recently by several authors; see e.g., Nguyen and Borkowski (2007), Dey (2009) and Dey and Kole (2013), where more references can also be found. The purpose of this paper is to provide additional orthogonally blocked 3-level designs for 5-11 factors in 100 runs or less with high D-efficiency and Q^* rotatability measure (Draper and Pukelsheim, 1990).

2 Method of construction

All designs in this paper are constructed from resolvable incomplete block designs (IBDs). Recall that an IBD with parameters (v, k, r) is an arrangement of v treatments in b $(= vr/k)$ blocks, each of size k $(< v)$ such that each treatment occurs in r blocks and each treatment occurs at most once in any block. An IBD is said to be t-resolvable if its blocks can be divided into s replicate sets of blocks, each of which is an IBD with parameters (v, k, t), i.e., $r = ts$. A 1-resolvable IBD is a resolvable IBD. See e.g., Dey (2010) for more on IBDs or Nguyen and Blagoeva (2010) for a brief introduction to this subject. The advantage of using a resolvable IBD in conjunction with the runs of a 2-level factorial with levels ± 1 or, a suitable fraction of a 2-

level factorial is that orthogonal blocking can be achieved without any extra effort. Note that since the information matrix of an orthogonally blocked response surface design under a model that includes the block effects, apart from the surface parameters, equals the information matrix under a model with no block effects, the efficiency of an orthogonally blocked design equals the corresponding efficiency of an unblocked design.

Let λ_{ij} $(i \neq j)$ be the number of blocks in an IBD in which both treatments i and j concur. If the λ_{ij}'s differ by at most one, the IBD is called a regular graph design (RGD) (John and Mitchell, 1977), who conjectured that D-, A- and E-optimal IBDs are also RGDs. The class of RGDs thus includes balanced IBDs (IBDs whose λ_{ij}'s are all the same) and all IBDs whose λ_{ij}'s differ by one. All IBDs used in this paper are RGDs.

All BBDs except the one for 11 factors are constructed by superimposing the 2-level factorials with levels ± 1 onto treatments in each block of an IBD (which can be resolvable or non-resolvable). On the other hand, all designs in this paper are constructed by superimposing a 2-level fractional factorial and its fold-over onto treatments in each block of a resolvable IBD. As an example, suppose we start with the following 2-resolvable RGD with parameters (v, k, r)=(6, 3, 4), whose treatments are labeled $0, 1, \ldots, 5$ and the blocks are

$$(2,3,4),(0,5,2),(0,1,3),(1,4,5);(0,4,5),(1,3,5),(0,1,2),(2,3,4).$$

Here, the first 4 blocks constitute a replicate set and the next four blocks constitute the second replicate set. Each treatment appears twice within a replicate set. If we now impose a half fraction of a 2^3 factorial, say (1, 1, 1), (1, -1, -1), (-1, 1, -1) and (-1, -1, 1) onto treatments in each odd block and its fold-over in each even block, we get the following 6-factor 3-level second order design in two orthogonal blocks (without the center points):

$$\begin{array}{cccccc}
0 & 0 & \pm1 & \pm1 & \pm1 & 0 \\
\mp1 & 0 & \mp1 & 0 & 0 & \mp1 \\
\pm1 & \pm1 & 0 & \pm1 & 0 & 0 \\
0 & \mp1 & 0 & 0 & \mp1 & \mp1 \\
\hline
\pm1 & 0 & 0 & 0 & \pm1 & \pm1 \\
0 & \mp1 & 0 & \mp1 & 0 & \mp1 \\
\pm1 & \pm1 & \pm1 & 0 & 0 & 0 \\
0 & 0 & \mp1 & \mp1 & \mp1 & 0
\end{array}$$

Here $(\pm1 \pm 1 \pm 1)$ represents the four points of a half fraction of a 2^3, $(\mp1 \mp 1 \mp 1)$ represents the fold-over of this half fraction and 0 represents a column vector of four 0's. At least one center point has to be added in each block to ensure the non-singularity of the information matrix and, an equal number center runs are to be added to each block to ensure orthogonal blocking. It is easy to verify that this orthogonally blocked design has $\sum x_i^2 x_j^2 = \frac{1}{2} 2^3 \ \lambda_{ij}$ where λ_{ij} is the concurrencies of the mentioned RGD.

With reference to an n-run second order design d involving m factors, let X_d denote the $n \times p$ design matrix of d, where the ith row of X_d is written as

$$(1, x_{i1}^2, x_{i2}^2, \ldots, x_{im}^2, x_{i1}, x_{i2}, \ldots, x_{im}, x_{i1}x_{i2}, \ldots, x_{i,m-1}x_{im})$$

and $p = (m+2)(m+1)/2$. Then, the $X_d' X_d$ matrices of the designs in this paper, the augmented-pair designs (Morris, 2000) and small CCDs (Nguyen and Lin, 2011) have the form

$$\left(\begin{array}{c|c} A & \mathbf{0} \\ \hline \mathbf{0} & B \end{array} \right), \tag{1}$$

where A is a square matrix of order $m+1$ and B is a square matrix of order $m + \binom{m}{2}$ $(= \frac{1}{2}m(m+1))$. The quadratic effects of these designs are always orthogonal to all main- and interaction effects. Nguyen and Lin (2011) called this property the orthogonal quadratic effect (OQE) property. Unlike BBDs (except the one for 11 factors) and CCDs, where the matrix B in (1) is a diagonal matrix, certain $\sum x_i x_j x_l$ terms in the off-diagonal elements of B will be non-zero.

To construct the designs in this paper we first construct a large number of resolvable RGDs using the algorithm of Nguyen (1994). For each RGD we construct an orthogonally blocked 3-level second order design using the method in the previous paragraphs and compute its D-efficiency relative to a D-optimal continuous (approximate) design measure over an m-ball of radius unity (see e.g., Dey, 2009 and Dey and Kole, 2013 for the computation of this D-efficiency). The design with the highest D-efficiency is then selected. Since the D-efficiency is computed relative to a hypothetical (approximate) D-optimal design, the efficiencies reported in Table 1 are in fact a lower bound to the actual D-efficiency of the design.

3 Results and Discussion

Table 1. Goodness measures of new designs

m	p	Design	t	(v, k, r)	n (n_0†)	D-eff	Q^*
5	21	5a	3	(5, 3, 6)	42 (2)	87.93	0.9351
		5b	3	(5, 3, 9)	63 (3)	94.39	0.9802
		5c	2	(6, 3, 4)	34 (2)	68.97	0.9644
		5d	2	(6, 3, 6)	51 (3)	73.88	0.9835
		5e	2	(6, 3, 8)	68 (4)	75.66	0.9908
6	28	6a	2	(6, 3, 4)	34 (2)	75.95	0.9240
		6b	2	(6, 3, 6)	51 (3)	91.49	0.9643
		6c	2	(6, 3, 8)	68 (4)	96.38	0.9858
7	36	7a	3	(7, 3, 6)	58 (2)	99.93	1
		7b	3	(7, 3, 9)	87 (3)	97.67	0.9854
8	45	8a	3	(8, 3, 6)	66 (2)	84.99	0.9479
		8b	3	(8, 3, 9)	99 (3)	93.32	0.9720
		8c	3	(8, 4, 6)	98 (2)	82.57	0.9778
		8d	2	(8, 4, 6)	99 (3)	83.14	0.9778
		8e	1	(9, 3, 5)	65 (5)	69.43	0.9581
		8f	1	(9, 3, 6)	78 (6)	72.97	0.9770
		8g	1	(9, 3, 8)	100 (4)	82.81	0.9985
9	55	9a	1	(9, 3, 5)	65 (5)	79.07	0.9465
		9b	1	(9, 3, 6)	78 (6)	85.35	0.9710
		9c	2	(9, 3, 8)	100 (4)	98.18	0.9985
10	66	10a	3	(10, 3, 6)	82 (2)	80.63	0.9466
		10b	3	(10, 5, 6)	98 (2)	80.81	0.9563
11	78	11a	3	(11, 3, 6)	90 (2)	70.64	0.9334
		11b	2	(12, 3, 6)	99 (3)	67.06	0.9393

†Number of center points (which is also the number of orthogonal blocks).

Table 1 displays 24 orthogonally blocked 3-level second order designs for 5-11 factors with 100 runs or less. This table includes for each design, the number of factors m, the number of parameters p in the second-order response surface model, the design identification, the associated t-resolvable RGD with parameters (v, k, r), the total number of runs n, the number of center runs n_0 (which is also the number of orthogonal blocks of each design), the D-efficiency and rotatability measure Q^* (see Draper and Pukelsheim (1990) for the computation of this measure). Below are some general observations for the new designs in Table 1:

(i) Although all the designs in Table 1 are available with at most 100 runs, they have reasonably high D-efficiencies and rotatability measures in most cases. With the exception of two designs 5b and 11b, the D-efficiencies of these designs are between 70-100%. As stated earlier, the D-efficiencies reported in Table 1 are in fact a lower bound to the actual D-efficiency of the design.

(ii) Designs 5a, 5d, 5c, 6b, 6c, 8a, 8b, 9a, 10a, 11a also appear in Dey and Kole (2013). With the exception of two designs 9a and 8a, the new designs show substantial improvement in D-efficiency over the corresponding designs of Dey and Kole. For example, while the D-efficiencies of our designs 8b (for eight factors in 99 runs and three orthogonal blocks) and 10a (for 10 factors in 82 runs and two orthogonal blocks) are 93.32% and 80.63% respectively, the ones of the corresponding Dey-Kole designs are only 82.85% and 67.35%, respectively.

(iii) Designs 7a and 9c were constructed from resolvable balanced IBDs with repeated blocks. While 7a could be obtained from the algoithm, 9c was constructed manually. These designs are not new: 7a with a different number of center runs has appeared in Box and Behnken (1960) and Dey and Kole (2013), 9c with a different number of center runs has appeared in Nguyen and Borkowski (2007).

(iv) Designs 5c, 5d, 5e, 8e, 8f, 8g and 11b were obtained by deleting one column from designs with larger number of factors. Some new designs in Morris (2000) and Dey (2009) were constructed this way.

(v) Some designs in Table 1 use resolvable RGDs with block sizes other than three and fractional factorial other than a half fraction of a 2^3 : designs 8c and 8d use resolvable RGDs with block size four and a half fraction of a 2^4, design 10b uses a resolvable RGD with block size five and a quarter fraction of a 2^5.

4 Concluding remarks

This paper gives a catalog of 24 orthogonally blocked 3-level second order designs for 5-11 factors involving 100 runs or less. All designs have the QDF property and reasonably high D-efficiencies. Design with the number of factors larger than 11 can also be constructed by the method in this paper. However, these designs require more than 100 runs which might not be useful in practice. For experiments with a large number of factors, we recommend the use of the first-order designs in the first stage or screening stage and the designs in this paper only in the second stage of the experiment. All designs in this paper are available at `http://designcomputing.net/smallBBD/`.

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