Small Box–Behnken design

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ABSTRACT

Box–Behnken design has been popularly used for the second-order response surface model. It is formed by combining two-level factorial designs with incomplete block designs in a special manner—the treatments in each block are replaced by an identical design. In this paper, we construct small Box–Behnken design. These designs can fit the second-order response surface model with reasonably high efficiencies but with only a much smaller run size. The newly constructed designs make use of balanced incomplete block design (BIBD) or partial BIBD, and replace treatments partly by 2 3−1 III designs and partly by full factorial designs. It is shown that the orthogonality properties in the original Box and Behnken designs will be kept in the new designs. Furthermore, we classify the parameters into groups and introduce Group Moment Matrix (GMM) to estimate all the parameters in each group. This allows us to significantly reduce the amount of computational costs in the construction of the designs.

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1. Introduction

Consider k factors, x1, . . . , xk, under investigation to determine their effects on a response variable y. Often we approximate the functional relationships over a limited experimental region by a polynomial representation (see, for example, Draper and Lin, 1990). We start with the first-order model

\[ y_t = \beta_0 + \beta_1 x_{1t} + \cdots + \beta_k x_{kt} + \epsilon_t, \]

where \( t = 1, \ldots, n \) is the number of runs, and \( \epsilon_t \) is the error term at the \( t \)-th run with zero mean and variance \( \sigma^2 \). If it suffers with lack of fit, a few more runs may be added to allow the full second-order model to be fitted,

\[ y_t = \beta_0 + \sum_{i=1}^{k} \beta_i x_{it} + \sum_{i=1}^{k} \beta_i x_{it}^2 + \sum_{j=1}^{k} \sum_{j \neq i}^{k} \beta_{ij} x_{it} x_{jt} + \epsilon_t. \]  

There is a total of \((k + 2)(k + 1)/2\) parameters to be estimated, including a constant term, \( k \) first-order terms, \( k \) quadratic terms, and \( k(k - 1)/2 \) interaction terms. For second-order response surface design, the central composite design (Box and Wilson, 1951; Box and Hunter, 1957) and the Box–Behnken design (Box and Behnken, 1958) are probably two most popular ones among practitioners. These designs have some desirable properties, such as, orthogonality and high efficiency. The run size of these designs increases rapidly as the number of factors \( k \) increases, however. For central composite design, efforts have been made to reduce the run size (see, for example, Draper, 1985; Draper and Lin, 1990, 1996; Jensen, 1994). For Box–Behnken design, little is known on reducing the run size. The objective here is to find small Box–Behnken designs which could maintain as many good properties as the original Box and Behnken designs, but with far fewer runs.

An alternative replacement method for the construction of small Box–Behnken designs is proposed in Section 2. These newly obtained small Box–Behnken designs are then compared with the other Box–Behnken designs in Section 3. An
algorithm is proposed in Section 4 to simplify the computation efforts (this is particularly important for large $k$). The conclusions and discussions are given in Section 5.

2. Alternative replacement

The Box–Behnken design, proposed by Box and Behnken (1958), combines two-level factorial designs with incomplete block designs in a special manner. For instance, an incomplete block design with six treatments and six blocks is given by

$$
\begin{bmatrix}
* & * & 0 & 0 & 0 & 0 \\
0 & * & * & 0 & 0 & \\
0 & 0 & * & * & 0 & * \\
* & 0 & 0 & * & 0 & \\
0 & * & 0 & 0 & * & \\
* & 0 & 0 & 0 & 0 & *
\end{bmatrix}.
$$

(2)

Take the six columns as the six input factors $x_1, x_2, x_3, x_4, x_5, x_6$ in a response surface study. Replace the three asterisks in each block by a $2^3$ full design and insert a column of zeros wherever the asterisk does not appear. Repeating the procedure for each block and adding a few central points lead to the following Box–Behnken design with $k = 6$ factors as displayed in Eq. (3). The resulting design will have 48 runs plus the center points. These designs are popularly used (see, for example, Box and Draper, 1987; Myers et al., 2009; Khuri and Cornell, 1996)

$$
\begin{bmatrix}
\pm 1 & \pm 1 & 0 & \pm 1 & 0 & 0 \\
0 & \pm 1 & \pm 1 & 0 & \pm 1 & 0 \\
0 & 0 & \pm 1 & \pm 1 & 0 & \pm 1 \\
\pm 1 & 0 & 0 & \pm 1 & \pm 1 & 0 \\
0 & \pm 1 & \pm 0 & \pm 1 & \pm 1 & \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}.
$$

Note: $(\pm 1, \pm 1, \pm 1)$ denotes all $2^3$ combinations of the plus and minus levels.

Box and Behnken (1958) replaced the treatments in each block by the same design (typically $2^2$ or $2^3$). Keeping the BIBD (or PBIBD) structure unchanged, the run size of the resulting design could be smaller if alternative designs are used. As an illustrative example, consider the above design for $k = 6$. We first divide the six blocks (as shown in Eq. (2)) into two parts. Suppose that we put the first two blocks as part I and the rest as part II. The three treatments of each block in Part I is replaced by a $2^3$ design, while the treatments of each block in part II is replaced by a $2_{III}^{3-1}$ design. The results can be shown as follows.

$$
\begin{bmatrix}
\pm 1 & \pm 1 & 0 & \pm 1 & 0 & 0 \\
0 & \pm 1 & \pm 1 & 0 & \pm 1 & 0 \\
0 & 0 & \pm 1 & \pm 1 & 0 & \pm 1 \\
\pm 1 & 0 & 0 & \pm 1 & \pm 1 & 0 \\
0 & \pm 1 & \pm 0 & \pm 1 & \pm 1 & \\
\pm 1 & 0 & \pm 1 & 0 & 0 & \pm 1
\end{bmatrix} \quad 2^3
$$

$$
2_{III}^{3-1}.
$$

In Part I, $(\pm 1, \pm 1, \pm 1)$ denotes all $2^3$ combinations of the plus and minus levels; while in Part II, $(\pm 1, \pm 1, \pm 1)$ is the short form of $\begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix}$, a $2_{III}^{3-1}$ design. The newly constructed design will have 32 runs plus center points, as compared to 48 runs in the original Box–Behnken design.

3. Construction and comparison

Next, we discuss in detail on the construction method of the small Box–Behnken designs in general. The construction method involves the following three steps:

Step 1 : (Construction of block designs.) The incomplete block designs used must satisfy the following properties: (i) each block contains no more than three treatments, (ii) any pair of treatments has to coincide in some block, but with as few times as possible. The block designs satisfying (i) and (ii) are listed in the Appendix.

Step 2 : (Treatments replacement.) Use proper factorial design to replace the treatments of each block. If the block size is two, then a $2^2$ design is adopted. If the block size is three, either a $2^3$ design or a $2_{III}^{3-1}$ design is adopted (this will be explained in detail later–see Steps 2a–2c).
Step 3: (Adding central points.) Some central points, if desirable, can be added to estimate the grand mean.

For each BIBD (or PBIBD) chosen in Step 1, let $b_0$ be the number of blocks with three treatments and $b_1$ be the number of blocks in which treatments are replaced by a $2^3$ design. Then the treatments in the rest $b_0 - b_1$ blocks will be replaced by a $2^1_{-1}$ design. Obviously, the total number of runs is $4(b_0 - b_1) + 8b_1$. Note that the total number of parameters in the second-order model is $(k + 2)(k + 1)/2 - 1$ (excluding the constant term). The inequality

$$4(b_0 - b_1) + 8b_1 \geq \frac{(k + 2)(k + 1)}{2} - 1 \tag{4}$$

holds if the small Box–Behnken design is capable of estimating all parameters in this model (excluding the constant term). Denote $b^* = \lceil((k + 2)(k + 1)/2 - 1)/4 - b_0\rceil$ the smallest integer $b_1$ satisfying the inequality (4). We discuss details of the replacement method mentioned in Step 2:

Step 2a: For the fixed $b^*$ blocks, calculate the $D$-efficiency (labeled $D$-eff) of the moment matrix $M = Z'Z/n$, where $Z$ is the model matrix excluding the column of all ones. For a fair comparison, we define the $D$-eff as $(\|\hat{Z}Z\|)^{1/p}/n \times 100\%$, where $\hat{Z}$ is the $Z$ matrix corrected by the method of Nguyen and Borkowski (2008). Other types of $D$-efficiency (for example, Kiefer, 1960) can be used as well. If the matrix is nonsingular, go to Step 2b. Otherwise select a new non-isomorphic $b^*$ blocks to repeat the above process (two different $b^*$ blocks are called isomorphic if their moment matrices resemble each other). If there is no nonsingular moment matrix, after an exhausted search among all the non-isomorphic $b^*$ blocks, go to Step 2c.

Step 2b: If the moment matrix is nonsingular, we search all non-isomorphic $b^*$ blocks to update the block scheme which maximizes the $D$-eff. The algorithm stops until all the non-isomorphic $b^*$ blocks are compared.

Step 2c: If $b^* < b_0$, update $b^*$ by $b^* + 1$. Select the first $b^*$ blocks and go to Step 2a. If $b^* = b_0$, then select all blocks and the algorithm stops.

As a result, there will be $b^*$ blocks chosen to be replaced by a $2^3$ design and the rest will be replaced by a $2^{k-1}$ design. When $b^* = b_0$, the resulting is indeed the original Box and Behnken design. The newly constructed designs ensure all the parameters in model (1) can be estimated with reasonably high efficiencies, while the number of runs are reduced.

Through the construction method, small Box–Behnken designs are obtained in Appendix. The moment matrices for newly constructed designs have the following three properties. It can be shown that all the orthogonal properties in the original Box–Behnken designs are kept. The proofs are straightforward and thus are omitted here. Following the notations used in Box and Draper (1987), define $[i] = \frac{1}{n} \sum_{t=1}^{n} x_{ti}$, $[ij] = \frac{1}{n} \sum_{t=1}^{n} x_{ti} x_{tj}$, $[ijk] = \frac{1}{n} \sum_{t=1}^{n} x_{tij}$, and so on. It can be verified that

1. $[i] = 0$; and $[ij] = 0$, for $i \neq j$.
2. $[ijk] = 0$, for the position that *** appears in $i$, $j$, $k$ simultaneously in Part II, otherwise $[ijk] = 0$, for $i \neq j \neq k$; $[ij] = 0$, for $i \neq j$; $[ii] = 0$.
3. $[ijkl] = 0$, for $i \neq j \neq k \neq l$; $[ijkl] = 0$, for $i \neq j \neq k$; $[iii] = 0$, for $i \neq j$.

The newly constructed small Box–Behnken designs (SBBD) are next compared with original Box–Behnken designs (BBD) and 3-level designs given in Nguyen and Borkowski (2008, labelled NBD) in terms of the total number of runs and their corresponding $D$-efficiencies. The comparisons are displayed in Table 1.

The following observations are clear from Table 1:

1. (Run size). The run sizes for the proposed SBBD are clearly smaller than the original BBD and NBD, especially for the larger $k$. For example, when $k = 8$, the run size for SBBD is about 25% (56 vs. 192) of the original BBD and 50% (56 vs. 128) of NBD. And it is very close to the minimal number of points (the total number of parameters to be estimated).
2. (Efficiency). The proposed SBBDs, even with very few runs, still have high $D$-efficiencies, although these are lower than BBD and NBD. All their $D$-efficiencies are over 70%, for example.

<table>
<thead>
<tr>
<th>Number of factors $k$</th>
<th>Number of parameters $p = \frac{(k+2)(k+1)}{2} - 1$</th>
<th>Total points $(n)$</th>
<th>$D$-efficiency $(%)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>BBD</td>
<td>NBD</td>
<td>SBBD</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
<td>12</td>
<td>12</td>
</tr>
<tr>
<td>4</td>
<td>14</td>
<td>24</td>
<td>16</td>
</tr>
<tr>
<td>5</td>
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<td>40</td>
<td>24</td>
</tr>
<tr>
<td>6</td>
<td>27</td>
<td>48</td>
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</tr>
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<td>7</td>
<td>35</td>
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<td>40</td>
</tr>
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<td>8</td>
<td>44</td>
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<td>56</td>
</tr>
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<td>9</td>
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<td>10</td>
<td>64</td>
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<td>76</td>
</tr>
<tr>
<td>11</td>
<td>77</td>
<td>176</td>
<td>96</td>
</tr>
</tbody>
</table>

Table 1
Total points (excluding central points) and $D$-efficiency comparison.
4. A new algorithm for construction of higher dimensional designs

To fit the second-order response model, the inverse of the moment matrix needs to be calculated. When \( k \) is small, it can be easily calculated. As \( k \) increases, the calculation becomes troublesome. For instance, when \( k = 9 \) the moment matrix is a \( 54 \times 54 \) matrix. The calculation of its inverse may not be straightforward. The small Box–Behnken design has a good property—we could reduce the computational effort by classifying the parameters into groups. For example, for \( k = 9 \), by properly grouping the parameters we only need to compute the inverses of a \( 4 \times 4 \) matrix and another \( 9 \times 9 \) matrix. This can be much more easily done as opposed to the inverse of a \( 54 \times 54 \) matrix. Based on the parameter grouping, a new algorithm is proposed in this section to significantly reduce the computational effort.

According to the structure of the design matrix \( X \), we can classify the parameters into groups, each of which can be computed independently. Again, take \( k = 9 \) as an example. From the Appendix A, let

\[
X = \begin{bmatrix}
\pm 1 & 0 & 0 & \pm 1 & 0 & 0 & \pm 1 & 0 & 0 \\
0 & \pm 1 & 0 & 0 & \pm 1 & 0 & 0 & \pm 1 & 0 \\
0 & 0 & \pm 1 & 0 & 0 & \pm 1 & 0 & 0 & \pm 1 \\
\end{bmatrix}
\]

where \( X_{11}, X_{12}, X_{13}, X_{21}, X_{22}, X_{23}, X_{24}, X_{25}, X_{26}, X_{27}, X_{28} \) and \( X_{29} \) correspond to all blocks of \( X \). Note that each of \( X_{11}, X_{12} \) and \( X_{13} \) is replaced by a \( 2^3 \) full design, which makes all main effects and their interactions orthogonal in each block. Meanwhile, each of \( X_{21}, X_{22}, X_{23}, X_{24}, X_{25}, X_{26}, X_{27}, X_{28} \) and \( X_{29} \) is replaced by a \( 2^4 \)-1 design, which makes the main effects and the corresponding interactions aliased in each block of this part. For example in the block \( X_{21} \), the 1st, 2nd and 3rd column are "\( \pm 1 \)" which results in the alias of \( \beta_1 \) and \( \beta_{21} \). Here, \( \beta_i \) stands for the main effect of factor \( X_i \) while \( \beta_{ij} \) stands for the interaction effect between factors \( X_i \) and \( X_j \). Therefore, we put \( \beta_1 \) and \( \beta_{21} \) in one group, denoted by Group 1. It is obvious that \( \beta_1 \) is aliased again with \( \beta_{59} \) in \( X_{24} \) and with \( \beta_{68} \) in \( X_{27} \). So \( \beta_{59} \) and \( \beta_{68} \) are also put into Group 1. Since any parameter in Group 1 is not aliased with any other parameter in the rest blocks of Part II, all parameters \( \{ \beta_1, \beta_{23}, \beta_{59}, \beta_{68} \} \) constitute a single group.

Group 1 with the Group Moment Matrix (GMM) being

\[
G_1 = \begin{bmatrix}
11 & 123 & 159 & 168 \\
123 & 2233 & 2359 & 2368 \\
159 & 2359 & 5599 & 5689 \\
168 & 2368 & 5689 & 6688 \\
\end{bmatrix} \times \begin{bmatrix}
5 & 1 & 1 & 1 \\
1 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 \\
\end{bmatrix}
\]

Similarly, the following eight groups can be obtained: \( \{ \beta_2, \beta_{13}, \beta_{49}, \beta_{67} \} \); \( \{ \beta_3, \beta_{12}, \beta_{48}, \beta_{57} \} \); \( \{ \beta_4, \beta_{46}, \beta_{29}, \beta_{38} \} \); \( \{ \beta_5, \beta_{46}, \beta_{19}, \beta_{37} \} \); \( \{ \beta_6, \beta_{45}, \beta_{27}, \beta_{18} \} \); \( \{ \beta_7, \beta_{39}, \beta_{26}, \beta_{35} \} \); \( \{ \beta_8, \beta_{79}, \beta_{34}, \beta_{16} \} \); \( \{ \beta_9, \beta_{78}, \beta_{25}, \beta_{24} \} \). Each of them has the same GMM \( G_1 \) as Group 1.

The complete group used to estimate the quadratic terms is \( \{ \beta_{11}, \beta_{22}, \beta_{33}, \beta_{44}, \beta_{55}, \beta_{66}, \beta_{77}, \beta_{88}, \beta_{99} \} \) with the GMM denoted by

\[
G_2 = \begin{bmatrix}
1111 & 1122 & 1133 & 1144 & 1155 & 1166 & 1177 & 1188 & 1199 \\
1122 & 2222 & 2233 & 2244 & 2255 & 2266 & 2277 & 2288 & 2299 \\
1133 & 2233 & 3333 & 3344 & 3355 & 3366 & 3377 & 3388 & 3399 \\
1144 & 2244 & 3344 & 4444 & 4455 & 4466 & 4477 & 4488 & 4499 \\
1155 & 2255 & 3355 & 4455 & 5555 & 5566 & 5577 & 5588 & 5599 \\
1166 & 2266 & 3366 & 4466 & 5566 & 6666 & 6677 & 6688 & 6699 \\
1177 & 2277 & 3377 & 4477 & 5577 & 6677 & 7777 & 7788 & 7799 \\
1188 & 2288 & 3388 & 4488 & 5588 & 6688 & 7788 & 8888 & 8899 \\
1199 & 2299 & 3399 & 4499 & 5599 & 6699 & 7799 & 9988 & 9999 \\
\end{bmatrix}
\]

Finally, each of the rest parameters constitute a single group, such as \( \beta_{14} \) itself.

Note that the moment matrix \( M \) for such a design can be decomposed as

\[
M = \text{diag} \left( G_1, \ldots, G_1, G_2, c_1, \ldots, c_9 \right)
\]

where \( \text{diag} \) denotes a block diagonal matrix and \( c_j \)'s are constants corresponding to single groups. So we only need to calculate the inverses of \( G_1 \) (a \( 4 \times 4 \) matrix) and \( G_2 \) (a \( 9 \times 9 \) matrix) to fit the model.
5. Conclusions and discussions

Box–Behnken design is a popular response surface design. In this paper, we construct Box–Behnken designs with a small number of runs. Such designs make use of BIBD (or PBIBD), and replace treatments, partly by a $2^3_{III}$ design and partly by a $2^3$ design. It is shown that the orthogonality properties in the original Box and Behnken designs will be kept in the new designs. These designs can fit the second-order response surface model with reasonably high efficiencies but with only much smaller run sizes. To reduce the computational efforts for large $k$, we classify the parameters into groups. All parameters in each group are expressed by a Group Moment Matrix (GMM). A new algorithm based on such a GMM is also proposed to make the design construction possible for large $k$.

Acknowledgement

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Appendix A. Small Box and Behnken designs for $3 \leq k \leq 11$

<table>
<thead>
<tr>
<th>$k$</th>
<th>Block design (without central points)</th>
<th>Replacement design</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>$[\pm 1 \pm 1 0 \pm 1 ]$</td>
<td>$2^2$</td>
</tr>
<tr>
<td>4</td>
<td>$[\pm 1 \pm 1 0 0 \pm 1 ]$</td>
<td>$2^2$</td>
</tr>
<tr>
<td>5</td>
<td>$[\pm 1 \pm 1 0 \pm 1 0 \pm 1 ]$</td>
<td>$2^3_{III}$</td>
</tr>
<tr>
<td>6</td>
<td>$[\pm 1 \pm 1 0 \pm 1 0 \pm 1 ]$</td>
<td>$2^3$</td>
</tr>
<tr>
<td>7</td>
<td>$[\pm 1 \pm 1 0 0 \pm 1 \pm 1 0 \pm 1 ]$</td>
<td>$2^3_{III}$</td>
</tr>
<tr>
<td>8</td>
<td>$[\pm 1 \pm 1 0 0 \pm 1 \pm 1 0 \pm 1 ]$</td>
<td>$2^3_{III}$</td>
</tr>
</tbody>
</table>

(continued on next page)
### Appendix B. Supplementary data

Supplementary material related to this article can be found online at [doi:10.1016/j.spl.2011.02.024](https://doi.org/10.1016/j.spl.2011.02.024).
References


