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# NEW THREE-LEVEL EXPERIMENTAL DESIGNS FOR QUALITATIVE AND QUANTITATIVE FACTORS

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***ABSTRACT***

*Jones and Nachtsheim (2011a) have introduced a class of economical three-level designs for screening quantitative factors in the presence of active second-order effects. In this paper, some new three-level designs are constructed involving both quantitative and qualitative factors using the designs given by Jones and Nachtsheim (2011a). The D- and A-optimal values of these designs are obtained. The relative D-efficiencies of these designs are also computed.*

***Keywords:*** *Screening experiments; Three-level designs; Quantitative factor; Qualitative factor; D-efficiency; D- and A-optimal values.*

***AMS Subject Classification:*** *62K20.*

## 1. INTRODUCTION

Screening designs are widely used in industrial experiments. Screening experiments are experiments in which many factors are considered with the purpose of identifying those factors (if any) that have large effects. These experiments are usually performed early in a response surface study when it is likely that many of the factors initially considered have little or no effect on the response. The factors that are identified as important are then investigated more thoroughly in subsequent experiments.

Jones and Nachtsheim (2011a) proposed a new class of three level designs for screening quantitative factors in the presence of active second-order effects. These designs provide a definitive approach to screening in that main effects are not biased by any second-order effect and all quadratic effects are estimable. Moreover, in the presence of sparsity in the number of active factors, these designs project to highly efficient response surface designs. They have also provided an algorithm for generating these designs for any number of factors. These designs have the minimum possible number of runs for estimating both main and pure quadratic effects of the factors. Some references for three level designs are Box and Behnken (1960), Tsai *et al.* (2000), Mee (2007), Nguyen and Borkowski (2008), Dey (2009) and Jones and Nachtsheim (2011b).

In response surface designs, mostly, factors are quantitative in nature, but quite often in practice, experimenter needs to conduct an experiment where at least one of the factors is qualitative. For example, in agricultural experiment one may be interested to know the effect of fertilizers as well as irrigation methods on the yield of a crop. Here fertilizers are considered as quantitative factors whereas irrigation methods as qualitative. Some references include Draper and John (1988), Wu and Ding (1998), Aggarwal and Bansal (1998), Aggarwal *et al.* (2000) and Joseph *et al.* (2009).

The purpose of this paper is to construct a class of three-level designs involving both quantitative and qualitative factors using the designs given by Jones and Nachtsheim (2011a). The D- and A-optimal values of these designs are obtained. The D-efficiencies of these designs relative to Plackett-Burman (PB) designs are also computed.

The rest of the paper is organized as follows. In Section 2, we discuss the model along with the selection criteria. Method of construction is given in Section 3. The concluding remark is given in Section 4. The D- and A-optimal values and D-efficiencies of the designs for different number of factors ($4 \leq m \leq 12$) are given in Annexure I.

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## 2. MODEL AND DESIGN SELECTION CRITERIA

Consider the design consisting of *m* factors, denoted by $x_j$; $j$ = 1, 2, …, *m*, of which one factor is qualitative in nature and the remaining (*m* - 1) factors are quantitative type. In this paper, the model consists of the intercept term and all *m* linear effects and is defined as

$$y_i = \beta_0 + \beta_1 z_i + \sum_{j=2}^{m} \beta_j x_{ij} + \varepsilon_i ; i = 1, ..., 2m \tag{2.1}$$

where, $y_i$ is the response; $\beta_0$ is a fixed and unknown constant; $\beta_j$'s are regression coefficients; *z* is a qualitative factor and $\varepsilon_i$'s are the *iid* N(0, $\sigma^2$ ).

There are several optimality criteria. Here we have used D-optimal values for selection of our designs. It is known that the larger the D-optimal value the better the design is while the smaller the A-optimal value the better the design.

The D-optimal value of the design is obtained as

$$D = \frac{\left| X'X \right|^{\frac{1}{p}}}{N} \tag{2.2}$$

where, X is a model matrix, N (= 2*m*) is the number of runs in the design and *p* is the number of parameters to be estimated in the model.

The formula for A-optimal value is

$$A = tr\left( X'X \right)^{-1} \tag{2.3}$$

The D-efficiency of any design $d_1$, relative to a nonsingular design $d_2$, is given by

$$D_\varepsilon\left(d_1, d_2\right) = \left( \frac{\left| X\left(d_1\right)' X\left(d_1\right) \right|}{X\left(d_2\right)' X\left(d_2\right)} \right)^{1/p} \times 100 \tag{2.4}$$

where $X\left(d_i\right)$ is the model matrix of the design $d_i$ ($i$ = 1, 2), in the model.

## 3. METHOD OF CONSTRUCTION

Here we construct the designs involving two types of factors; qualitative and quantitative, using the designs given by Jones and Nachtsheim (2011a). The procedure for constructing the design is as follows:

First we consider the design with *m* factors, developed by Jones and Nachtsheim (2011a). We remove the last row consisting of all zeroes from the designs. The factor corresponding to the first column of the design is taken as a qualitative factor. We have considered the levels of the qualitative factor as 1 and -1. So we replace the zeroes in the column corresponding to the qualitative factor by -1 and 1. Since every column of the design has two entries at zero level so the total number of combinations of ±1 will be $2^2$ i.e. {(-1 -1), (-1 1), (1 -1), (1 1)}. We replace all the zeroes in first column of the design by one of the possible combination of ±1. We also observe that on replacing zeroes of the column by the two possible combinations of ±1 having equal number of +1 and -1 i.e. (1 -1) and (-1 1), the design retains its original property of orthogonality. Next, the model matrix is generated according to equation (2.1) and D-and A-optimal values of the design are obtained. This procedure is repeated for all possible combinations of ±1. The design giving the highest D-optimal value and least A-optimal value is selected.

If any other column of the design is considered as qualitative factor, we observe that the same D- and A-optimal values are obtained for the same combination of ±1.

In order to obtain the D-efficiencies, we have compared our designs with D-optimal designs for N = 2*m* runs. When *m* is even, the D-efficiency is obtained relative to Plackett-Burman (PB) designs with 2*m* runs and when *m* is odd, the D-efficiency is obtained relative to D-optimal designs of size 2*m* constructed using coordinate exchange algorithm in the JMP statistical software.

The above procedure is explained with the help of the following example:

**Example 1:** Consider the design, constructed by Jones and Nachtsheim (2011a), for *m* = 6. After deleting the last row of center runs, the design is given in Table 1:

 

**Table-1:** Design for $m$ = 6 factors

| $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ |
|---|---|---|---|---|---|
| 0 | 1 | -1 | -1 | -1 | -1 |
| 0 | -1 | 1 | 1 | 1 | 1 |
| 1 | 0 | -1 | 1 | 1 | -1 |
| -1 | 0 | 1 | -1 | -1 | 1 |
| -1 | -1 | 0 | 1 | -1 | -1 |
| 1 | 1 | 0 | -1 | 1 | 1 |
| -1 | 1 | 1 | 0 | 1 | -1 |
| 1 | -1 | -1 | 0 | -1 | 1 |
| 1 | -1 | 1 | -1 | 0 | -1 |
| -1 | 1 | -1 | 1 | 0 | 1 |
| 1 | 1 | 1 | 1 | -1 | 0 |
| -1 | -1 | -1 | -1 | 1 | 0 |

The factor $x_1$ is considered as qualitative factor $z$. The zeros in the column corresponding to the qualitative factor $z$ are replaced by the first combination of ±1. Let the combination be (-1 -1). The model matrix is then generated according to equation (2.1) and is given in Table 2:

**Table-2:** Model matrix for $m$ = 6 factors

| $k$ | $z$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ |
|---|---|---|---|---|---|---|
| 1 | -1 | 1 | -1 | -1 | -1 | -1 |
| 1 | -1 | -1 | 1 | 1 | 1 | 1 |
| 1 | 1 | 0 | -1 | 1 | 1 | -1 |
| 1 | -1 | 0 | 1 | -1 | -1 | 1 |
| 1 | -1 | -1 | 0 | 1 | -1 | -1 |
| 1 | 1 | 1 | 0 | -1 | 1 | 1 |
| 1 | -1 | 1 | 1 | 0 | 1 | -1 |
| 1 | 1 | -1 | -1 | 0 | -1 | 1 |
| 1 | 1 | -1 | 1 | -1 | 0 | -1 |
| 1 | -1 | 1 | -1 | 1 | 0 | 1 |
| 1 | 1 | 1 | 1 | 1 | -1 | 0 |
| 1 | -1 | -1 | -1 | -1 | 1 | 0 |

Here, the column vector $k$ is the coefficient of the intercept term of the model given in equation (2.1). The D- and A-optimal values of the design are then obtained using equation (2.2) and (2.3) respectively. The highest D-optimal value and the least A-optimal value of the design are 0.8744 and 0.6714 respectively.

The D-efficiency of our design relative to Plackett-Burman design using equation (2.4) is then obtained and is 87.44%.

If the experimenter wants to retain the orthogonal property of the design, the two zeroes of the first column are replaced by two possible combination of ±1 having equal number of -1 and +1 i.e. (-1, 1) and (1, -1). The model matrix is generated in the same manner as explained above. D- and A-optimal values are computed. The D-efficiency of the design is also obtained.

For the above example with $m$ = 6 factors, the D-and A-optimal values are 0.8553 and 0.7033 respectively. The D-efficiency relative to Plackett-Burman designs is 85.53%.

In Annexure I, we give the D- and A-optimal values, D-efficiencies and level combinations corresponding to zeroes of the qualitative factor of the designs for different number of factors ($4 \le m \le 12$).

## 4. CONCLUSIONS

Screening designs are widely used in industrial experiments. Most of the screening experiments involve factors of quantitative type but there are many situations where the factors are of both quantitative and qualitative types. In this paper, we have considered the designs which involve both types of factors. We have restricted ourselves with the designs having only one qualitative factor and rest quantitative factors. We have also computed D- and A-optimal values of the designs. On comparing with D-optimal designs we observe that our designs have high D-efficiencies. The designs involve less number of runs and are orthogonal in some cases. When running an experiment is costly, then our designs are more economical.

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## ANNEXURE I

**Table-3:** D-and A-optimal values, D-efficiencies and level combinations of the designs

| No. of Factors | Level Combinations | A-optimal value of our Designs | D-optimal value of our Designs | D-optimal value of PB/D-optimal Designs | D-efficiency (in %) |
|---|---|---|---|---|---|
| 4 | 1, 1 | 0.7667 | 0.8307 | 1.0000 | 83.07 |
| 5 | 1, -1 | 0.9200 | 0.7647 | 0.9641 | 79.32 |
| 6 | -1, -1 | 0.6714 | 0.8744 | 1.0000 | 87.44 |
| 7 | 1, 1 | 0.7453 | 0.8277 | 0.9739 | 84.99 |
| 8 | -1, -1 | 0.6270 | 0.8998 | 1.0000 | 89.98 |
| 9 | 1, 1 | 0.6825 | 0.8606 | 0.9789 | 87.92 |
| 10 | 1, 1 | 0.6010 | 0.9166 | 1.0000 | 91.66 |
| 11 | -1, -1 | 0.6441 | 0.8825 | 0.9823 | 89.84 |
| 12 | -1, -1 | 0.6165 | 0.9044 | 1.0000 | 90.44 |

 

**Table-4:** D- and A-optimal values, D-efficiencies and level combinations of the designs with orthogonal property

| No. of Factors | Level Combinations | A-optimal value of our Designs | D-optimal value of our Designs | D-optimal value of PB/D-optimal Designs | D-efficiency (in %) |
|---|---|---|---|---|---|
| 4 | -1, 1 | 0.8472 | 0.7944 | 1.0000 | 79.44 |
| 5 | 1, -1 | 0.9200 | 0.7647 | 0.9641 | 79.32 |
| 6 | -1, 1 | 0.7033 | 0.8553 | 1.0000 | 85.53 |
| 7 | 1, -1 | 0.7523 | 0.8243 | 0.9739 | 84.64 |
| 8 | -1, 1 | 0.6441 | 0.8881 | 1.0000 | 88.81 |
| 9 | -1, 1 | 0.6989 | 0.851 | 0.9789 | 86.93 |
| 10 | 1, -1 | 0.6117 | 0.9087 | 1.0000 | 90.87 |
| 11 | -1, 1 | 0.6559 | 0.8757 | 0.9823 | 89.15 |
| 12 | -1, 1 | 0.6178 | 0.9034 | 1.0000 | 90.34 |

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