Constructing Definitive Screening Designs Using Conference Matrices

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Jones and Nachtsheim (2011) propose a new class of designs for definitive screening. These designs have very nice properties for practical use. Their construction approach requires a computerized search. This short note provides a theoretical basis for design construction, making use of conference matrices. The design construction is straightforward, and the resulting design is always a global optimum definitive screening design. The proposed method only works when the number of factors is even, however.

Key Words: Alias Matrix; Foldover; Interaction Effects; Main Effects; Orthogonal Design.

Introduction

Consider fitting the following linear model for m factors.

$$Y = X_1 \beta_1 + \epsilon$$
.

Suppose the true model is in fact

$$\mathbf{Y} = \mathbf{X}_1 \boldsymbol{\beta}_1 + \mathbf{X}_2 \boldsymbol{\beta}_2 + \boldsymbol{\epsilon},$$

where X_2 is the model matrix corresponding to terms of the model other than those in X_1 . Then the expected value of the least-squares estimator $\hat{\beta}_1 = (X_1'X_1)^{-1}X_1'Y$ of β_1 for the model excluding the X_2 term can be shown to be

$$E(\hat{\beta}_1) = \beta_1 + \mathbf{A}\beta_2,$$

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where A is the alias matrix defined as $A = (X_1'X_1)^{-1}X_1'X_2$. For robustness purposes in various factor-screening contexts, it is desirable to minimize such a matrix in some sense.

Jones and Nachtsheim (2011) propose a series of designs, called definitive screening designs, with 2m+1 runs to investigate m factors. These 2m+1 degrees of freedom comprise the minimal number possible for estimates of the intercept, all m main effects, and all m quadratic effects. Furthermore, the estimated main effects are orthogonal to all two-factor interaction effects, namely, the alias matrix $\mathbf{A}=0$ when \mathbf{X}_1 consists of main effects and \mathbf{X}_2 consists of two-factor interactions. Their construction approach requires a computerized search. In this paper, we propose a simple procedure for constructing designs having the same structure by using conference matrices.

Proposed Designs

For m even, an $m \times m$ matrix C is a conference matrix if it satisfies $C'C = (m-1)I_{m \times m}$, with $C_{ii} = 0, (i = 1, 2, ..., m)$ and $C_{ij} \in \{-1, 1\}, (i \neq j, i, j = 1, 2, ..., m)$ (see, for example, Goethals and Seidel (1967)). These matrices were first introduced for

dealing with conference telephony (Belevitch (1950)) but not directly for design of experiments.

The design matrix \mathbf{D} for the definitive screening designs of Jones and Nachtsheim (2011) can be constructed as

$$\mathbf{D} = \begin{pmatrix} \mathbf{C} \\ -\mathbf{C} \\ \mathbf{0} \end{pmatrix},$$

where C is an $m \times m$ conference matrix and 0 is a $1 \times m$ zero matrix. This design has the same size and all the desirable properties as those proposed by Jones and Nachtsheim (2011). In other words, the proposed design will automatically inherit all their nice properties (the proof of which is provided in Appendix A). Specifically,

1. It is a saturated design for estimating the in-

tercept, all m main effects, and all m quadratic effects.

- 2. All main effects are orthogonal to all quadratic effects.
- 3. All main effects are orthogonal to all two-factor interactions, that is, the alias matrix, A, is a zero matrix.

Moreover, the proposed designs are always orthogonal (in term of main and quadratic effects), a desirable property that is not always shared by designs given in Jones and Nachtsheim (2011). Of course, such an orthogonality constraint can be added to their algorithm, if so desired.

Some conference matrices of small sizes are given in Appendix B (for $m=2,4,\ldots,18$). Take the case m=12 as an example. If C denotes the conference matrix of order m=12, the resulting design will be shown in Equation (1).

$$\mathbf{D} = \begin{pmatrix} \mathbf{C} \\ \mathbf{O} \\ \mathbf{O} \\ \mathbf{I} \\ \mathbf{I} \\ \mathbf{I} \\ \mathbf{I} \\ \mathbf{J} \\ \mathbf{I} \\ \mathbf{J} \\ \mathbf{J}$$

It is straightforward to verify that its D-efficiency is 92.3%, higher than the 89.8% for the design given

in Jones and Nachtsheim (2011). For a fair comparison, we adapt the D-efficiency criterion defined in

Number D-efficiency of D-efficiency of Relative of Jones and Nachtsheim's the proposed Ratio factors design (%) design (%) $(\%)^*$ 4 79.4 79.4 100.0 6 85.5 85.5 100.0 8 88.8 88.8 100.0 10 90.9 90.9 100.0 12 89.8 92.3 102.8 14 90.1 93.3 103.6 16 91.5 94.1 102.8 18 89.4 94.7 105.920 89.5 95.2 106.4 22 89.8 NA** NA** 24 90.0 96.0 106.7 26 90.2 96.3106.8 28 90.4 96.5106.7 30 90.7 96.8 106.7

TABLE 1. Relative D-Efficiencies for the Main Effect Model

Jones and Nachtsheim (2011),

$$D_e(d, d_D) = \left(\frac{|\mathbf{X}(\mathbf{d})'\mathbf{X}(\mathbf{d})|}{|\mathbf{X}(\mathbf{d_D})'\mathbf{X}(\mathbf{d_D})|}\right)^{1/p},$$

where X(d) is the design matrix of design d, d_D is the D-optimal design, and p is the number of intercept and main effects terms in the model. Furthermore, we define the relative ratio as

relative ratio =
$$\frac{D_e(d_P, d_D)}{D_e(d_{J\&N}, d_D)}$$
,

where d_P is the proposed design and $d_{J\&N}$ is Jones and Nachtsheim's design.

The relative D-efficiency between Jones and Nachtsheim's design and the proposed design for the main-effect model is shown in Table 1. The proposed designs for m=6 through 30 (except 22) are all orthogonal for main effects. For m=12,14,16,18,20,24,26,28,30, the proposed designs are all superior to those in Jones and Nachtsheim (2011) in terms of D-efficiency. If a quadratic model is considered (with main and quadratic effects), the relative ratio can be verified as 100% for $4 \le m \le 10$ and between 101.4% to 103.4% for $12 \le m \le 30$ (except 22).

Discussion and Conclusion

For the definitive screening design, the model matrix can be represented as

$$\mathbf{M} = \begin{pmatrix} 1 & x_1, \cdots, x_m & x_1^2, \cdots, x_m^2 & x_1x_2, \cdots, x_{m-1}x_m \\ \mathbf{1}_{m \times 1} & \mathbf{C}_{m \times m} & \mathbf{Q}_{m \times m} & \mathbf{P}_{m \times m(m-1)/2} \\ \mathbf{1}_{m \times 1} & -\mathbf{C}_{m \times m} & \mathbf{Q}_{m \times m} & \mathbf{P}_{m \times m(m-1)/2} \\ \mathbf{1}_{1 \times 1} & \mathbf{0}_{1 \times m} & \mathbf{0}_{1 \times m} & \mathbf{0}_{1 \times m(m-1)/2} \end{pmatrix},$$

where

$$\begin{pmatrix} \mathbf{C} \\ -\mathbf{C} \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \mathbf{Q} \\ \mathbf{Q} \\ \mathbf{0} \end{pmatrix}, \text{ and } \begin{pmatrix} \mathbf{P} \\ \mathbf{P} \\ \mathbf{0} \end{pmatrix}$$

represent main effects, pure-quadratic effects, and

two-factor interaction effects, respectively; $\mathbf{1}_{m\times 1}$ is an $m\times 1$ matrix with all entries equal to one, $\mathbf{0}_{1\times m}$ is a $1\times m$ zero matrix, and $\mathbf{C}_{m\times m}$ is an $m\times m$ conference matrix. The inner product matrix can then be represented as follows:

^{*}Relative Ratio = $D_e(d_P, d_D)/D_e(d_{J\&N}, d_D)$, where $D_e(d_P, d_D)$ is the D-efficiency of the proposed design and $D_e(d_{J\&N}, d_D)$ is the D-efficiency of Jones and Nachtsheim's design.

^{**}NA = "not available". Conference matrix of order 22 does not exist.

where ${\bf I}$ is the identity matrix and ${\bf J}$ is the matrix with all 1's. It is clear that

- 1. All main effects are orthogonal to each other.
- 2. All main effects and quadratic effects are orthogonal.
- 3. All main effects and two-factor interaction effects are orthogonal.
- 4. The inner products among quadratic effects can be represented as $2(m-2)\mathbf{J} + 2\mathbf{I}$, i.e., the diagonal element is 2m-2 and the off-diagonal element is 2m-4.
- 5. The inner products between the pure-quadratic effects and the two-factor interaction effects can be represented as $2\mathbf{Q}'\mathbf{P}$, whose entries belong to the set $\{-2,0,2\}$. Consequently, the correlation between the two columns is

$$r_{qq,st}^{c}(m) = \pm \sqrt{\frac{2m+1}{3(m-1)(m-2)}},$$

as shown in Jones and Nachtsheim (2011). Thus, Columns 4 and 5 in their Table 3 should be identical for even m. Namely, $\overline{|r_{qq,st}^c(m)|} = |r_{qq,st}^c(m)|^{\max}$.

6. The inner products among two-factor interaction effects are rather complicated. The inner-product matrix $2\mathbf{P}'\mathbf{P}$ has its diagonal entries 2(m-2), and off-diagonal entries belong to the set $\{0, \pm 2, \pm 4, \cdots, \pm 2(m-4)\}$.

The construction of conference matrices is well studied in the literature. For $m \equiv 0 \pmod{4}$, a multiple of four, a conference matrix can be obtained via a Hadamard matrix by $\mathbf{C} = \mathbf{H} - \mathbf{I}$, where \mathbf{H} is a skew-Hadamard matrix and \mathbf{I} is the identity matrix (see, for example, Koulouvinos and Stylianou (2008)). For $m \equiv 2 \pmod{4}$, an even number but not a multiple

of four, conference matrices can be found for m=2, 6, 10, 14, 18, 26, 30, 38, 42, 46, 50, 54, 62. Especially when (m-1) is a sum of two squares, some related theorems can be found in Van Lint and Seidel (1966).

The method proposed in this paper only works when m is even. When the number of factors mis odd, we suggest deleting the last column of an $(m+1)\times(m+1)$ conference matrix. However, this will be two more runs than necessary and is no longer a definitive design by definition. For an odd number of factors and 2m+1 runs, we cannot find better designs than the ones proposed by Jones and Nachtsheim (2011). For saturated cases, we suggest using their designs. It might occur to some practitioners after dropping the column to further remove the two rows having no zero values to form a potential definitive design for odd m. This would be a bad idea, as the resulting design will be singular for the main-effect model. One referee pointed out that it is not advisable to use a conference matrix itself for a screening design. This is sensible advice.

A conference matrix is a special case of a weighing matrix (Raghavarao (1959)). We may replace the conference matrix in the proposed design by a weighing matrix and get a series of orthogonal maineffect designs that have the same properties as shown above. This deserves further study.

Appendix A Theoretical Properties of the Proposed Design

1. It is a saturated design for estimating the intercept, all m main effects, and all m quadratic effects. Assume the model contains the intercept, m main effects, and m pure quadratic effects,

so the model matrix is

$$\mathbf{X} = \begin{pmatrix} \mathbf{1}_{m\times 1} & \mathbf{C}_{m\times m} & \mathbf{Q}_{m\times m} \\ \mathbf{1}_{m\times 1} & -\mathbf{C}_{m\times m} & \mathbf{Q}_{m\times m} \\ \mathbf{1}_{1\times 1} & \mathbf{0}_{1\times m} & \mathbf{0}_{1\times m} \end{pmatrix},$$

where

$$\begin{pmatrix} \mathbf{Q} \\ \mathbf{Q} \\ \mathbf{0} \end{pmatrix}$$

denote the matrix for m pure quadratic effects, \mathbf{Q} is $m \times m$ matrix with zero diagonal entries, and other entries are all 1's. Let $\|\mathbf{X}\|$ denote the determinant of a square matrix \mathbf{X} , then we have

$$\|\mathbf{X}\| = \begin{pmatrix} \mathbf{1}_{m \times 1} & \mathbf{C}_{m \times m} & \mathbf{Q}_{m \times m} \\ \mathbf{1}_{m \times 1} & -\mathbf{C}_{m \times m} & \mathbf{Q}_{m \times m} \\ \mathbf{1}_{1 \times 1} & \mathbf{0}_{1 \times m} & \mathbf{0}_{1 \times m} \end{pmatrix}$$

$$= (-1)^{2m+1+1} \times 1 \times \begin{pmatrix} \mathbf{C} & \mathbf{Q} \\ -\mathbf{C} & \mathbf{Q} \end{pmatrix}$$

$$= \|\mathbf{C}\| \times \|2\mathbf{Q}\|$$

$$= (m-1)^{m/2} \times 2^m \times (-1)^{m-1} \times (m-1)$$

$$= (-1)^{m-1} \times 2^m \times (m-1)^{m/2+1}.$$

When m is even, this determinant cannot be zero. Namely, the model matrix is invertible. Therefore, it is possible to estimate the intercept, all m main effects, and all m quadratic effects.

2. All main effects are orthogonal to all quadratic effects. The design matrix for main effects is

$$\mathbf{X}_1 = \begin{pmatrix} \mathbf{C}_{m \times m} \\ -\mathbf{C}_{m \times m} \\ \mathbf{0}_{1 \times m} \end{pmatrix},$$

while the matrix for quadratic effects can be expressed as

$$\mathbf{X}_{22} = \begin{pmatrix} \mathbf{Q}_{m \times m} \\ \mathbf{Q}_{m \times m} \\ \mathbf{0}_{1 \times m} \end{pmatrix}.$$

Thus, we have

$$\mathbf{X}_1'\mathbf{X}_{22} = (\mathbf{C}' \quad -\mathbf{C}' \quad \mathbf{0}_{m \times 1}) \times \begin{pmatrix} \mathbf{Q} \\ \mathbf{Q} \\ \mathbf{0}_{1 \times m} \end{pmatrix}$$

$$= (\mathbf{C}'\mathbf{Q} - \mathbf{C}'\mathbf{Q} + \mathbf{0}_{m \times 1} \times \mathbf{0}_{1 \times m})$$

$$= \mathbf{0}_{m \times m}.$$

That is, all main effects are orthogonal to all quadratic effects.

3. All main effects are orthogonal to all two-factor interactions, that is, the alias matrix, A, is a zero matrix. The design matrix for main effects is

$$\mathbf{X}_1 = \begin{pmatrix} \mathbf{C}_{m \times m} \\ -\mathbf{C}_{m \times m} \\ \mathbf{0}_{1 \times m} \end{pmatrix},$$

while the matrix for two-factor interactions has the following structure:

$$\mathbf{X}_2 = egin{pmatrix} \mathbf{P}_{m imes m(m-1)/2} \ \mathbf{P}_{m imes m(m-1)/2} \ \mathbf{0}_{1 imes m(m-1)/2} \end{pmatrix}.$$

Thus, the alias matrix is

$$\begin{split} \mathbf{A} &= (\mathbf{X}_1'\mathbf{X}_1)^{-1} \times \mathbf{X}_1'\mathbf{X}_2 \\ &= (\mathbf{X}_1'\mathbf{X}_1)^{-1} \times (\mathbf{C}' - \mathbf{C}' \quad \mathbf{0}) \times \begin{pmatrix} \mathbf{P} \\ \mathbf{P} \\ \mathbf{0} \end{pmatrix} \\ &= (\mathbf{X}_1'\mathbf{X}_1)^{-1} \times (\mathbf{C}'\mathbf{P} - \mathbf{C}'\mathbf{P} + \mathbf{0}) \\ &= \mathbf{0}_{m \times m(m-1)/2}. \end{split}$$

A is identically zero; therefore, all main effects are orthogonal to all two-factor interactions.

Appendix B Conference Matrices for m = 2, 4, ..., 18

$$C_{2} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ -1 & 0 & -1 & 1 \\ -1 & 1 & 0 & -1 \\ -1 & -1 & 1 & 0 \end{pmatrix}$$

$$C_{4} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ -1 & 1 & 0 & -1 \\ -1 & -1 & 1 & 0 \end{pmatrix}$$

$$C_{6} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & -1 & -1 \\ 1 & 1 & 0 & -1 & -1 & 1 \\ 1 & 1 & -1 & 0 & 1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 1 \\ 1 & -1 & 1 & -1 & 1 & 0 \end{pmatrix}$$

$$C_{8} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 0 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 0 & 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & 0 & 1 & 1 & -1 & -1 \\ -1 & 1 & 1 & -1 & 0 & -1 & 1 & -1 \\ -1 & -1 & 1 & -1 & 1 & 0 & -1 \\ -1 & -1 & 1 & 1 & -1 & 1 & 0 & -1 \\ -1 & -1 & -1 & 1 & 1 & -1 & 1 & 0 \end{pmatrix}$$

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