

Proofs and Selected Design Augmentations

Supplement to “An Integrative Framework for Geometric and Hidden Projections in Three-Level Fractional Factorial Designs”

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1. Proofs

Proof of Lemma 1. We have $|\mathcal{F}| = \sum_{x \in \mathcal{D}_s} F_{\mathcal{F}}(x) = \sum_{x \in \mathcal{D}_s} \sum_{I \in \mathcal{I}} \sum_{T \in \mathcal{T}_I} b_{\mathcal{F}, I, T} X_{I, T}(x) = 3^s b_{\mathcal{F}, \phi, \phi}$, and so $b_{\mathcal{F}, \phi, \phi} = 3^{-s} |\mathcal{F}|$. $\square$

Proof of Lemma 2. For one factor A_{j_1} , as $b_{\mathcal{H}, \phi, \phi} = 3^{-p}(|\mathcal{F}| + |\mathcal{G}|) = 3^{s-p} b_{\mathcal{F}, \phi, \phi} + b_{\mathcal{G}, \phi, \phi}$,

$$\begin{aligned} \begin{pmatrix} b_{\mathcal{H}, j_1, L} \\ b_{\mathcal{H}, j_1, Q} \end{pmatrix} &= 2^{-1} 3^{1-p} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} |\mathcal{F}_{j_1, L}| + |\mathcal{G}_{j_1, L}| \\ |\mathcal{F}_{j_1, Q}| + |\mathcal{G}_{j_1, Q}| \end{pmatrix} - \begin{pmatrix} 0 \\ 3^{s-p} b_{\mathcal{F}, \phi, \phi} + b_{\mathcal{G}, \phi, \phi} \end{pmatrix} \\ &= 3^{s-p} \begin{pmatrix} b_{\mathcal{F}, j_1, L} \\ b_{\mathcal{F}, j_1, Q} \end{pmatrix} + \begin{pmatrix} b_{\mathcal{G}, j_1, L} \\ b_{\mathcal{G}, j_1, Q} \end{pmatrix}. \end{aligned}$$

For distinct A_{j_1} and A_{j_2} , $B_{\mathcal{H}, j_1 j_2, LQ} = 3^{s-p} b_{\mathcal{F}, j_1, L} + b_{\mathcal{G}, j_1, L}$, $B_{\mathcal{H}, j_1 j_2, QL} = 3^{s-p} b_{\mathcal{F}, j_2, L} + b_{\mathcal{G}, j_2, L}$, and $B_{\mathcal{H}, j_1 j_2, QQ} = 3^{s-p} (b_{\mathcal{F}, \phi, \phi} + b_{\mathcal{F}, j_1, Q} + b_{\mathcal{F}, j_2, Q}) + b_{\mathcal{G}, \phi, \phi} + b_{\mathcal{G}, j_1, Q} + b_{\mathcal{G}, j_2, Q}$. As $|\mathcal{H}_{j_1 j_2, TS}| = |\mathcal{F}_{j_1 j_2, TS}| + |\mathcal{G}_{j_1 j_2, TS}|$ for all $T, S \in \{L, Q\}$, we have that $(A_{j_1} \otimes A_{j_2})_{\mathcal{H}} = 3^{s-p} (A_{j_1} \otimes A_{j_2})_{\mathcal{F}} + (A_{j_1} \otimes A_{j_2})_{\mathcal{G}}$. The general result then follows by induction. $\square$

Proof of Theorem 1. By Lemma 1, the construction of the smallest follow-up design is equivalent to identifying a valid set of indicator function coefficients $\mathbf{b}_{\mathcal{G}}$ with minimum $b_{\mathcal{G}, \phi, \phi}$. In order for $\mathbf{b}_{\mathcal{G}}$ to be valid, each row of $\mathbf{M}_p \mathbf{b}_{\mathcal{G}}$ must be either 0 or 1,

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which holds if and only if $(\mathbf{M}_p \mathbf{b}_G) \odot (\mathbf{1}_{|\mathcal{D}_p|} - \mathbf{M}_p \mathbf{b}_G) = (0, \dots, 0)^\top$. Lemma 2 specifies the indicator function coefficients for $\mathcal{G}$ that are necessary to yield the desired aliasing structure for $\mathcal{H}$. Thus, the construction of the smallest follow-up design is equivalent to finding $\mathbf{b}_G$ that minimizes $b_{G,\phi,\phi}$ subject to these constraints. $\square$

Proof of Corollary 1. By inspection of the second-order model, an augmented design $\mathcal{H}$ satisfies the second-order orthogonality criterion if and only if all of its indicator function coefficients of the form $b_{\mathcal{H},i,L}$, $b_{\mathcal{H},i,Q}$, $b_{\mathcal{H},ij,LL}$, $b_{\mathcal{H},ij,LQ}$, $b_{\mathcal{H},ij,QQ}$, and $b_{\mathcal{H},ijk,LLL}$ are zero. We enter these conditions into Theorem 1 to obtain the optimization. $\square$

Proof of Lemma 3. For $(i, j) \in \{1, \dots, (p+1)(p+2)/2\}$, entry (i, j) of $\mathbf{X}_{\mathcal{F}}^\top \mathbf{X}_{\mathcal{F}}$ is the dot product of columns i and j of $\mathbf{X}_{\mathcal{F}}$, which is equivalently expressed as

$$\sum_{x \in \mathcal{F}} Z_{(i)}(x) Z_{(j)}(x) = \sum_{x \in \mathcal{D}_p} F_{\mathcal{F}}(x) Z_{(i)}(x) Z_{(j)}(x).$$

$\square$

Proof of Theorem 2. The entries of $\mathbf{X}_{\mathcal{H}}^\top \mathbf{X}_{\mathcal{H}}$ are derived by combining Lemma 3 with the aliasing relations induced by the second-order orthogonality criterion to calculate the inner products of contrast vectors across the columns of $\mathbf{X}_{\mathcal{H}}$. Then $\det(\mathbf{X}_{\mathcal{H}}^\top \mathbf{X}_{\mathcal{H}})$ and $(\mathbf{X}_{\mathcal{H}}^\top \mathbf{X}_{\mathcal{H}})^{-1}$ follow from the block-matrix structure for $\mathbf{X}_{\mathcal{H}}^\top \mathbf{X}_{\mathcal{H}}$. $\square$

2. Selected Designs and Augmentations

Selected three-level fractional factorial designs, their augmentations, and further details for the case studies considered in Sections 1, 3.2, 4.2, and 4.3 are summarized in the following tables and figures.

Table 1: The DSD(13), with $A_1, \dots, A_6$ denoting its six factors and $-1, 0$, and 1 their levels (Jones and Nachtsheim, 2011, p. 5).

Run	A_1	A_2	A_3	A_4	A_5	A_6
1	0	1	-1	-1	-1	-1
2	0	-1	1	1	1	1
3	1	0	-1	1	1	-1
4	-1	0	1	-1	-1	1
5	-1	-1	0	1	-1	-1
6	1	1	0	-1	1	1
7	-1	1	1	0	1	-1
8	1	-1	-1	0	-1	1
9	1	-1	1	-1	0	-1
10	-1	1	-1	1	0	1
11	1	1	1	1	-1	0
12	-1	-1	-1	-1	1	0
13	0	0	0	0	0	0

Table 2: The 3_{III}^{3-1} regular fractional factorial design. Under the orthogonal components system, in which our levels of $-1, 0$, and 1 are coded as $0, 1$, and 2 modulo 3 , the third factor is defined as the sum of the first two factors modulo 3 .

Run	A_1	A_2	A_3
1	-1	-1	-1
2	-1	0	0
3	-1	1	1
4	0	-1	0
5	0	0	1
6	0	1	-1
7	1	-1	1
8	1	0	-1
9	1	1	0

Table 3: A follow-up design to the 3_{III}^{3-1} regular fraction in Table 2 that yields an augmentation satisfying the second-order orthogonality criterion for all factors.

Run	A_1	A_2	A_3
10	-1	-1	1
11	-1	0	0
12	-1	1	-1
13	0	-1	0
14	0	0	-1
15	0	1	1
16	1	-1	-1
17	1	0	1
18	1	1	0

Table 4: The DSD(11) with five factors (Jones and Nachtsheim, 2011, p. 5).

Run	A_1	A_2	A_3	A_4	A_5
1	0	1	1	-1	-1
2	0	-1	-1	1	1
3	1	0	-1	-1	1
4	-1	0	1	1	-1
5	1	-1	0	1	-1
6	-1	1	0	-1	1
7	1	-1	1	0	1
8	-1	1	-1	0	-1
9	1	1	1	1	0
10	-1	-1	-1	-1	0
11	0	0	0	0	0

Table 5: Two follow-up designs to the projection onto factors A_1, A_2, A_3 , and A_4 of the DSD(11) in Table 4 that yield augmented designs satisfying the second-order orthogonality criterion. The right set of runs yields an augmented design that is A- and D-optimum with respect to the second-order model among all candidate augmentations.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
12	-1	-1	0	0	12	-1	-1	0	0
13	-1	-1	1	-1	13	-1	-1	1	-1
14	-1	0	0	1	14	-1	0	-1	1
15	-1	0	1	1	15	-1	0	1	0
16	-1	1	-1	0	16	-1	1	0	1
17	0	-1	-1	1	17	0	-1	-1	0
18	0	-1	0	-1	18	0	-1	1	1
19	0	0	-1	0	19	0	0	0	-1
20	0	0	1	0	20	0	0	0	1
21	0	1	0	1	21	0	1	-1	-1
22	0	1	1	-1	22	0	1	1	0
23	1	-1	1	0	23	1	-1	0	-1
24	1	0	-1	-1	24	1	0	-1	0
25	1	0	0	-1	25	1	0	1	-1
26	1	1	-1	1	26	1	1	-1	1
27	1	1	0	0	27	1	1	0	0

Table 6: The second follow-up design of size 16 to the first four factors of the DSD(11) that yields an augmented design that is A- and D-optimum with respect to the second-order model and satisfies the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4
12	-1	-1	0	1
13	-1	-1	1	-1
14	-1	0	-1	1
15	-1	0	0	0
16	-1	1	1	0
17	0	-1	0	-1
18	0	-1	1	0
19	0	0	-1	-1
20	0	0	1	1
21	0	1	-1	0
22	0	1	0	1
23	1	-1	-1	0
24	1	0	0	0
25	1	0	1	-1
26	1	1	-1	1
27	1	1	0	-1

Table 7: The follow-up design of size 16 to the first four factors of the DSD(11) that yields an augmented design that is E- and G-optimum with respect to the second-order model and satisfies the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4
12	-1	-1	0	0
13	-1	-1	1	-1
14	-1	0	-1	1
15	-1	0	0	1
16	-1	1	1	0
17	0	-1	0	-1
18	0	-1	1	1
19	0	0	-1	0
20	0	0	1	0
21	0	1	-1	-1
22	0	1	0	1
23	1	-1	-1	0
24	1	0	0	-1
25	1	0	1	-1
26	1	1	-1	1
27	1	1	0	0

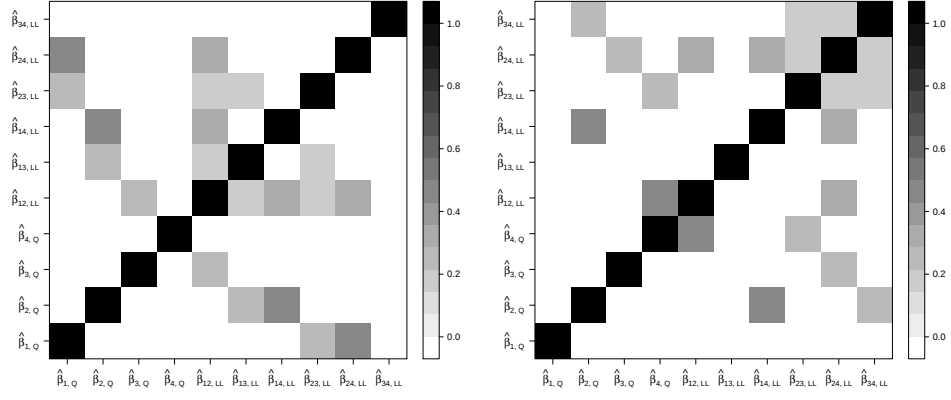


Figure 1: Absolute correlations among second-order contrasts for the A- and D-optimum augmented designs for factors A_1, A_2, A_3 , and A_4 of the DSD(11) that are formed from the corresponding follow-up runs in Tables 5 and 6. The absolute correlations are in grayscale, with white denoting zero correlation and black an absolute correlation of one. Under the second-order orthogonality criterion, all cells involving at least one linear main effect (excluding diagonals) or two distinct quadratic main effects are white.

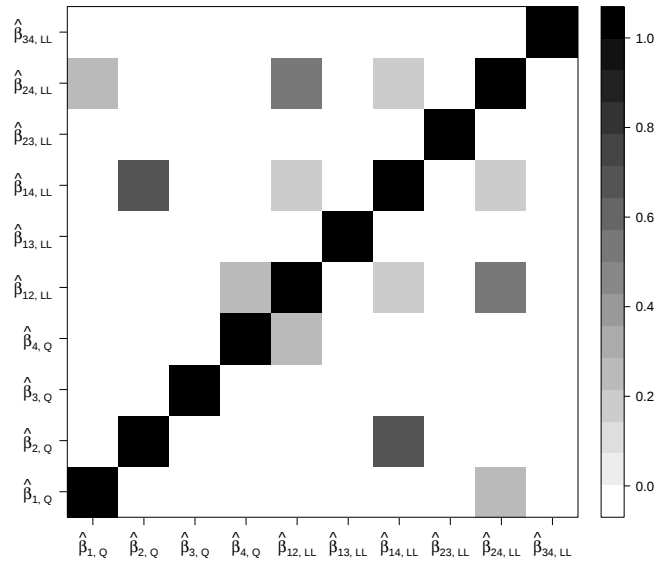


Figure 2: Absolute correlations among second-order contrasts for the E- and G-optimum augmented design for factors A_1, A_2, A_3 , and A_4 of the DSD(11) that is formed from the corresponding follow-up runs in Table 7.

Table 8: Two sets of follow-up runs to the projection onto factors A_1, A_2, A_3 , and A_4 of the DSD(13) in Table 1 that yield augmented designs satisfying the second-order orthogonality criterion. The right set of runs yields an augmented design that is A-, D-, and E-optimum with respect to the second-order model among all candidate augmentations.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	1	1	1	0	14	-1	-1	1	0
15	1	0	0	1	15	-1	0	-1	0
16	1	0	-1	0	16	-1	0	0	1
17	1	-1	0	-1	17	-1	1	0	-1
18	0	1	0	0	18	0	-1	-1	-1
19	0	1	-1	-1	19	0	-1	0	0
20	0	0	1	-1	20	0	0	-1	1
21	0	0	-1	1	21	0	0	1	-1
22	0	-1	1	1	22	0	1	0	0
23	0	-1	0	0	23	0	1	1	1
24	-1	1	0	1	24	1	-1	0	1
25	-1	0	1	0	25	1	0	0	-1
26	-1	0	0	-1	26	1	0	1	0
27	-1	-1	-1	0	27	1	1	-1	0

Table 9: Two sets of follow-up runs to the projection onto factors A_1, A_2, A_3 , and A_4 of the DSD(13) in Table 1 that yield augmented designs satisfying the second-order orthogonality criterion and are A- and E-optimum (left), and G-optimum (right), respectively, with respect to the second-order model among all candidate augmentations.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	0	0	14	-1	-1	0	0
15	-1	0	-1	0	15	-1	0	0	1
16	-1	0	1	1	16	-1	0	1	0
17	-1	1	0	-1	17	-1	1	-1	-1
18	0	-1	-1	0	18	0	-1	-1	0
19	0	-1	1	-1	19	0	-1	0	-1
20	0	0	0	-1	20	0	0	-1	1
21	0	0	0	1	21	0	0	1	-1
22	0	1	-1	1	22	0	1	0	1
23	0	1	1	0	23	0	1	1	0
24	1	-1	0	1	24	1	-1	1	1
25	1	0	-1	-1	25	1	0	-1	0
26	1	0	1	0	26	1	0	0	-1
27	1	1	0	0	27	1	1	0	0

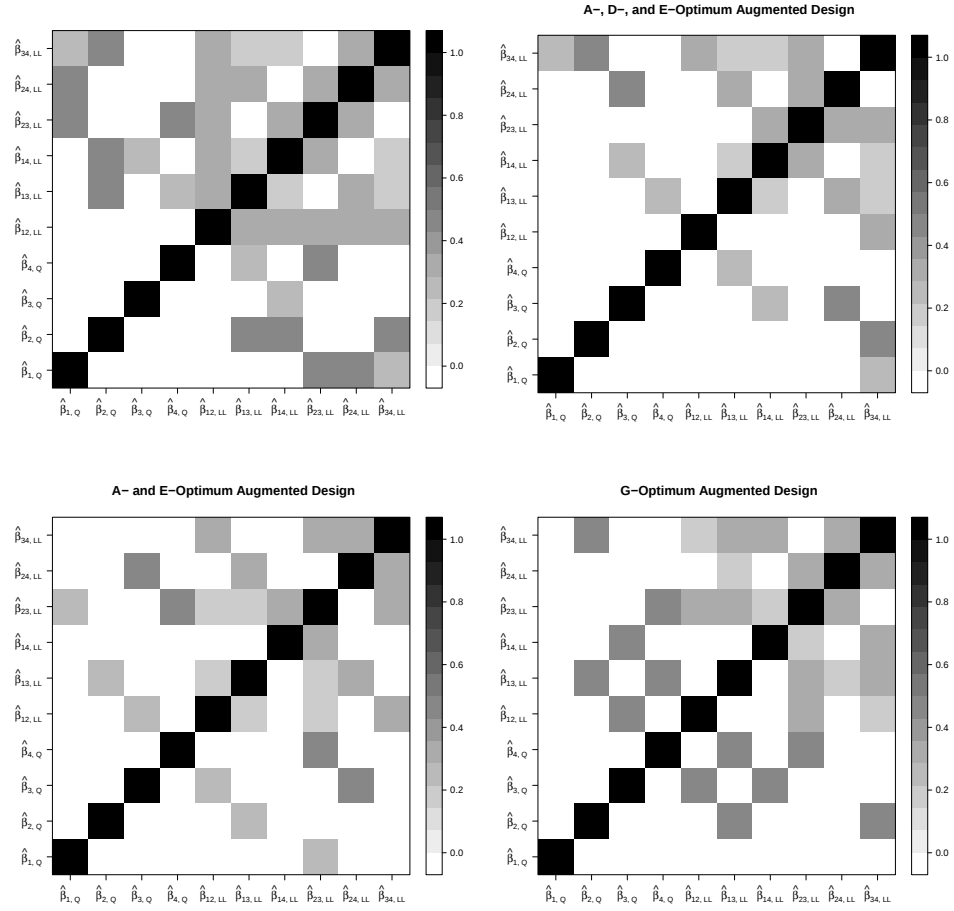


Figure 3: Absolute correlations of second-order contrasts for distinct candidate augmented designs for the first four factors of the DSD(13) that correspond to the follow-up runs in Tables 8 and 9. One candidate design is optimum with respect to the A-, D-, and E-optimality criteria, another is optimum only with respect to the A- and E-optimality criteria, and the last is optimum only with respect to the G-optimality criteria, for the second-order model.

Table 10: The first two follow-up designs of size 14 to the factors A_1, A_2, A_3 , and A_4 of the DSD(13) that yield augmented designs that are A-, D-, and E-optimum with respect to the second-order model and satisfy the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	1	0	14	-1	-1	0	0
15	-1	0	-1	0	15	-1	0	0	-1
16	-1	0	0	1	16	-1	0	1	1
17	-1	1	0	-1	17	-1	1	-1	0
18	0	-1	-1	-1	18	0	-1	-1	1
19	0	-1	0	0	19	0	-1	0	-1
20	0	0	-1	1	20	0	0	-1	0
21	0	0	1	-1	21	0	0	1	0
22	0	1	0	0	22	0	1	0	1
23	0	1	1	1	23	0	1	1	-1
24	1	-1	0	1	24	1	-1	1	0
25	1	0	0	-1	25	1	0	-1	-1
26	1	0	1	0	26	1	0	0	1
27	1	1	-1	0	27	1	1	0	0

Table 11: The second two follow-up designs of size 14 to the factors A_1, A_2, A_3 , and A_4 of the DSD(13) that yield augmented designs that are A-, D-, and E-optimum with respect to the second-order model and satisfy the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	1	0	14	-1	-1	-1	0
15	-1	0	-1	-1	15	-1	0	0	0
16	-1	0	0	1	16	-1	0	1	1
17	-1	1	0	0	17	-1	1	0	-1
18	0	-1	-1	1	18	0	-1	0	-1
19	0	-1	0	-1	19	0	-1	1	0
20	0	0	-1	0	20	0	0	-1	1
21	0	0	1	0	21	0	0	1	-1
22	0	1	0	1	22	0	1	-1	0
23	0	1	1	-1	23	0	1	0	1
24	1	-1	0	0	24	1	-1	0	1
25	1	0	0	-1	25	1	0	-1	-1
26	1	0	1	1	26	1	0	0	0
27	1	1	-1	0	27	1	1	1	0

Table 12: The final two follow-up designs of size 14 to the factors A_1, A_2, A_3 , and A_4 of the DSD(13) that yield augmented designs that are A-, D-, and E-optimum with respect to the second-order model and satisfy the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	0	-1	14	-1	-1	1	0
15	-1	0	-1	0	15	-1	0	-1	1
16	-1	0	1	1	16	-1	0	0	0
17	-1	1	0	0	17	-1	1	0	-1
18	0	-1	-1	1	18	0	-1	-1	0
19	0	-1	1	0	19	0	-1	0	-1
20	0	0	0	-1	20	0	0	-1	-1
21	0	0	0	1	21	0	0	1	1
22	0	1	-1	0	22	0	1	0	1
23	0	1	1	-1	23	0	1	1	0
24	1	-1	0	0	24	1	-1	0	1
25	1	0	-1	-1	25	1	0	0	0
26	1	0	1	0	26	1	0	1	-1
27	1	1	0	1	27	1	1	-1	0

Table 13: The two follow-up designs of size 14 to the factors A_1, A_2, A_3 , and A_4 of the DSD(13) that yield augmented designs that are only A- and E-optimum with respect to the second-order model and satisfy the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	0	0	14	-1	-1	1	0
15	-1	0	-1	0	15	-1	0	-1	0
16	-1	0	1	1	16	-1	0	0	-1
17	-1	1	0	-1	17	-1	1	0	1
18	0	-1	-1	0	18	0	-1	-1	1
19	0	-1	1	-1	19	0	-1	0	0
20	0	0	0	-1	20	0	0	-1	-1
21	0	0	0	1	21	0	0	1	1
22	0	1	-1	1	22	0	1	0	0
23	0	1	1	0	23	0	1	1	-1
24	1	-1	0	1	24	1	-1	0	-1
25	1	0	-1	-1	25	1	0	0	1
26	1	0	1	0	26	1	0	1	0
27	1	1	0	0	27	1	1	-1	0

Table 14: The first two follow-up designs of size 14 to the factors A_1, A_2, A_3 , and A_4 of the DSD(13) that yield augmented designs that are only G-optimum with respect to the second-order model and satisfy the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	0	0,	14	-1	-1	0	0
15	-1	0	0	1	15	-1	0	-1	0
16	-1	0	1	0	16	-1	0	0	-1
17	-1	1	-1	-1	17	-1	1	1	1
18	0	-1	-1	0	18	0	-1	0	1
19	0	-1	0	-1	19	0	-1	1	0
20	0	0	-1	1	20	0	0	-1	1
21	0	0	1	-1	21	0	0	1	-1
22	0	1	0	1	22	0	1	-1	0
23	0	1	1	0	23	0	1	0	-1
24	1	-1	1	1	24	1	-1	-1	-1
25	1	0	-1	0	25	1	0	0	1
26	1	0	0	-1	26	1	0	1	0
27	1	1	0	0	27	1	1	0	0

Table 15: The second two follow-up designs of size 14 to the factors A_1, A_2, A_3 , and A_4 of the DSD(13) that yield augmented designs that are only G-optimum with respect to the second-order model and satisfy the second-order orthogonality criterion.

Run	A_1	A_2	A_3	A_4	Run	A_1	A_2	A_3	A_4
14	-1	-1	1	-1	14	-1	-1	-1	1
15	-1	0	-1	0	15	-1	0	0	-1
16	-1	0	0	1	16	-1	0	1	0
17	-1	1	0	0	17	-1	1	0	0
18	0	-1	-1	0	18	0	-1	0	-1
19	0	-1	0	1	19	0	-1	1	0
20	0	0	-1	-1	20	0	0	-1	-1
21	0	0	1	1	21	0	0	1	1
22	0	1	0	-1	22	0	1	-1	0
23	0	1	1	0	23	0	1	0	1
24	1	-1	0	0	24	1	-1	0	0
25	1	0	0	-1	25	1	0	-1	0
26	1	0	1	0	26	1	0	0	1
27	1	1	-1	1	27	1	1	1	-1

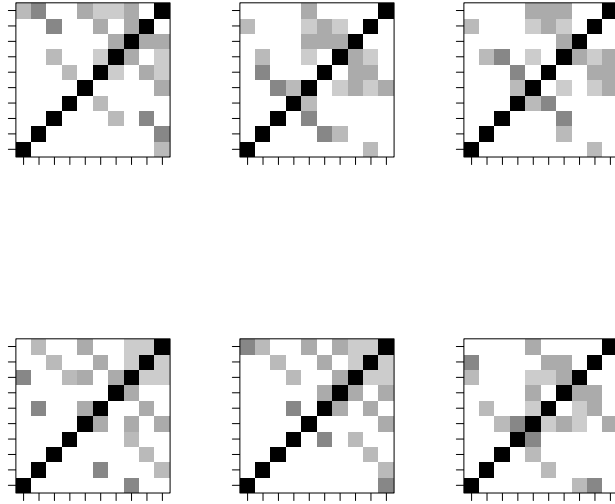


Figure 4: Absolute correlations among second-order contrasts for the A-, D-, and E-optimum augmented designs for the first four factors of the DSD(13).

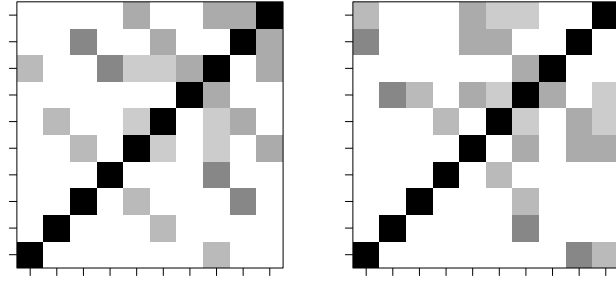


Figure 5: Absolute correlations among second-order contrasts for the A- and E-optimum augmented designs for the first four factors of the DSD(13).

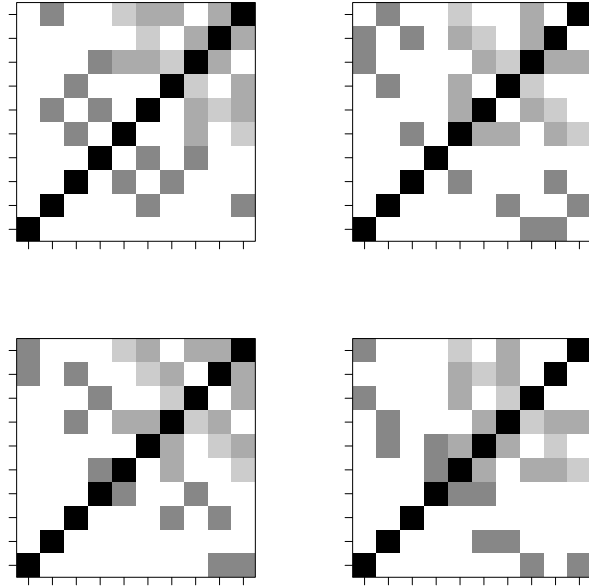


Figure 6: Absolute correlations among second-order contrasts for the G-optimum augmented designs for the first four factors of the DSD(13).

Table 16: Two follow-up designs to the DSD(13) that yield augmented designs satisfying the second-order orthogonality criterion for all factors.

Run	A_1	A_2	A_3	A_4	A_5	A_6	Run	A_1	A_2	A_3	A_4	A_5	A_6
14	1	1	1	0	0	-1	14	-1	-1	0	-1	1	0
15	1	0	0	1	-1	1	15	-1	0	-1	0	-1	1
16	1	0	-1	0	1	0	16	-1	0	0	1	0	-1
17	1	-1	0	-1	0	0	17	-1	1	1	0	0	0
18	0	1	0	0	1	1	18	0	-1	0	0	-1	-1
19	0	1	-1	-1	-1	0	19	0	-1	1	1	0	1
20	0	0	1	-1	0	1	20	0	0	-1	1	1	0
21	0	0	-1	1	0	-1	21	0	0	1	-1	-1	0
22	0	-1	1	1	1	0	22	0	1	-1	-1	0	-1
23	0	-1	0	0	-1	-1	23	0	1	0	0	1	1
24	-1	1	0	1	0	0	24	1	-1	-1	0	0	0
25	-1	0	1	0	-1	0	25	1	0	0	-1	0	1
26	-1	0	0	-1	1	-1	26	1	0	1	0	1	-1
27	-1	-1	-1	0	0	1	27	1	1	0	1	-1	0

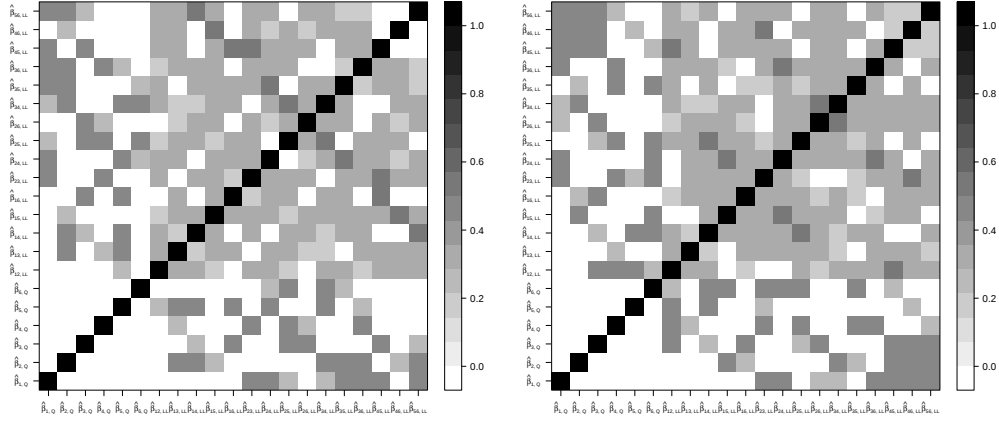


Figure 7: Absolute correlations among second-order contrasts for the designs formed by augmenting the DSD(13) with the follow-up runs in Table 16, respectively.

References

- Jones, B., Nachtsheim, C. J., 2011. A class of three-level designs for definitive screening in the presence of second-order effects. *Journal of Quality Technology* 43 (1), 1–15.