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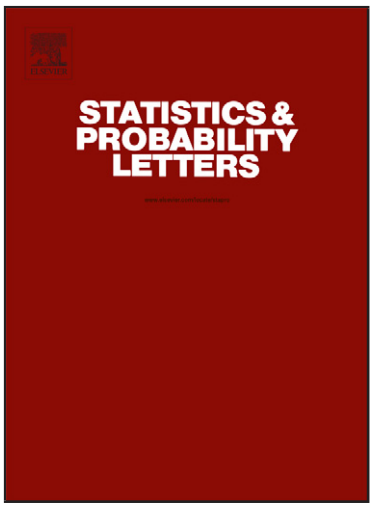

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Schur- and E-Optimal Two-Level Factorial Designs

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Summary

Schur-optimality is a very general class of optimality criteria that includes, as special cases, A- D- and E-optimality and Cheng (1978) Type 1 optimality. In this paper, Schur-optimal two-level factorial designs under a second-order model are derived for 3 and 5 factors for all numbers of runs where the model is estimable. In addition, orthogonal arrays of strength 4 (resolution V) with e added runs are shown to be E-optimal under a second-order model for $e \leq 10$ and $m = 4$ factors and for $e \leq 15$ and $m \geq 5$ factors. Corresponding results for third-order models are also given.
Some key words: Defining contrasts; Fractional factorial; Main effect; Majorization; Optimum design; Regular design; Two-factor interaction.

1 Introduction

There are various known optimality results for two-level factorial designs in cases where an orthogonal design is not possible. For first-order models, consisting of main effects and a mean, an orthogonal design exists for $n \equiv 0 \bmod 4$ runs by using columns from a Hadamard matrix or Plackett & Burman (1946) design. Cheng (1980) showed that adding any extra two-level run is optimal for first-order models under the Cheng (1978) Type 1 optimality criteria. Jacroux, Wong & Masaro (1983) showed that adding two specific extra runs is also Type 1 optimal. The case of $n \equiv 3 \bmod 4$ is more problematic and different Type 1 optimality criteria, such as A-, D- and E-optimality, tend to have different optimal designs.

For second-order models, consisting of main effects, two-factor interactions and a mean, orthogonality is achieved using orthogonal arrays of strength 4 (Rao, 1947), or regular designs of resolution V or more (Finney, 1945; Box & Hunter, 1961a,b). Type 1 optimality for one extra run and two specific runs is respectively shown by Cheng (1980) and Chadjiconstantinidis, Cheng & Moyssiadis (1989). Butler & Ramos (2007) provide optimal additions and deletions to orthogonal arrays of strength 4 under the very general Schur-optimality criteria (Marshall & Olkin, 1979; Giovagnoli & Wynn, 1981).

Mukerjee (1995) derives E-optimality results under various order models for multi-level orthogonal arrays with additional runs; see also Dey & Mukerjee (1999). In this paper, the results are extended in the case of two-level factorial designs. It is shown that two-level orthogonal arrays of strength 4 with e additional runs are E-optimal under a second-order model for $e \leq 10$ and $m = 4$ factors and for $e \leq 15$ and $m \geq 5$ factors. This compares with the previously known result of $e \leq 5$. In addition, Schur-optimal designs under a second-order model are derived for 3 and 5 factors for all possible numbers of runs. Third-order models are also considered briefly in the final section.

2 Background

Optimal designs will be derived for two-level factorial designs in m factors under the second-order model

$$y = \mu + \sum_{i=1}^{m} \alpha_i x_i + \sum_{i_1=1}^{m-1} \sum_{i_2=i_1+1}^{m} \beta_{i_1 i_2} x_{i_1} x_{i_2} + \epsilon$$

for observations y, mean μ, factorial main effects α_i, factor levels $x_i = \pm 1$, two-factor interactions $\beta_{i_1 i_2}$, and independent errors $\epsilon \sim N(0, \sigma^2)$.

The model for n runs may also be expressed in matrix form as

$$Y = Z\beta + \epsilon, \qquad \epsilon \sim N(0, \sigma^2 I_n),$$

where Z is the $n \times t$ design, and $t = m(m+1)/2+1$ is the number of parameters in the model. For two-level designs, there are a total of 2^m possible factorial combinations or runs with levels ± 1 in each of the m factors. Each run i has a design vector z_i of length t, and number of replicates r_i. The information matrix $Z'Z$ for these designs is given by

$$Z'Z = \sum_{i=1}^{2^m} r_i z_i z_i' \tag{1}$$

with $\sum_{i=1}^{2^m} r_i = n$. Note that for a full 2^m factorial,

$$Z'Z = \sum_{i=1}^{2^m} z_i z_i' = 2^m I_t.$$

Designs will be compared on the basis of the eigenvalues $\lambda_1 \geq ... \geq \lambda_t$ of the information matrix $Z'Z$. The optimality criteria considered will be E-optimality and Schur-optimality. The E-optimality criterion simply maximises $\min \lambda_i = \lambda_{min} = \lambda_t$. Equivalently, E-optimality minimises the maximum

eigenvalue of the variance matrix $\sigma^2(Z'Z)^{-1}$ of the least squares parameter estimates.

Schur-optimality is a very general class of criteria that includes A-, D- and E-optimality and Cheng (1978) Type 1-optimality as special cases. Schur-optimal designs minimise all Schur-convex functions of the $Z'Z$-matrix eigenvalues, including

$$\sum_{i=1}^{t} f(\lambda_i) \tag{2}$$

for any convex function f. Note that A-optimality has $f(\lambda) = 1/\lambda$ and D-optimality has $f(\lambda) = -\log \lambda$. For more information on the theory and applications of Schur-optimality, see Marshall & Olkin (1979) Giovagnoli & Wynn (1981), Shah & Sinha (1989), Bailey, Monod & Morgan (1995), Bagchi & Bagchi (2001) and Butler & Ramos (2007).

A Schur-optimal design is required to majorise every other design. A design with $Z'Z$-matrix eigenvalues $\lambda_1^* \geq ... \geq \lambda_t^*$ is said to majorise, or be Schur-better, than a design with $Z'Z$-matrix eigenvalues $\lambda_1 \geq ... \geq \lambda_t$ if

$$\lambda_1^* + ... + \lambda_t^* = \lambda_1 + ... + \lambda_t \tag{3}$$

and

$$\lambda_k^* + ... + \lambda_t^* \geq \lambda_k + ... + \lambda_t \tag{4}$$

for $k = 2, ..., t$. Observe that, as (3) fixes the sum of the eigenvalues, a design satisfies (4) for $k = k'$ if and only if it satisfies

$$\lambda_1^* + ... + \lambda_k^* \leq \lambda_1 + ... + \lambda_k \tag{5}$$

for $k = k' - 1$. Both majorization conditions (4) and (5) will be used in the proofs that follow. The other condition (3) holds for all two-level designs as trace$(Z'Z)$ always equals nt, as a result of every diagonal element of $Z'Z$ equalling n.

Schur-optimal designs can trivially be found for $m = 2$ factors and $n = 4r + e$ runs. In this case, the design vectors z_i of length 4 are orthogonal to each other. Hence, from (1), the eigenvalues of $Z'Z$ are $4r_i$ with corresponding eigenvectors z_i. Thus, it follows that any design with $r + 1$ replicates of e of the runs and r replicates of the other runs is Schur-optimal.

3 Three Factors

The following theorem provides Schur-optimal two-level designs for 3 factors for all numbers of runs where the model is estimable, i.e. $n \geq t = 7$.

THEOREM 1. *For 3 factors and $n = 8r+e$ runs ($1 \le e \le 7$), r replicates of the full 2^3 factorial design with any e additional distinct runs is Schur-optimal.*

Proof. Note that $Z'Z$ is a 7×7 matrix. Let the designs in the theorem have eigenvalues $\lambda_1^* \ge ...\lambda_7^*$. The information matrix of these designs is $Z'Z = 8rI_7 + Z_0'Z_0$, where Z_0 is the design matrix of the additional runs. Hence, $\lambda_i^* = 8r + \mu_i$, where $\mu_i \ge 0$ are the eigenvalues of $Z_0'Z_0$, and so each $\lambda_i^* \ge 8r$. Similarly, $Z'Z = 8(r+1)I_7 - Z_1'Z_1$, where Z_1 is the design matrix of the runs not replicated $r+1$ times, and hence $\lambda_i^* \le 8(r+1)$. Thus, $8(r+1) \ge \lambda_1^* \ge \lambda_7^* \ge 8r$.

For each possible two-level design, define the set $S = \{1 \le i \le 8 : r_i > r\}$ and let a ($1 \le a \le 7$) be the design-dependent number of elements in S. For $a \le 6$, let $u_1, ..., u_{a+1}$ be orthogonal eigenvectors associated with the $a+1$ biggest eigenvalues of $Z'Z$. Then there is a unit vector v that is a linear combination of $u_1, ..., u_{a+1}$ that is orthogonal to each of the a vectors z_i ($i \in S$). Now

$$\begin{aligned} v'Z'Zv &= v'\left(\sum_{i=1}^{8} r_i z_i z_i'\right) v = v'\left(\sum_{i \in S^c} r_i z_i z_i'\right) v \\ &\le v'\left(r\sum_{i \in S^c} z_i z_i'\right) v = v'\left(r\sum_{i=1}^{8} z_i z_i'\right) v = 8rv'v \\ &= 8r. \end{aligned}$$

As v is a linear combination of $u_1, ..., u_{a+1}$ and is a unit vector, if $\lambda_{a+1} > 8r$, then $v'Z'Zv > 8r$. Hence, $\lambda_{a+1} \le 8r \le \lambda_7^*$ for $a \le 6$. Consequently, the majorization condition (4) is satisfied for $k = a+1, ..., 7$ and $a \le 6$.

Similarly, for $a \ge 2$, let $u_{a-1}, ..., u_7$ be orthogonal eigenvectors associated with the $9-a$ smallest eigenvalues of $Z'Z$. Then there is a unit vector v that is a linear combination of $u_{a-1}, ..., u_7$ that is orthogonal to each of the $8-a$ vectors z_i ($i \in S^c$). Thus,

$$\begin{aligned} v'Z'Zv &= v'\left(\sum_{i=1}^{8} r_i z_i z_i'\right) v = v'\left(\sum_{i \in S} r_i z_i z_i'\right) v \\ &\ge v'\left((r+1)\sum_{i \in S} z_i z_i'\right) v = v'\left((r+1)\sum_{i=1}^{8} z_i z_i'\right) v = 8(r+1)v'v \\ &= 8(r+1). \end{aligned}$$

As v is a linear combination of $u_{a-1}, ..., u_7$ and is a unit vector, if $\lambda_{a-1} < 8(r+1)$, then $v'Z'Zv < 8(r+1)$. Hence, $\lambda_{a-1} \ge 8(r+1) \ge \lambda_1^*$ for $a \ge 2$. Therefore, the majorization condition (5) is satisfied for $k = 1, ..., a-1$ and $a \ge 2$. This implies that the majorization condition (4) holds for $k = 2, ...a$.

On combining this with the last sentence of the previous paragraph, the majorization condition (4) holds for $k = 2, ..., 7$, and so the designs in the theorem are Schur-optimal. ■

4 Four Factors

THEOREM 2. *For 4 factors and $n = 16r + e$ runs ($1 \leq e \leq 15$), there is an E-optimal design that contains r replicates of the full 2^4 factorial design.*

Proof. A design containing r replicates of a 2^4 factorial design has $\lambda_{min} \geq 16r$, as $Z'Z = 16rI_{11} + Z_0'Z_0$ where Z_0 is the design matrix of the additional runs. It will be shown that for any other design $\lambda_{min} \leq 16r$ if $e \leq 14$.

Suppose that this is not the case, so $\lambda_{min} > 16r$ for a design with $\min r_i = r - a$ and $a \geq 1$. In this scenario, the set $S = \{1 \leq i \leq 8 : r_i > r\}$ will be shown to contain at least 11 elements. If it does not, then there exists a unit vector v of length $t = 11$ that is orthogonal to all the vectors z_i $(i \in S)$. Consequently,

$$\begin{aligned} v'Z'Zv &= v'\left(\sum_{i=1}^{16} r_i z_i z_i'\right) v = v'\left(\sum_{i \in S^c} r_i z_i z_i'\right) v \\ &\leq v'\left(\sum_{i \in S^c} r z_i z_i'\right) v = v'\left(\sum_{i=1}^{16} r z_i z_i'\right) v = 16r. \end{aligned}$$

This contradicts the assumption that $\lambda_{min} > 16r$. Hence, S must contain 11 or more runs.

We now define the Hamming distance between two runs to be the number of main effects for which the two runs differ. For instance, the run with main effects $(+, +, -, -)$ is at distance 2 to $(+, -, +, -)$ as factors 2 and 3 differ. It is easily shown using the confounding between runs ideas in Butler (2006) that $z_i'z_j = 3$ if runs i and j are at distance 1 or 4, and $z_i'z_j = -1$ if i and j are at distance 2 or 3. Thus, for each run j, the set $S_3(j) = \{1 \leq i \leq 16 : z_i'z_j = 3\}$ contains 5 elements, and the set $S_1(j) = \{1 \leq i \leq 16 : z_i'z_j = -1\}$ contains 10 elements. The only other possibility is $i = j$ when $z_i'z_j = 11$.

Suppose, without loss of generality, that run 1 has the minimum number of replicates $r - a$. Then

$$\begin{aligned} z_1'Z'Zz_1 &= z_1'\left(\sum_{i=1}^{16} r_i z_i z_i'\right) z_1 \\ &= z_1'\left((r-a)z_1z_1 + \sum_{i \in S_3(1)} r_i z_i z_i' + \sum_{i \in S_1(1)} r_i z_i z_i'\right) z_1 \end{aligned}$$

$$= \quad 121(r-a) + 9 \sum_{i \in S_3(1)} r_i + \sum_{i \in S_1(1)} r_i.$$

Now

$$(r-a) + \sum_{i \in S_3(1)} r_i + \sum_{i \in S_1(1)} r_i \quad = \quad \sum_{i=1}^{16} r_i = 16r + e.$$

Therefore

$$z_1' Z' Z z_1 \quad = \quad 9(16r+e) + 112(r-a) - 8 \sum_{i \in S_1(1)} r_i.$$

There are 10 runs in $S_1(1)$. At least six of these must have $r_i > r$ as S contains 11 elements, and $i = 1 \notin S$. The other four runs must have $r_i \geq r - a$. Hence

$$\sum_{i \in S_1(1)} r_i \geq 6(r+1) + 4(r-a) = 10r + 6 - 4a.$$

Consequently,

$$\begin{aligned} z_1' Z' Z z_1 &\leq 9(16r+e) + 112(r-a) - 8(10r + 6 - 4a) \\ &= 176r + 9e - 48 - 80a \\ &< 16r z_1' z_1 \end{aligned} \tag{6}$$

for $1 \leq e \leq 14$ and $a \geq 1$. This implies that $Z'Z$ must have $\lambda_{min} < 16r$, and a contradiction is obtained for $1 \leq e \leq 14$.

For $e = 15$, it follows from (6) that

$$\begin{aligned} \lambda_{min} &\leq \frac{z_1' Z' Z z_1}{z_1' z_1} \leq \frac{176r + 9e - 48 - 80a}{11} \\ &\leq 16r + \frac{7}{11}. \end{aligned}$$

This compares with $\lambda_{min} = 16r + 5$ for a design with $r+1$ replicates of a 2^4 design with one run z deleted, as $Z'Z = 16(r+1)I_{11} - zz'$. Thus, for $e = 15$, a design that does not contain r replicates of a 2^4 factorial cannot be E-optimal.

■

THEOREM 3. *For 4 factors and $n = 16r + e$ runs ($1 \leq e \leq 10$), r replicates of the 2^4 factorial design with any e additional runs is E-optimal and $\lambda_{min} = 16r$.*

Proof. From the proof of Theorem 2, the only designs that could have $\lambda_{min} > 16r$ would contain r replicates of a 2^4 factorial design. Such a design would have information matrix

$$Z'Z = 16rI_{11} + Z_0'Z_0$$

where Z_0 is the $e \times 11$ design matrix of the e additional runs. The eigenvalues of $Z'Z$ are $\lambda_i = 16r + \mu_i$, where μ_i are the eigenvalues of $Z_0'Z_0$. However, Z_0 is of rank at most e and so $Z_0'Z_0$ has at least one zero eigenvalue. Consequently, λ_{min} cannot be greater than $16r$, and the designs in the theorem are E-optimal. ■

THEOREM 4. *For 4 factors and $n = 16r + e$ runs ($11 \leq e \leq 15$), r replicates of a 2^4 factorial design with an E-optimal design for 4 factors and e runs is E-optimal.*

Proof. This result follows from Theorems 2 and 3 and the fact that with $e \geq 11$, $Z_0'Z_0$ can be non-singular. The E-optimal design for $e = 11$ runs is proved in Butler & Ramos (2007). ■

Theorems 3 and 4 together cover all cases $1 \leq e \leq 15$. Note that the additional runs in Theorem 3 could be added using the distance-based methods in the aforementioned paper, Butler & Ramos (2007).

5 Five or More Factors

In this section, we require orthogonal arrays of strength 4. By definition, a two-level design is an orthogonal array of strength $s \geq 2$ if, for each subset of s factors, each of the 2^s factorial combinations occurs equally often. Obviously, n must equal $2^s q$ for some integer q.

For an orthogonal array of strength 4, main effects, two-factor interactions and the mean are all orthogonal to each other. Consequently, $Z'Z = 16qI_t$. If the design is regular, i.e. it can be defined in terms of defining contrasts, then it has resolution V or more.

With $m = 5$ factors, orthogonal arrays of strength 4 can easily be formed for $16q$ runs for any positive integer q by combining $w \leq q$ replicates of the half-fraction design $ABCDE = +$ with $q - w$ replicates of the design $ABCDE = -$. For $m = 6$ factors, it is possible to form nonregular orthogonal arrays of strength 4, for example when $n = 80$. Other nonregular orthogonal arrays of strength 4 can be formed for $n = 80 + 32r$ by adding r half-fraction designs $ABCDEF = \pm$. Thus, it follows that orthogonal arrays of strength 4 exist for $m = 6$ factors and $16q$ runs for all $q \geq 4$. This means that Theorem 5

below cannot be extended to $e > 15$ for $m = 6$, and may be difficult to extend for higher values of m.

THEOREM 5. *For $m \geq 5$ factors and $n = 16q + e$ runs (q an integer, $1 \leq e \leq 15$), an orthogonal array of strength 4 for $16q$ runs with any e additional runs is E-optimal and $\lambda_{min} = 16q$.*

Proof. First consider the case of $m = 5$ factors. Let $z_{1,i}$ $(i = 1, ...16)$ be the design vectors and $r_{1,i}$ be the corresponding number of replicates for the runs in a 2^{5-1} design with defining contrast $ABCDE = +$. Similarly, let $z_{2,i}$ $(i = 1, ...16)$ be the design vectors and $r_{2,i}$ be the corresponding number of replicates for the runs in a 2^{5-1} design with defining contrast $ABCDE = -$. Then

$$Z'Z = \sum_{j=1}^{2} \sum_{i=1}^{16} r_{j,i} z_{j,i} z'_{j,i}$$

and

$$\sum_{i=1}^{16} z_{j,i} z'_{j,i} = 16 I_{16}$$

for $j = 1, 2$. Let $N(S)$ be the number of elements in any set S. Then

$$\begin{aligned} n &= \sum_{j=1}^{2} \sum_{i=1}^{16} r_{j,i} = \sum_{j=1}^{2} \sum_{p \geq 1} p N(i : r_{j,i} = p) = \sum_{j=1}^{2} \sum_{p \geq 1} N(i : r_{j,i} \geq p) \\ &= \sum_{p=1}^{q+1} (N(i : r_{1,i} \geq p) + N(i : r_{2,i} \geq q + 2 - p)) + \sum_{j=1}^{2} \sum_{p \geq q+2} N(i : r_{j,i} \geq p). \end{aligned}$$

Hence,

$$\sum_{p=1}^{q+1} (N(i : r_{1,i} \geq p) + N(i : r_{2,i} \geq q + 2 - p)) \quad \leq \quad n < 16(q + 1).$$

Therefore, as there are $q + 1$ terms in the above sum, there exists a p_0 $(1 \leq p_0 \leq q + 1)$ such that

$$N(i : r_{1,i} \geq p_0) + N(i : r_{2,i} \geq q + 2 - p_0) < 16.$$

Consequently, there is a unit vector v of length $t = 16$ that is orthogonal to all the vectors

$$z_{1,i} \ (i : r_{1,i} \geq p_0) \qquad\qquad z_{2,i} \ (i : r_{2,i} \geq q + 2 - p_0).$$

Thus,

$$\begin{aligned}
v'Z'Zv &= v'\left(\sum_{i=1}^{16} r_{1,i}z_{1,i}z'_{1,i} + \sum_{i=1}^{16} r_{2,i}z_{2,i}z'_{2,i}\right)v \\
&= v'\left(\sum_{i:r_{1,i}<p_0} r_{1,i}z_{1,i}z'_{1,i} + \sum_{i:r_{2,i}<q+2-p_0} r_{2,i}z_{2,i}z'_{2,i}\right)v \\
&\leq v'\left(\sum_{i:r_{1,i}<p_0} (p_0-1)z_{1,i}z'_{1,i} + \sum_{i:r_{2,i}<q+2-p_0} (q+1-p_0)z_{2,i}z'_{2,i}\right)v \\
&= v'\left(\sum_{i=1}^{16}(p_0-1)z_{1,i}z'_{1,i} + \sum_{i=1}^{16}(q+1-p_0)z_{2,i}z'_{2,i}\right)v \\
&= 16(p_0-1)v'I_{16}v + 16(q+1-p_0)v'I_{16}v \\
&= 16qv'v \\
&= 16q.
\end{aligned}$$

As v is of unit length, this implies that $\lambda_{min} \leq 16q$ for any design. The designs stated in the theorem have $\lambda_{min} \geq 16q$ as they contain an orthogonal array of strength 4 for $16q$ runs. Consequently, they are E-optimal for $m = 5$ factors.

For $m > 5$ factors, partition the design matrix $Z = (Z_1, Z_2)$ where Z_1 is an $n \times 16$ design matrix containing the mean, 5 main effects and 10 two-factor interactions of a five-factor design, and Z_2 is the design matrix for all remaining effects. Then

$$Z'Z = \begin{pmatrix} Z'_1Z_1 & Z'_1Z_2 \\ Z'_2Z_1 & Z'_2Z_2 \end{pmatrix}.$$

The lowest eigenvalue of $Z'Z$ cannot be greater than the lowest eigenvalue of the principal submatrix Z'_1Z_1, and hence $\lambda_{min} \leq 16q$. The designs in the theorem again have $\lambda_{min} \geq 16q$ as they contain an orthogonal array of strength 4 for $16q$ runs, and so they are E-optimal. ■

THEOREM 6. *For 5 factors and $n = 16q + e$ runs ($1 \leq e \leq 15$), an orthogonal array of strength 4 for $16q$ runs with any e additional distinct runs from the same half-fraction design $ABCDE = \pm$ is Schur-optimal.*

Proof. First note that the information matrix may be expressed as

$$Z'Z = \sum_{j=1}^{2}\sum_{i=1}^{16} r_{j,i}z_{j,i}z'_{j,i} = \sum_{j=1}^{2}\sum_{p\geq 1}\sum_{i:r_{j,i}\geq p} z_{j,i}z'_{j,i}$$

$$= \sum_{p=1}^{q+1} \left(\sum_{i:r_{1,i} \geq p} z_{1,i} z'_{1,i} + \sum_{i:r_{2,i} \geq q+2-p} z_{2,i} z'_{2,i} \right) + \sum_{j=1}^{2} \sum_{p \geq q+2} \sum_{i:r_{j,i} \geq p} z_{j,i} z'_{j,i}.$$

From the proof of Theorem 5,

$$\sum_{p=1}^{q+1} \left(N(i : r_{1,i} \geq p) + N(i : r_{2,i} \geq q+2-p) \right) \quad \leq \quad n.$$

Define, for $1 \leq p \leq q+1$,

$$h_p = \max\left(0, 16 - N(i : r_{1,i} \geq p) - N(i : r_{2,i} \geq q+2-p)\right).$$

Then

$$\begin{aligned} \sum_{p=1}^{q+1} h_p &\geq \sum_{p=1}^{q+1} \left(16 - N(i : r_{1,i} \geq p) - N(i : r_{2,i} \geq q+2-p)\right) \\ &= 16(q+1) - \sum_{p=1}^{q+1} \left(N(i : r_{1,i} \geq p) + N(i : r_{2,i} \geq q+2-p)\right) \\ &\geq 16(q+1) - n \\ &= 16 - e. \end{aligned}$$

Now, from the definition of h_p, there are $h_p \geq 0$ orthogonal vectors $v_{p,i}$ $(i = 1, ..., h_p)$ that are orthogonal to all the vectors

$$z_{1,i} \ (i : r_{1,i} \geq p) \qquad\qquad z_{2,i} \ (i : r_{2,i} \geq q+2-p)$$

for $1 \leq p \leq q+1$. The vectors $v_{p,i}$ $(p = 1, ..., q+1; i = 1, ..., h_p)$ form a subspace of dimension $a \leq \sum_{p=1}^{q+1} h_p$. Suppose that $u_1, ..., u_a$ form an orthonormal basis for the subspace and let $U_1 = (u_1, ..., u_a)$. Then, $P = U_1 U_1'$ is the $t \times t$ projection matrix of rank a spanned by the vectors $v_{p,i}$ $(p = 1, ..., q+1; i = 1, ..., h_p)$.

The projection matrix P may be expressed for each $p \geq 1$ as

$$P = Q_p^{(1)} + R_p^{(1)}$$

where $Q_p^{(1)}$ and $R_p^{(1)}$ are projection matrices with $Q_p^{(1)}$ spanned by the subset of vectors $v_{p',i}$ $(p' \leq p; i = 1, ..., h_p)$. Thus, $R_p^{(1)}$ is the projection matrix spanned by the subspace of $v_{p',i}$ $(p' > p; i = 1, ..., h_p)$ that is orthogonal to $Q_p^{(1)}$. Alternatively,

$$P = Q_p^{(2)} + R_p^{(2)}$$

where $Q_p^{(2)}$ and $R_p^{(2)}$ are projection matrices with $Q_p^{(2)}$ spanned by the different subset of vectors $v_{p',i}$ $(p' \geq p; i = 1, ..., h_p)$.

Now consider

$$Z'ZP = \sum_{p=1}^{q+1} \left(\sum_{i:r_{1,i} \geq p} z_{1,i} z'_{1,i} P + \sum_{i:r_{2,i} \geq q+2-p} z_{2,i} z'_{2,i} P \right) + \sum_{j=1}^{2} \sum_{p \geq q+2} \sum_{i:r_{j,i} \geq p} z_{j,i} z'_{j,i} P.$$

Then

$$\text{trace}(Z'ZP) = \sum_{p=1}^{q+1} \left(\sum_{i:r_{1,i} \geq p} z'_{1,i} P z_{1,i} + \sum_{i:r_{2,i} \geq q+2-p} z'_{2,i} P z_{2,i} \right) + \sum_{j=1}^{2} \sum_{p \geq q+2} \sum_{i:r_{j,i} \geq p} z'_{j,i} P z_{j,i}.$$

From their definition, all the vectors $v_{p,i}$ $(p = 1, ..., q+1; i = 1, ..., h_p)$ spanning P are orthogonal to $z_{j,i}$ $(i : r_{j,i} \geq q + 2)$. Hence

$$\sum_{j=1}^{2} \sum_{p \geq q+2} \sum_{i:r_{j,i} \geq p} z'_{j,i} P z_{j,i} = 0.$$

Now, for $j = 1$ and each $1 \leq p \leq q + 1$,

$$\sum_{i:r_{1,i} \geq p} z'_{1,i} P z_{1,i} = \sum_{i:r_{1,i} \geq p} z'_{1,i} Q_p^{(1)} z_{1,i} + \sum_{i:r_{1,i} \geq p} z'_{1,i} R_p^{(1)} z_{1,i}.$$

Also from their definition, the vectors $v_{p',i}$ $(p' \leq p; i = 1, ..., h_p)$ spanning $Q_p^{(1)}$ are all orthogonal to the vectors $z_{1,i}$ $(i : r_{1,i} \geq p)$. Hence, the first term in the above sum disappears and

$$\sum_{i:r_{1,i} \geq p} z'_{1,i} P z_{1,i} = \sum_{i:r_{1,i} \geq p} z'_{1,i} R_p^{(1)} z_{1,i} = \sum_{i:r_{1,i} \geq p} \text{trace}(R_p^{(1)} z_{1,i} z'_{1,i})$$

$$\leq \sum_{i=1}^{16} \text{trace}(R_p^{(1)} z_{1,i} z'_{1,i}) = 16\text{trace}(R_p^{(1)}).$$

Following a similar procedure, it can be shown for $j = 2$ and each $1 \leq p \leq q+1$ that

$$\sum_{i:r_{2,i} \geq q+2-p} z'_{2,i} P z_{2,i} \leq 16\text{trace}(R_p^{(2)}).$$

Thus

$$\text{trace}(Z'ZP) \leq 16 \sum_{p=1}^{q+1} \left(\text{trace}(R_p^{(1)}) + \text{trace}(R_p^{(2)}) \right).$$

Note that $\text{trace}(R_p^{(1)})$ is the dimension of the subspace added by the vectors $v_{p',i}$ $(p' > p)$ after allowing for $v_{p',i}$ $(p' \leq p)$. This is obviously less than or equal to the dimension added by the same vectors $v_{p',i}$ $(p' > p)$ only allowing for $v_{p,i}$. The latter equals $\text{trace}(Q_p^{(2)}) - h_p$. Hence

$$\begin{aligned}
\text{trace}(Z'ZP) &\leq 16\sum_{p=1}^{q+1}\left(\text{trace}(Q_p^{(2)}) + \text{trace}(R_p^{(2)}) - h_p\right) \\
&= 16\sum_{p=1}^{q+1}(\text{trace}(P) - h_p) \\
&= 16(q+1)a - 16\sum_{p=1}^{q+1} h_p.
\end{aligned}$$

Now define the $t \times t$ orthogonal matrix $U = (U_1, U_2)$ where the $t \times a$ matrix U_1 is defined as before so that $P = U_1U_1'$. We will use the fact that the matrix $U'Z'ZU$ has the same eigenvalues as $Z'Z$. The sum of the first a diagonal elements of $U'Z'ZU$ is

$$\text{trace}(U_1'Z'ZU_1) = \text{trace}(Z'ZP) \leq 16(q+1)a - 16\sum_{p=1}^{q+1} h_p.$$

It is well known that the diagonal elements of an information matrix majorise the matrix's eigenvalues (see Bagchi & Bagchi, 2001). Thus, for any design the sum of the a smallest eigenvalues is less than or equal to the sum of the a smallest diagonal elements, and so is at most $16qa$ as $a \leq \sum_{p=1}^{q+1} h_p$. Hence, the average of the a smallest eigenvalues is less than or equal to $16q$. Similarly, the sum of the largest $16-a$ eigenvalues for any design is greater than or equal to

$$\begin{aligned}
\text{trace}(Z'Z) - \text{trace}(U_1'Z'ZU_1) &\geq 16(16q+e) - \left(16(q+1)a - 16\sum_{p=1}^{q+1} h_p\right) \\
&= 16(q+1)(16-a) + 16(\sum_{p=1}^{q+1} h_p + e - 16) \\
&\geq 16(q+1)(16-a)
\end{aligned}$$

as $\sum_{p=1}^{q+1} h_p \geq 16 - e$. Thus, the average of the largest $16-a$ eigenvalues is greater than or equal to $16(q+1)$.

The designs stated in the theorem have all eigenvalues $\lambda_i^* \geq 16q$ as $Z'Z = 16qI_{16} + Z_0'Z_0$ where Z_0 is the design matrix of the extra runs. Similarly, by considering deletions to an orthogonal array for $16(q+1)$ runs, $\lambda_i^* \leq 16(q+1)$. As the average of the lowest a eigenvalues of any other design is less than or

equal to $16q$, majorization condition (4) holds for $k = 17-a, ..., 16$. Similarly, as the average of the largest $16-a$ eigenvalues is greater then or equal to $16(q+1)$, majorization condition (5) holds for $k = 1, ..., 16-a$. On combining these, the designs in the theorem are proved to be Schur-optimal. ■

6 Third-Order Model

The results obtained can be extended to two-level factorial designs under a third-order model

$$y = \mu + \sum_{i=1}^{m} \alpha_i x_i + \sum_{i_1=1}^{m-1} \sum_{i_2=i_1+1}^{m} \beta_{i_1 i_2} x_{i_1} x_{i_2} + \sum_{i_1=1}^{m-2} \sum_{i_2=i_1+1}^{m-1} \sum_{i_3=i_2+1}^{m} \gamma_{i_1 i_2 i_3} x_{i_1} x_{i_2} x_{i_3} + \epsilon$$

where $\gamma_{i_1 i_2 i_3}$ are three-factor interactions. For $m = 3$ factors, the problem is trivial in the same way as for $m = 2$ factors under a second-order model. The following results can be proved in almost exactly the same way as Theorems 1, 5 and 6 respectively.

THEOREM 7. *For 4 factors and $n = 16r + e$ runs ($1 \leq e \leq 15$), r replicates of the full 2^4 factorial design with any e additional distinct runs is Schur-optimal under a third-order model.*

THEOREM 8. *For $m \geq 7$ factors and $n = 64q + e$ runs (q an integer, $1 \leq e \leq 63$), an orthogonal array of strength 6 for $64q$ runs with any e additional runs is E-optimal under a third-order model and $\lambda_{min} = 64q$.*

THEOREM 9. *For 7 factors and $n = 64q + e$ runs ($1 \leq e \leq 63$), an orthogonal array of strength 6 for $64q$ runs with any e additional distinct runs from the same half-fraction design $ABCDEFG = \pm$ is Schur-optimal under a third-order model.*

In Theorem 7, the model contains all possible effects except the four-factor interaction, and so is analogous to Theorem 1 where the model contains all possible effects except the three-factor interaction. Theorems 8 and 9 use the fact that a 2^{7-1} design $ABCDEFG = \pm$ is saturated and orthogonal under a third-order model for 64 runs in the same way that a 2^{5-1} design $ABCDE = \pm$ is saturated and orthogonal under a second-order model for 16 runs.

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