

Discriminating Between Superior $UE(s^2)$ -optimal Supersaturated Designs

Feng- Shun Chai¹, Ashish Das², Rakhi Singh³ and John Stufken³

¹*Academia Sinica, Taipei, Taiwan*

²*Indian Institute of Technology Bombay, Mumbai, India*

³*University of North Carolina at Greensboro, Greensboro, NC, USA*

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Abstract

For binary factors, a design is supersaturated for the main effects model if the number of runs is smaller than the number of factors. Supersaturated designs (SSDs) cannot have all orthogonal columns, and so, the traditional notions of D -, A -, E -optimality are not applicable here. SSDs are studied under criteria such as $E(s^2)$ or $UE(s^2)$ which are near-orthogonality measures. In this work, following some of the latest works, we provide algorithms to construct better $UE(s^2)$ -optimal designs. We also provide a few design examples to demonstrate the proposed algorithms.

Key words: Constructions; Hadamard matrices; Superior designs; $UE(s^2)$ -optimal designs.

1. Introduction

Factor-screening experiments are performed in situations when a large number of factors could potentially be affecting the response but only a limited number of runs can be performed. The main goal of these studies is to screen (or, identify) the most important factors. Supersaturated designs are useful in factor-screening experiments and they work under the effect sparsity assumption that only a small number of factors are active. For m binary factors and n runs, under a main-effects model, supersaturated designs require n to be smaller than $m + 1$.

An n -run supersaturated design d for m two-level factors is represented by an $n \times m$ matrix X_d of 1's and -1's, where the i th column of X_d corresponds to the i th factor. Let $Z_d = [1 \ X_d]$ be the model matrix of the main-effects model for d . Since $n < m + 1$, it is not possible to have Z_d with mutually orthogonal columns, even though orthogonality is a desirable property. To assess non-orthogonality of supersaturated designs, the available literature on the topic involves finding lower bounds to the popular $E(s^2)$ -criterion and constructing designs satisfying these lower bounds. Designs that have an equal number of ± 1 s in each column of X_d for even n are called level-balanced designs. An $E(s^2)$ -optimal

design is a level-balanced design that minimizes the sum of the squares of the inner products of columns of X_d among all level-balanced designs. A review paper by Georgiou (2014) and the references therein are a good source for the available literature on $E(s^2)$ -optimal supersaturated designs.

Jones and Majumdar (2014) extended the class of available designs by removing the imposition of level-balance from the designs. To keep the definition of $E(s^2)$ sensible in the broader class of designs, they included the sums of squares of the inner product of columns of X_d with the column of all 1s in the existing definition and called it unrestricted $E(s^2)$, or $UE(s^2)$. For a design d , the

$$UE_d(s^2) = \frac{1}{\binom{m+1}{2}} \left[\sum_{i=1}^m (1^T x_i)^2 + \sum_{1 \leq i < j \leq m} (x_i^T x_j)^2 \right], \quad (1)$$

where x_i is the i th column of X_d . The $E(s^2)$ -criterion minimizes the second quantity in (1) among all level balanced designs (the first quantity is 0 for level-balanced designs), whereas the $UE(s^2)$ -criterion minimizes (1) among all possible designs with ± 1 s. Jones and Majumdar (2014) obtained lower bounds to $UE_d(s^2)$ and provided constructions of $UE(s^2)$ -optimal supersaturated designs. $UE(s^2)$ -optimal supersaturated designs are easy to construct and are available for any parameter sets, whereas $E(s^2)$ -optimal designs are difficult to construct and are available only for selected parameter sets.

Since many $UE(s^2)$ -optimal designs exist, Jones and Majumdar (2014) and Cheng et al. (2018) suggested various criteria to choose the better design among all available designs. Using the same notations as in Cheng et al. (2018), following are a few definitions:

- $SS = \sum_{i=1}^m (1^T x_i)^2 = 1^T X_d X_d^T 1$;
- LB = the number of level-balanced factors for n even;
- OF = the number of orthogonal pairs of factors among the $\binom{m}{2}$ pairs for n even;
- $Q = LB + OF$.

For odd n , these definitions are easily generalized. For example, when n is odd, LB is the number of nearly-level-balanced factors, that is the number of factors with the corresponding column sums of X_d equal to ± 1 . Similarly, OF is the number of nearly orthogonal pairs of factors among the $\binom{m}{2}$ pairs, that is, the number of pairs of factors having an inner product equal to ± 1 . For even n , Q is half the number of zeros in the matrix $Z_d^T Z_d$, whereas for odd n , Q is half the number of ± 1 s in the matrix $Z_d^T Z_d$.

Cheng et al. (2018) defined a $UE(s^2)$ -optimal design to be a superior $UE(s^2)$ -optimal design if it additionally minimizes SS among the class of $UE(s^2)$ -optimal designs constructed in a restricted class. Singh et al. (2020) then extended the definition of superior $UE(s^2)$ -optimal designs in a global class of all $UE(s^2)$ -optimal designs, also providing the constructions of the superior $UE(s^2)$ -optimal designs in a global class. In this work, we restrict ourselves to the superior $UE(s^2)$ -optimal designs constructed in Cheng et al. (2018). Since the class of superior $UE(s^2)$ -optimal designs is still very large, Cheng et al. (2018) further proposed that

Q should be minimized to find a better design among superior $UE(s^2)$ -optimal designs. This minimization reduces the spread among the off-diagonal elements of $Z_d^T Z_d$, and because the minimization is restricted to superior $UE(s^2)$ -optimal designs it favors such designs with uniformly relatively small correlations between the columns of Z_d . The superior $UE(s^2)$ -optimal designs with small Q tend to perform very well on the projection-based measures such as average D-efficiency when only a small number of factors are active.

In this paper, we propose algorithms to find designs with minimum Q among the class of superior $UE(s^2)$ -optimal designs constructed by Cheng et al. (2018). These algorithms differ based on whether $m = 4t, 4t + 1, 4t + 2$, or $4t + 3$ and are provided in Section 2 along with an example each.

2. Algorithms for Constructing Q -superior $UE(s^2)$ -optimal Designs

Constructions of superior $UE(s^2)$ -optimal designs (Cheng et al. (2018)) differ based on the type of values that m has. Let H be a $4t \times 4t$ normalized Hadamard matrix with all the entries in the first row and first column equal to 1. If $m = 4t - 1$, then any $UE(s^2)$ -optimal design is superior and these designs are constructed by deleting any $4t - n$ rows and the first column of a normalized Hadamard matrix H . If $m = 4t$, adding a level-balanced column to the $UE(s^2)$ -optimal design with $m = 4t - 1$ gives a superior $UE(s^2)$ -optimal design. If $m = 4t - 2$, deleting a column having maximum absolute column sum from a $UE(s^2)$ -optimal design with $m = 4t - 1$ gives a superior $UE(s^2)$ -optimal design. If $m = 4t + 1$, two columns are added to a $UE(s^2)$ -optimal design with $m = 4t - 1$ so that the pairs $(1, 1)$, $(-1, -1)$, $(1, -1)$ and $(-1, 1)$ appear in these columns as close to equal as possible; moreover, if $n \equiv 2 \pmod{4}$, the two columns must be orthogonal. Note that superior $UE(s^2)$ -optimal designs can be constructed using other methods which do not necessarily add or delete one or two columns to a Hadamard matrix; some of such construction methods have been studied in Singh et al. (2020). We restrict ourselves to superior $UE(s^2)$ -optimal designs constructed by Cheng et al. (2018).

We provide algorithms to find the designs with minimum Q among the superior $UE(s^2)$ -optimal designs. Before we do that, we need the following result due to Singh et al. (2020). This result gives the values of SS for superior $UE(s^2)$ -optimal designs in a restricted class, that is, the class of designs constructed using the methods of Cheng et al. (2018).

Theorem 1 (Theorem 1 of Singh et al. (2020)) *The values of SS for a superior $UE(s^2)$ -optimal design d in restricted class are*

$$C(m, n) = \begin{cases} n(m - n + 1) & \text{for } m = 4t - 1 \\ n(m - n) + x & \text{for } m = 4t \\ n(m - n - 1) + z & \text{for } m = 4t + 1 \\ n(m - 2n + 2) + 4s(n - s) & \text{for } m = 4t - 2 \text{ and } s = \min(n, 2t) \end{cases} \quad (2)$$

where $x = 0$ for n even and $x = 1$ for n odd, and $z = 0$ for $n \equiv 0 \pmod{4}$, $z = 4$ for $n \equiv 2 \pmod{4}$, $z = 2$ for $m \neq n \equiv 1$ or $3 \pmod{4}$, and $z = 4n - 10$ for $n = m$.

We now consider four cases depending on whether m is of the form $4t - 1, 4t - 2, 4t$, or $4t + 1$, where t is a positive integer.

(A) Construction for $m = 4t - 1$. Let X_b be a matrix obtained by deleting the first column of all 1s and $4t - n$ rows of H . Irrespective of the Hadamard matrix used, and irrespective of the rows deleted, each X_b has $SS = C(n, 4t - 1)$ as in Theorem 1, and hence is a superior $UE(s^2)$ -optimal design (Cheng et al., 2018; Singh et al., 2020). We call X_b the base matrix. All such X_b 's form the set of base design matrices for the other three cases. For X_b , with $m = 4t - 1 = m_b$ (say), we denote the parameters SS, LB, OF, Q by SS^b, LB^b, OF^b, Q^b respectively. To find a superior $UE(s^2)$ -optimal supersaturated design with minimum Q , the following steps are proposed:

- (i) Find the parameter values for all the $\binom{4t}{n}$ superior $UE(s^2)$ -optimal designs obtained from every available non-isomorphic Hadamard matrix H of order $4t$. Collect designs with the same parameters in the same class, thereby forming I classes of designs with distinct parameters $(SS^b, LB_i^b, OF_i^b, Q_i^b)$, $i = 1, \dots, I$.
- (ii) Without loss of generality, let parameters satisfy $Q_1^b \leq Q_2^b \leq \dots \leq Q_I^b$. Any superior $UE(s^2)$ -optimal design with $Q^b = Q_1^b$ is, therefore, a design as proposed.

For a large m , many non-isomorphic Hadamard matrices exist and it is not possible to do (i) for all non-isomorphic Hadamard matrices. One could then do step (i) for as many non-isomorphic Hadamard matrices as possible. Then, there is a possibility of a design with smaller Q than the proposed design.

Example 1 For $m = 15, n = 12$, there are 5 non-isomorphic Hadamard matrices of order 16, the total number of possible superior $UE(s^2)$ -optimal designs are $\binom{16}{12} \times 5 = 1820 \times 5 = 9100$. Among these 9100 possibilities of X_b 's, we get only four distinct parameter sets given in Table 1. In Table 1, we also provide the respective number of designs in these classes under the 'Count' column.

Table 1: Four sets of parameters for $m = 15, n = 12$

i	SS^b	LB_i^b	OF_i^b	Q_i^b	Count
1	48	6	42	48	7248
2	48	3	57	60	384
3	48	9	51	60	1152
4	48	12	84	96	316
				Total	9100

Any superior $UE(s^2)$ -optimal designs corresponding to the first row in Table 1, that is, designs with $Q_1^b = 48$ are the proposed designs. One such example of a superior $UE(s^2)$ -optimal design with $Q = 48$ is given below.

-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1
-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1
1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1
-1	-1	-1	1	1	1	1	-1	-1	-1	-1	1	1	1	1
1	-1	1	1	-1	1	-1	-1	1	-1	1	1	-1	1	-1
-1	1	1	1	1	-1	-1	-1	1	1	1	1	1	-1	-1
1	1	-1	1	-1	-1	1	-1	1	1	-1	1	-1	-1	1
-1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	1	1
-1	-1	-1	1	1	1	1	1	1	1	1	-1	-1	-1	-1
-1	1	1	-1	1	-1	1	1	1	-1	-1	1	-1	1	-1
1	-1	1	1	-1	-1	1	1	-1	1	-1	1	1	1	-1

(B) Construction for $m = 4t - 2$. For $m = 4t - 2$, a column with the maximum absolute column sum is deleted from X_b to get a superior $UE(s^2)$ -optimal design. Starting from X_b with $m_b = 4t - 1$, we construct a superior $UE(s^2)$ -optimal design with $m = 4t - 2$ and minimum Q as follows.

- (i) For the i -th set, there are $m - LB_i^b$ number of columns in the corresponding X_b 's which are not (nearly) level-balanced. Let x_u be the number of columns for a design in the i -th class with the column sums equal to $\pm 2u$ (for n even) and equal to $\pm(2u + 1)$ (for n odd), $u = 1, \dots, k$. Then, for all designs in the i -th class, $i = 1, \dots, I$, we check whether

$$4 \sum_{u=1}^k u^2 x_u = C(4t - 2, n) \text{ for } n \text{ even, and}$$

$$\sum_{u=1}^k (2u + 1)^2 x_u = C(4t - 2, n) - LB_i^b \text{ for } n \text{ odd.}$$

Assume that the conditions are true for $I_1 \leq I$ sets of parameters. Only keep these I_1 sets and number the sets as $i = 1, \dots, I_1$ such that $Q_1^b \leq Q_2^b \leq \dots \leq Q_{I_1}^b$.

- (ii) Starting from $i = 1$, for the designs in the i -th class, we delete a column with column sum as $\pm n$ for $n \leq 2t$ or as $\pm(4t - n)$ for $n > 2t$ (note that this can always be done, see, Singh et al. (2020)). Then for each i , designs could have J_i possible sets of parameters $(C(4t - 2, n), LB_i = LB_i^b, OF_{i(j)}, Q_{i(j)})$, where $OF_i^b - m \leq OF_{i(j)} \leq OF_i^b$, $j = 1, \dots, J_i$. Without loss of generality, let $Q_{i(1)} \leq Q_{i(2)} \leq \dots \leq Q_{i(J_i)}$. Define $q_i = \min\{Q_{i(1)}, q_{i-1}\}$ for $i = 2, \dots, I$ and $q_1 = Q_{i(1)}$.
- (iii) If $q_i \leq Q_{i+1}^b - m$, then a superior $UE(s^2)$ -optimal design with $Q = q_i$ is the proposed design, otherwise the steps (ii)-(iii) are sequentially repeated for $i = 2, \dots, I_1$. If we reach $i = I_1$, then a superior $UE(s^2)$ -optimal design with $Q = q_{I_1}$ is the proposed design.

Example 2 For constructing a superior $UE(s^2)$ -optimal design, with $m = 14, n = 12$ having minimum Q , from Table 1, the base design with $m_b = 15, n = 12$ has $I = 4$ sets of parameters. With $C(14, 12) = 32$, the condition in step (i) of the algorithm is not met for $i = 2$. This allows us to reduce the number of sets of parameters to $I_1 = 3$. Now, for the designs in the set $i = 1$, deleting a column with the desired property gives superior $UE(s^2)$ -optimal designs with $J_1 = 1$ parameters ($SS = 32, LB_1 = 6, OF_{1(1)} = 36, Q_{1(1)} = 42$). Since, $q = 42 < 60 - 14 = 46$, the design with $Q = q = 42$ is the proposed design and is given below.

1	1	1	1	1	1	1	1	1	1	1	1	1	1
1	1	-1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1
-1	-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1
-1	-1	-1	-1	1	1	1	1	-1	-1	-1	-1	1	1
-1	-1	-1	-1	1	1	-1	-1	1	1	1	1	-1	-1
-1	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	1	1
1	1	-1	-1	-1	-1	-1	-1	-1	-1	1	1	1	1
1	1	1	1	1	1	-1	-1	-1	-1	-1	-1	-1	-1
1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
1	-1	-1	1	-1	1	1	-1	1	-1	-1	1	-1	1
-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1
-1	1	-1	1	1	-1	-1	1	1	-1	1	-1	-1	1

(C) Construction for $m = 4t$. For $m = 4t$, a level-balanced column should be added to X_b to get a superior $UE(s^2)$ -optimal design. Our algorithm to construct a superior $UE(s^2)$ -optimal design with $m = 4t$, having the minimum value of Q is as follows. We start with X_b 's as in Construction (A) corresponding to $m_b = 4t - 1$. Then, the i th set of parameters corresponding to the base matrices is $(SS^b, LB_i^b, OF_i^b, Q_i^b)$, $i = 1, \dots, I$. Note that these i sets are such that $Q_1^b \leq Q_2^b \leq \dots \leq Q_I^b$.

- (i) Starting from $i = 1$, for each design in the i -th class (that is, a design with minimum Q), we add all possible balanced columns to the existing $4t - 1$ columns. Then for each i , designs could have J_i resultant possible parameters $(C(4t, n), LB_i = LB_i^b + 1, OF_{i(j)}^b, Q_{i(j)}^b)$, where $OF_i^b \leq OF_{i(j)}^b \leq OF_i^b + m - 1$, $j = 1, \dots, J_i$. Without loss of generality, let $Q_{i(1)} \leq Q_{i(2)} \leq \dots \leq Q_{i(J_i)}$. Define $q_i = \min\{Q_{i(1)}, q_{i-1}\}$ for $i \geq 2$ and $q_1 = Q_{i(1)}$.
- (ii) If $q_i \leq Q_{i+1}^b$, then a superior $UE(s^2)$ -optimal design with $Q = q_i$ is the final design. Otherwise steps (i)-(ii) are repeated sequentially for $i = 2, \dots, I$. If we reach $i = I$, then a superior $UE(s^2)$ -optimal design with $Q = q_I$ is the proposed design.

Example 3 For constructing a superior $UE(s^2)$ -optimal design with $m = 16, n = 12$ having minimum Q , we make use of Table 1. For the designs in the set $i = 1$ in Table 1, adding level-balanced columns gives $J_1 = 7$ parameter sets of which the one with the minimum $Q_{1(j)}$ is $(SS = 48, LB_1 = 7, OF_{1(1)} = 42, Q_{1(1)} = 49)$. Since, $q = 49 < 60$, the design with $Q = q = 49$, given below, is a proposed superior $UE(s^2)$ -optimal design with minimum Q .

-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1
-1	1	1	-1	-1	1	1	-1	-1	1	1	-1	1	-1
1	1	-1	-1	1	1	-1	-1	1	1	-1	-1	1	-1
-1	-1	-1	1	1	1	1	-1	-1	-1	1	1	1	1
1	-1	1	1	-1	1	-1	-1	1	-1	1	1	-1	-1
-1	1	1	1	1	1	-1	-1	-1	1	1	1	-1	-1
-1	-1	-1	-1	-1	-1	-1	1	1	1	1	1	1	-1
-1	-1	1	-1	1	1	1	1	1	-1	1	-1	-1	1
-1	1	-1	1	1	1	-1	1	1	-1	1	-1	-1	1
-1	1	1	1	-1	-1	1	1	1	-1	-1	1	1	-1
1	-1	-1	1	-1	1	1	1	-1	1	1	-1	-1	-1

(D) Construction for $m = 4t + 1$. For $m = 4t + 1$, to get a superior $UE(s^2)$ -optimal design, two columns should be added to X_b so that the pairs $(1, 1)$, $(-1, -1)$, $(1, -1)$ and $(-1, 1)$ appear in these columns as close to equal as possible; moreover, if $n \equiv 2 \pmod{4}$, the two columns must be orthogonal. Our algorithm to construct a superior $UE(s^2)$ -optimal design with $m = 4t$, having the minimum value of Q is an adaptation of the algorithm in

Construction (C) in this paper. We again start with X_b 's as in Construction (A) corresponding to $m_b = 4t - 1$. Then, the i th set of parameters corresponding to the base matrices is $(SS^b, LB_i^b, OF_i^b, Q_i^b)$, $i = 1, \dots, I$ with $i = 1$ corresponding to the set with the minimum value of Q .

- (i) Starting from $i = 1$, for the designs in the i -th class, we add all possible sets of two level-balanced columns with 0 inner product. For each i , designs now have J_i resultant sets of possible parameters $(C(4t + 1, n), LB_i = LB_i^b + 2, OF_{i(j)}, Q_{i(j)})$, where $OF_i^b \leq OF_{i(j)} \leq OF_i^b + 2m - 3$, $j = 1, \dots, J_i$. Without loss of generality, let $Q_{i(1)} \leq Q_{i(2)} \leq \dots \leq Q_{i(J_i)}$. Define $q_i = \min\{Q_{i(1)}, q_{i-1}\}$ for $i \geq 2$ and $q_1 = Q_{i(1)}$.
- (ii) If $q_i \leq Q_{i+1}^b$, then a superior $UE(s^2)$ -optimal design with $Q = q_i$ is the proposed design. Otherwise steps (i)-(ii) are sequentially repeated for $i = 2, \dots, I$. If we reach $i = I$, then a superior $UE(s^2)$ -optimal design with $Q = q_I$ is the proposed design.

Example 4 For constructing a superior $UE(s^2)$ -optimal design with $m = 17, n = 12$ having minimum Q , we can again make use of the sets listed in Table 1. Now, for the designs in the set $i = 1$, adding two columns with required properties gives a large number of J_i . However, the set with the minimum $Q_{1(j)}$ is $(SS = 48, LB_1 = 8, OF_{1(1)} = 43, Q_{1(1)} = 51)$. Since, $q = 51 < 60$, the design with $Q = q = 51$, given below, is a proposed superior $UE(s^2)$ -optimal design with minimum Q .

$$\begin{array}{cccccccccccccccc}
 -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 \\
 -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 \\
 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\
 -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 \\
 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 \\
 -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\
 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\
 -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & -1 \\
 -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\
 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1
 \end{array}$$

3. Concluding Remarks

In this paper, we have provided algorithms for constructing superior $UE(s^2)$ -optimal designs with minimum Q starting from the class of designs in Cheng et al. (2018). If it is not feasible to identify the I sets of parameters for all non-isomorphic Hadamard matrices, we propose to run the algorithms on only a selected set of the available Hadamard matrices; however, then there is no guarantee that the designs proposed here would have the minimum value of Q . As mentioned previously, superior $UE(s^2)$ -optimal designs also exist outside the class of designs used here (Singh et al., 2020). A future direction is to identify the best designs using better algorithms (or, analytically) to identify superior $UE(s^2)$ -optimal designs with minimum Q among a broader class of all superior $UE(s^2)$ -optimal designs.

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