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Advanced Methods for Constructing $UE(S^2)$ Optimal Supersaturated Designs in Factor Screening Experiments

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Authors' contributions

This work was carried out in collaboration among all authors. All authors read and approved the final manuscript.

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ABSTRACT

Supersaturated designs (SSDs) are crucial in factor screening experiments, especially when factor sparsity is assumed, meaning only a few factors are expected to be significant. Building on the foundational work of Jones and Majumdar [1], who introduced the $UE(S^2)$ criterion as an

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improvement over the $E(S^2)$ criterion by Booth and Cox [2], this study simplifies the construction of $UE(S^2)$ -optimal designs. The $UE(S^2)$ criterion is similar to the $E(S^2)$ criterion but removes the requirement for factor level balance. Our contribution lies in further simplifying these methods, explaining them with practical examples, and providing proofs for lower bounds for $UE(S^2)$ designs. Through this study, we aim to make the concepts and applications of supersaturated designs more accessible and easier to understand for practitioners. These methods can significantly optimize resource use and reduce costs in industrial, biological, and agricultural experiments. The study's implications extend to any field requiring efficient factor screening, offering a robust framework for future research.

Keywords: Supersaturated design; $E(S^2)$-optimality; $UE(S^2)$-optimality; Hadamard matrix.

1. INTRODUCTION

Supersaturated designs (SSDs) have emerged as a pivotal tool in the realm of experimental design, particularly for scenarios where the number of potential factors exceeds the number of experimental runs. This methodological innovation provides a solution to the challenges posed by resource constraints in large-scale experiments, enabling researchers to identify significant factors efficiently without the need for prohibitively large sample sizes. The genesis of SSDs can be traced back to the growing demand for cost-effective experimental strategies in various scientific fields, including engineering, biotechnology, and industrial processes. By permitting the investigation of numerous factors simultaneously, SSDs facilitate the exploration of complex systems and the identification of key variables that influence system performance to achieve an unbiased estimate of the main effects for each factor, the number of runs must be at least equal to the number of factors plus one. When the number of runs equals the number of factors, the design is termed a saturated design. However, if the number of runs is less than the number of factors, it is referred to as a supersaturated design. Specifically, a supersaturated design is a factorial design with n observations and m factors, where m exceeds n - 1.

SSDs have evolved through various construction methods, allowing researchers to optimize designs for specific objectives while minimizing experimental costs. The pioneering work by Youden et al. [3] laid the foundation for this approach, which has since evolved with various methods and improvements. Lin [4] introduced a new class of SSDs, while Wu [5] used partially aliased interactions, and Tang and Wu [6] emphasized $E(S^2)$-optimality in their construction methods. Bulutoglu and Cheng [7] and Ryan and Bulutoglu [8] further refined these designs, emphasizing optimality and minimax properties. More advancements include the development of large SSDs by Eskridge et al. [9] and the construction of group-orthogonal SSDs by Jones et al. [10]. Other notable contributions include the review of two-level SSDs by Kole et al. [11], the examination of optimal SSDs for S^m Factorials in N≢ 0 (mod s) runs by Chai et al. [12] and the exploration of large row-constrained SSDs by Smucker et al. [13], and the study of discriminating between superior $UE(S^2)$ -optimal SSDs by Chai et al. [14]. The ongoing interest and research, as seen in the works of Singh and Stufken [15] and Georgiou [16], highlight the importance of SSDs in modern statistical practice, particularly in the context of high-throughput screening and electronic games [17].

Preliminary Definitions:

Level balanced designs: "A design is said to be Level balance if the numbers of times each level appear in a column is same, i.e., For balanced two level design the number of +1's and -1's is equal in the each column of design otherwise it is unbalanced".

Orthogonal Designs: "Let $\mathbf{X} = (x_{ij})$ be an n × m design matrix for a factorial experiment in m factors and n runs. For a two-level design, $x_{ij} = +1 \; or -1$.The design matrix $\mathbf{X}$ is called orthogonal if $\mathbf{X'X}$ is a diagonal matrix".

Hadamard Matrix: "Hadamard matrix is a square matrix whose entries are either +1 or −1 and whose rows are mutually orthogonal $(H_n {H^T}_n = nI_n)$. A Hadamard matrix is said to be Normalized if the first row and first column consists entirely of positive 1's".

2. OPTIMALITY CRITERIA FOR SUPERSATURATED DESIGNS

Consider experiments involving *p - 1* two-level factors and an a priori model that includes the main effects and an intercept term. Let $\mathbf{X}$ represent both the design and model matrix, where $\mathbf{X}$ is n × p matrix with entries of -1 or 1, and the first column consisting of 1's. Assuming $p > n$ and that the rank ($\mathbf{X}$) is n.

Let $\mathbf{S} = \mathbf{X}'\mathbf{X}$ be the information matrix, with s_{ij} as its elements. If s_{ij} = 0, then factors *i* and *j* are orthogonal. A design that satisfies this condition for all *i* and *j* ($i \neq j$) is an orthogonal design, which allows for the intercept and all main effects to be estimated with maximal efficiency. For an orthogonal design to exist, it is necessary that $n = 2$ or $n \equiv 0 \pmod 4$ and $n \geq p$. Since $p > n$ in supersaturated designs, orthogonal designs are not possible. Therefore, the efficiency of a two-level supersaturated design (SSD) is measured by its deviation from orthogonality, or the extent of non-orthogonality present in the design.

2.1 $E(S^2)$ Criterion (Booth and Cox, [2])

Booth and Cox [2] introduced the $E(S^2)$ criterion for selecting SSDs, which requires that the means of all main effects be orthogonal to the intercept

$$E(\boldsymbol{S^2}) = \sum_{i\neq j=1}^{p}\sum \boldsymbol{s^2}_{ij} \Big/ (\boldsymbol{p}-\mathbf{1})(\boldsymbol{p}-\mathbf{2}) \qquad (2.1)$$

A design d* is said to be $E(S^2)$ -optimal if $E\left({S_{d*}}^2\right) = min\left\{E\left({S_d}^2\right)\right\} \quad where\ d \in D$.

2.2 $UE(S^2)$ Criterion (Jones and Majumdar, [1])

Since the condition requires that all main effects be orthogonal to the intercept, $E(S^2)$ -optimality can be considered a form of conditional optimality. Jones and Majumdar [1] examine an unconditional version of this optimality criterion.

Let

$$\boldsymbol{O}(\boldsymbol{X}) = \sum_{i\neq j=1}^{p}\sum \boldsymbol{s^2}_{ij} \qquad (2.2)$$

Minimizing *O*(*X*) without imposing condition that means of all main effects are orthogonal to intercept. To distinguish it from $E(S^2)$ optimality calls this approach $UE(S^2)$ -optimality, where *U* stands for "unconditional." Given *n* and *p*, a design will be called $UE(S^2)$-optimal if it minimizes *O*(*X*) among all designs.

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \boldsymbol{O}(\boldsymbol{X}) \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \sum_{i\neq j=1}^{p}\sum \boldsymbol{s^2}_{ij} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})\ldots \qquad (2.3)$$

This formula can be expressed as

Let $\boldsymbol{R} = \mathbf{XX}'$ with elements denoted by r_{ij}; note that $r_{ii} = p$,i=1,…, n.

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \sum_{i\neq j=1}^{p}\sum \boldsymbol{s^2}_{ij} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \{\boldsymbol{trace}(\mathbf{X}'\mathbf{X})^2 - \boldsymbol{pn^2}\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \{\boldsymbol{trace}(\mathbf{XX}')^2 - \boldsymbol{pn^2}\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \left\{\sum_{i\neq j}^{p}\sum \boldsymbol{r^2}_{ij} + \boldsymbol{np^2} - \boldsymbol{pn^2}\right\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \left\{\sum_{i\neq j}^{p}\sum \boldsymbol{r^2}_{ij} + \boldsymbol{np}(\boldsymbol{p}-\boldsymbol{n})\right\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1}) \quad (2.4)$$

3. METHODS OF CONSTRUCTION OF $UE(S^2)$ -OPTIMAL DESIGNS (JONES AND MAJUMDAR, [1]) AND LOWER BOUNDS FOR $UE(S^2)$ DESIGNS

3.1 Method 1 for $p = 0 \pmod 4$, $2 \leq n \leq p - 1$.

Step 1: Start by selecting a Normalized Hadamard matrix of order p denoted as $\boldsymbol{H_p}$.

Step 2: From $\boldsymbol{H_p}$ matrix, we form the design matrix by selecting any n rows $\boldsymbol{H_p}$. These rows constitute an n×p matrix $\mathbf{X_0}$. The $\mathbf{X_0}$matrix will be asuper saturated design.

Step 3: Once the matrix is formed, the next step is to verify that $\mathbf{X_0}$ meets the criteria for a type $\mathbf{T_0}$ design. This verification is done by calculating $\mathbf{R_0} = \mathbf{X_0}\mathbf{X_0}'$. If $\mathbf{R_0}$ equals to p times the identity matrix $\boldsymbol{I_n}$, then $\mathbf{X_0}$ is confirmed as a type $\mathbf{T_0}$ supersaturated design.

Example 3.1: Let p =16 and n =10, so consider a Hadamard matrix of order 16.

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

From $\boldsymbol{H_{16}}$ select **any** 10 rows to form the 10×16 matrix $\mathbf{X_0}$,Thus $\mathbf{X_0}$ a supersaturated design

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

Calculate $\mathbf{R_0} = \mathbf{X_0}\mathbf{X_0}'$ the resulting matrix is given by

16	0	0	0	0	0	0	0	0	0
0	16	0	0	0	0	0	0	0	0
0	0	16	0	0	0	0	0	0	0
0	0	0	16	0	0	0	0	0	0
0	0	0	0	16	0	0	0	0	0
0	0	0	0	0	16	0	0	0	0
0	0	0	0	0	0	16	0	0	0
0	0	0	0	0	0	0	16	0	0
0	0	0	0	0	0	0	0	16	0
0	0	0	0	0	0	0	0	0	16

Since $\mathbf{R_0}$ is 16 times of times the identity matrix of order 10 ($\boldsymbol{R_0} = 16\mathbf{I_{10}}$),this condition is satisfied, and therefore, the design $\mathbf{X_0}$called a type $\mathbf{T_0}$design.

By using equation 2.3, the calculated value $UE(S^2)$ is 4. The lower bound for $UE(S^2)$, if *p* = 0 (mod 4), is given by

$$\mathbf{min}\boldsymbol{UE}(\boldsymbol{S}^2) = \boldsymbol{np}(\boldsymbol{p}-\boldsymbol{n}) \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1}) \tag{3.1}$$

Proof*:*

The result follows from the inequality:

$$\boldsymbol{trace}(\mathbf{XX'})^2 \geq {\{\boldsymbol{trace}(\mathbf{XX'})\}^2}/{\boldsymbol{n}}$$

We know that:

$$UE(S^2) = \{trace(XX')^2 - pn^2\} \Big/ p(p-1)$$

$$UE(S^2) = \left\{\frac{\{trace(XX')\}^2}{n} - pn^2\right\} \Big/ p(p-1)$$

We know that $R = XX' = pI_n$, we get:

$$UE(S^2) = \left\{\frac{\{np\}^2}{n} - pn^2\right\} \Big/ p(p-1)$$

Simplifying this, we obtain:

$$minUE(S^2) = np(p-n) \Big/ p(p-1)$$

Hence, the minimum value of $UE(S^2)$ is achieved when $R_0 = p\,I_n$, confirming that hence type $\mathbf{T_0}$ designs are $UE(S^2)$ -optimal.

3.2 Method 2 for p = 1(mod 4), 2 ≤ n ≤ p − 1.

Step 1: Start by selecting a Normalized Hadamard matrix of order *p-1* denoted as H_{p-1}

Step 2: From H_{p-1} matrix, we form the design matrix by selecting any n rows H_{p-1} ,these rows constitute an $n \times (p-1)$ matrix V.

Step 3: Create an $n \times 1$ vector φ with entries 1 or -1.

Step 4: Combine V and φ to form the design matrix $X_0 = (V, \varphi)$, which will be super saturated design.

Step 5: calculate $R_0 = X_0 X_0'$, if $R_0 = (p-1)I_n + \varphi\varphi'$, resulting in a matrix with diagonal entries p and off-diagonal entries 1 or -1, then design X_0 in this case will be called a type $\mathbf{T_1}$ design.

Example **3.2:** Let $p - 1 = 8$ and n =7, so consider a Hadamard matrix of order 8 (H_8).

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

V be the matrix of order 7 × 8 formed by first 7 rows of H_8

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

Let φ be the 7 × 1 vector with entries -1, then combined $\boldsymbol{V}$ and φ to form the design matrix $\mathbf{X_0}$ which will be super saturated design of order 7 × 9. The matrix $\mathbf{X_0}$ presented 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

$\mathbf{R}_{\mathbf{0}} = \boldsymbol{X_0}\boldsymbol{X_0}'$ is calculated it is of order 7 × 7

9	1	1	1	1	1	1
1	9	1	1	1	1	1
1	1	9	1	1	1	1
1	1	1	9	1	1	1
1	1	1	1	9	1	1
1	1	1	1	1	9	1
1	1	1	1	1	1	9

Verified that $\mathbf{R}_{\mathbf{0}} = 8\boldsymbol{I_n} + \varphi\varphi'$**,** hence design $\mathbf{X}_{\mathbf{0}}$ will be called a type $\boldsymbol{T_1}$ design.

The lower bound for $UE(S^2)$ If p = 1 (mod 4) is given by

$$\boldsymbol{minUE}(\boldsymbol{S^2}) = \{\boldsymbol{n}(\boldsymbol{n}-\mathbf{1}) + \boldsymbol{np}(\boldsymbol{p}-\boldsymbol{n})\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1}) \quad \ldots \quad (3.2)$$

Proof*:*

Let entries of **X** are x_{it}, then

$$r_{ij} = \sum_{t=1}^{p} x_{it}\, x_{jt}$$

Since $x_{it}\, x_{jt} \in \{-1,1\}$ and p is odd $|r_{ij}| \geq 1$, and therefore

$$min \sum_{i\neq j=1}^{p} \sum \boldsymbol{r^2}_{\boldsymbol{ij}} = n(n-1)$$

We know that

$$\boldsymbol{UE}(\boldsymbol{S^2}) = \left\{ \sum_{\boldsymbol{i}\neq \boldsymbol{j}}^{\boldsymbol{p}} \sum \boldsymbol{r^2}_{\boldsymbol{ij}} + \boldsymbol{np}(\boldsymbol{p}-\boldsymbol{n}) \right\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

And hence,

$$\boldsymbol{minUE}(\boldsymbol{S^2}) = \{\boldsymbol{n}(\boldsymbol{n}-\mathbf{1}) + \boldsymbol{np}(\boldsymbol{p}-\boldsymbol{n})\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1})$$

The minimum in (3.2) is attained whenever *R* is a matrix with diagonal entries *p* and off-diagonal entries either 1 or −1. Hence type T_1 designs are $UE(S^2)$ -optimal.

3.3 Method 3 for p = 2(mod 4), 2 ≤ n ≤ p − 2.

- **Case 1: n is even, n = 2m.**

Step 1: Start by selecting a Normalized Hadamard matrix of order *p-2* denoted as $\boldsymbol{H_{p-2}}$

Step 2: From $\boldsymbol{H_{p-2}}$ matrix, we form the design matrix by selecting any n rows $\boldsymbol{H_{p-2}}$,these rows constitute an $n \times (p-2)$ matrix $\boldsymbol{X}^*$.

Step 3: Create an $n \times 2$ matrix $\boldsymbol{U_1}$ with each of the first *m* rows either (1, 1) or (−1,−1) and each of the last *m* rows either (1,−1) or (−1, 1).

Step 4: Combine $\boldsymbol{X}^*$ and $\boldsymbol{U_1}$ to form the design matrix $\mathbf{X_0} = (\boldsymbol{X}^*, \boldsymbol{U_1})$, which will be super saturated design.

Step 5: calculate $\mathbf{R_0} = \mathbf{X_0}\mathbf{X_0}'$, The resulting $\mathbf{R_0}$ matrix has the block diagonal structure:

$$\begin{pmatrix} S_m & O_{m,m} \\ O_{m,m} & S_m \end{pmatrix}$$

Where the notation $O_{m,m}$ denotes a *m*× *m* matrix with entries 0, and S_m denotes a *m* × *m* matrix with diagonal entries *p* and off-diagonal entries either 2 or −2. If $\mathbf{R_0}$ has this specified block diagonal structure, then $\mathbf{X_0}$ is called a type $\mathbf{T_2}$ design.

Example 3.3.1: Let $p = 18$, n =10(even), m=5 and $p - 2 = 16$, so consider a Hadamard matrix of order 16 ($\boldsymbol{H_{16}}$).

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

$\boldsymbol{X}^*$ be the matrix of order 10×16 formed by first 10 rows of $\boldsymbol{H_{16}}$

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

Consider $\boldsymbol{U_1}$ be the 10 × 2 matrix with each of the first *5* rows (1, 1) and each of the last *5* rows (1,−1). Next by combining $\boldsymbol{X}^*$ and $\boldsymbol{U_1}$ to form the design matrix $\mathbf{X_0} = (\boldsymbol{X}^*, \boldsymbol{U_1})$, which will be super saturated design with p=18 and n=10 represented bellow

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

$\mathbf{R}_{\mathbf{0}} = \boldsymbol{X_0}\boldsymbol{X_0}'$ is calculated, it is of order 10 × 10

18	2	2	2	2	0	0	0	0	0
2	18	2	2	2	0	0	0	0	0
2	2	18	2	2	0	0	0	0	0
2	2	2	18	2	0	0	0	0	0
2	2	2	2	18	0	0	0	0	0
0	0	0	0	0	18	2	2	2	2
0	0	0	0	0	2	18	2	2	2
0	0	0	0	0	2	2	18	2	2
0	0	0	0	0	2	2	2	18	2
0	0	0	0	0	2	2	2	2	18

By using equation 2.3 Calculated $UE(S^2)$ of $\boldsymbol{X_0}$= 5.88. The lower bound for $UE(S^2)$ If p = 2 (mod 4) and n is even, then

$$\boldsymbol{minUE}(\boldsymbol{S^2}) = \{2\boldsymbol{n}(\boldsymbol{n}-\mathbf{2}) + \boldsymbol{np}(\boldsymbol{p}-\boldsymbol{n})\} \Big/ \boldsymbol{p}(\boldsymbol{p}-\mathbf{1}) \qquad \dots \qquad (3.3.1)$$

Proof:

Let entries of **X** are x_{it}, then

$$r_{ij} = \sum_{t=1}^{p} x_{it}\, x_{jt}$$

If there are a terms that are −1 in r_{ij} and p – a terms that are 1, then r_{ij} = p – 2a. Since p is even, | p – 2a | is either 0 or even. This means that for I ≠ j , $|r_{ij}| = 2$ whenever r_{ij} ≠ 0.

Strategy in this case has two parts. In the first part, for each n determine N(n), the maximal number of zeros among the off-diagonal entries of R. In the second step, derive the lower bounds by considering a matrix R with N(n) off-diagonal entries zero and the remaining off-diagonal entries either 2 or−2. Clearly this matrix attains $min \sum_{i\neq j=1}^{p} \sum r^2{}_{ij}$.

Part 1: Firstly determine the maximal number of pairs (I, j) , I <j, such that r_{ij} = 0. Let us define a graph G with n vertices, where each vertex corresponds to a row of X. Two vertices I and j of G are defined to be adjacent (there is an edge connecting them), if the corresponding rows of X are orthogonal, that is, r_{ij} = 0. Note that, since p ≠ 0(mod 4) no subset of three rows of X can be mutually orthogonal. This means that there are no triangles in the graph G. Viewed in these terms our problem is to determine the maximal number of edges in this graph. It follows from Turan's theorem

(Turan 1941; Harary 1972) that the maximal number of edges in a triangle-free graph with n vertices is $n^2/4$, and this maximal number is attained by a complete bipartite graph.

When n is even, n = 2m, the maximal number is attained by a complete bipartite graph where both sets of the partition are of size n/2 = m. This graph has m^2 edges; hence N(n) = $2m^2$.

Part 2: when n is even, n = 2m

$$\sum_{i \neq j=1}^{p} \sum \boldsymbol{r^2}_{ij} \geq \boldsymbol{4[n(n-1)-2m^2] = 2n(n-2)}$$

And hence

$$\boldsymbol{minUE(S^2)} = \{2\boldsymbol{n(n-2)} + \boldsymbol{np(p-n)}\} \Big/ \boldsymbol{p(p-1)}$$

The minimum in equation 3.3.1 is attained whenever the rows of $\boldsymbol{X}$ can be partitioned into two sets of size *n/*2 each such that if rows *I* and *j* belong to the same set then $|r_{ij}| = 2$, and if rows *I* and *j* belong to different sets then r_{ij} = 0*.* The above type *T*2 designs possess this property hence they are *UE*(*s*2)-optimal.

- **Case 2: n is odd, n = 2m+1.**

Step 1: Start by selecting a Normalized Hadamard matrix of order *p-2* denoted as $\boldsymbol{H_{p-2}}$

Step 2: From $\boldsymbol{H_{p-2}}$ matrix, we form the design matrix by selecting any n rows $\boldsymbol{H_{p-2}}$,these rows constitute an $n \times (p-2)$ matrix $\boldsymbol{X}^*$.

Step 3: Create an $n \times 2$ matrix $\boldsymbol{U_2}$ with each of the first *m* rows either (1*,* 1) or (−1*,*−1) and each of the last *m+1* rows either (1*,*−1) or (−1*,* 1).

Step 4: Combine $\boldsymbol{X}^*$ and $\boldsymbol{U_2}$ to form the design matrix $\mathbf{X_0} = (\boldsymbol{X}^*, \boldsymbol{U_2})$, which will be super saturated design.

Step 5: calculate $\mathbf{R_0} = \mathbf{X_0} \mathbf{X_0}'$**,** The resulting $\mathbf{R_0}$ matrix has the block diagonal structure:

$$\begin{pmatrix} S_m & O_{m,m+1} \\ O_{m+1,m} & S_{m+1} \end{pmatrix}$$

Where the notation $O_{m,m+1}$ and $O_{m+1,m}$ denotes matrices with entries 0, and S_m and S_{m+1} denotes matrices with diagonal entries *p* and off-diagonal entries either 2 or −2. If $\mathbf{R_0}$ has this specified block diagonal structure, then $\mathbf{X_0}$ is called a type $\mathbf{T_2}$ design.

Example 3.3.2: Let $p = 10$, n =7(odd), m=3 and $p - 2 = 8$, so consider a Hadamard matrix of order 8 ($\boldsymbol{H_8}$).

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

$\boldsymbol{X}^*$ be the matrix of order 7×8 formed by first 7 rows of $\boldsymbol{H_8}$

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

Consider $\boldsymbol{U_2}$ be the 7 × 2 matrix with each of the first *3* rows (-1, -1) and each of the last 4 rows (1,−1). Next by combining $\boldsymbol{X}^*$ and $\boldsymbol{U_2}$ to form the design matrix $\mathbf{X_0} = (\boldsymbol{X}^*, \boldsymbol{U_2})$, which will be super saturated design with p=10 and n=7 represented bellow

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

$\mathbf{R_0} = \boldsymbol{X_0}\boldsymbol{X_0}'$ is calculated it is of order 10 × 10

10	2	2	0	0	0	0
2	10	2	0	0	0	0
2	2	10	0	0	0	0
0	0	0	10	2	2	2
0	0	0	2	10	2	2
0	0	0	2	2	10	2
0	0	0	2	2	2	10

By using equation (2.3) Calculated $UE(S^2)$ of $\boldsymbol{X_0}$ = 3.133. The lower bound for $UE(S^2)$ If *p* = 2 (mod 4) and n is even, then

$$\mathrm{minUE(S^2)} = \{2(\mathrm{n}-1)^2 + \mathrm{np(p-n)}\} \Big/ \mathrm{p(p-1)} \qquad \text{… (3.3.2)}$$

Proof : The proof is similar to that provided for equation 3.3(1). When *n* is odd, *n* = 2*m* + 1, the maximal number is attained by a complete bipartite graph where the sets of the partition are of sizes *m* and *m* + 1*.* This graph has *m* (*m* + 1) edges, hence *N*(*n*) = 2*m*(*m* + 1).

$$\sum_{i \neq j=1}^{p} \sum \boldsymbol{r^2}_{\boldsymbol{ij}} \geq 4[n(n-1) - 2m(m+1)] = 2(n-1)^2$$

And hence

$$\mathrm{minUE(S^2)} = \{2(\mathrm{n}-1)^2 + \mathrm{np(p-n)}\} \Big/ \mathrm{p(p-1)}$$

The minimum in equation (3.3.2) is attained whenever the rows of X can be partitioned into two sets of sizes (n − 1)/2 and (n + 1)/2 such that if rows i and j belong to the same set then $|r_{ij}| = 2$ and if rows i and j belong to different sets then r_{ij} = 0. Above type $\mathbf{T_2}$ design possess this property hence they are $UE(S^2)$-optimal.

3.4 Method 4 for p = 3(mod 4), 2 ≤ n ≤ p − 1.

Step 1: Start by selecting a Normalized Hadamard matrix of order *p+1* denoted as $\boldsymbol{H_{p+1}}$

Step 2: From $\boldsymbol{H_{p+1}}$ matrix, we form the design matrix by selecting any n rows $\boldsymbol{H_{p+1}}$,these rows constitute an $n \times (p+1)$ matrix X^*

Step 3: last column of **X*** is denoted by $\boldsymbol{\delta}$

Step 4: remove the last column $\boldsymbol{\delta}$ from the design **X*** to form the design matrix $\mathbf{X_0}$, which will be super saturated design.

Step 5: calculate $\mathbf{R_0} = \mathbf{X_0}\mathbf{X_0}'$, if $\mathbf{R_0} = (\boldsymbol{p+1})\boldsymbol{I_n} - \boldsymbol{\delta}\boldsymbol{\delta}'$, resulting in a matrix with diagonal entries p and off-diagonal entries 1 or -1, then design $\mathbf{X_0}$ in this case will be called a type $\mathbf{T_3}$ design.

Example 3.4: Let $p = 15$, n =10 and $p + 1 = 16$, so consider a Hadamard matrix of order 16 ($\boldsymbol{H_{16}}$).

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

$\boldsymbol{X^*}$ be the matrix of order 10×16 formed by first 10 rows of $\boldsymbol{H_{16}}$

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

last column of **X*** is denoted by $\boldsymbol{\delta}$**,** remove the last column $\boldsymbol{\delta}$ from the design

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

$\mathbf{R}_0 = \boldsymbol{X_0}\boldsymbol{X_0}'$ is calculated, it is of order 10 × 10

15	1	1	-1	1	-1	-1	1	1	-1
1	15	-1	1	-1	1	1	-1	-1	1
1	-1	15	1	-1	1	1	-1	-1	1
-1	1	1	15	1	-1	-1	1	1	-1
1	-1	-1	1	15	1	1	-1	-1	1
-1	1	1	-1	1	15	-1	1	1	-1
-1	1	1	-1	1	-1	15	1	1	-1
1	-1	-1	1	-1	1	1	15	-1	1
1	-1	-1	1	-1	1	1	-1	15	1
-1	1	1	-1	1	-1	-1	1	1	15

$\boldsymbol{\delta}\,\boldsymbol{\delta}\,'$ matrix 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

Verified that $\mathbf{R}_0 = 16\boldsymbol{I_n} - \boldsymbol{\delta}\,\boldsymbol{\delta}\,'$ hence design $\mathbf{X}_0$ will be called a type **T3** design.

By using equation (2.3), the calculated $UE(S^2)$ of **Xo** is 4. The lower bound for $UE(S^2)$ If *p* = 3(mod 4) is given by:

$$\boldsymbol{UE(S^2)} = \{\boldsymbol{n(n-1)} + \boldsymbol{np(p-n)}\}\Big/\boldsymbol{p(p-1)} \quad (3.4)$$

Proof: is similar given to that given for equation **(3.2)**. The minimum in equation (3.4) is attained whenever $\mathbf{R}_0$ is a matrix with diagonal entries p and off- diagonal entries either 1 or −1. Hence type **T3** design are $UE(S^2)$ -optimal.

4. CONCLUSION

This study delves into the realm of supersaturated designs, offering valuable insights into their construction and optimization for efficient factor screening experiments. By exploring various design criteria such as $E(S^2)$-optimality and $UE(S^2)$ -optimality, the study highlights the significance of balancing efficiency and resource utilization in experimental design. The research primarily focuses on the utilization of Hadamard matrices to construct $UE(S^2)$ -optimal designs, thereby enhancing the understanding of design methodologies.

The methods outlined, including the selection and manipulation of Hadamard matrices, provide a robust framework for creating supersaturated designs that achieve near-optimal efficiency. These methods demonstrate that it is possible to maintain a high degree of efficiency even when the number of factors exceeds the number of runs, a common challenge in large-scale experiments. The practical examples and proofs provided for lower bounds of $UE(S^2)$ designs offer a comprehensive guide for practitioners aiming to implement these designs in various fields such as industrial, biological, and agricultural experiments. By bridging theoretical concepts with practical applications, this research contributes to the advancement of experimental design strategies, paving the way for more effective and cost-efficient factor screening studies. Overall, the study underscores the importance of developing and utilizing optimal SSDs to maximize resource use and reduce costs, thereby providing a robust framework for future research and application in any field requiring efficient factor screening.

our study acknowledges certain limitations. The methods described are primarily based on the use of Hadamard matrices, which may not be available or easily constructed for all parameter configurations. Future research could explore alternative construction methods that do not rely solely on Hadamard matrices, thereby broadening the applicability of the optimal SSDs. Investigating the integration of other optimality criteria and their impact on design efficiency would also be valuable.

DISCLAIMER (ARTIFICIAL INTELLIGENCE)

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc) and text-to-image generators have been used during writing or editing of manuscripts.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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