Exploratory Study of Construction Techniques for Optimal Supersaturated Designs in Factor Screening Experiments

Abstract:

Supersaturated designs are valuable for factor screening experiments, particularly under the assumption of factor sparsity, where only a few factors are expected to be significant. Box (1959) proposed using supersaturated designs when the number of parameters exceeds the number of observations. Booth and Cox (1962) introduced efficiency measures for these designs, specifically the $E(S^2)$ criterion, which minimizes the sum of squares of the entries in the information matrix for designs where each factor's two levels appear an equal number of times. Jones and Majumdar (2014) later suggested the $UE(S^2)$ criterion, which is similar to the $E(S^2)$criterion but removes the requirement for factor level balance. This relaxation simplifies the construction of $UE(S^2)$optimal designs. This study explores various methods for constructing $UE(S^2)$optimal designs.

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

1.Introduction

In industrial, biological, and agricultural experiments, there are often scenarios where a large number of factors need to be tested, but only a few are actually significant. The challenge lies in identifying which and how many of these factors are active. The experimenter's goal is to minimize the number of experimental runs required to detect the active factors, thereby optimizing resource use and reducing cost and time. One effective approach in such situations is to use Supersaturated Designs (SSDs). Satterthwaite (1959) proposed the construction of these designs, which are fractional factorial designs with a number of runs insufficient to estimate the main effects of all the factors in the experiment.

To obtain an unbiased estimate of the main effects of each factor run size must exceed (or at least equal to) the number of factors plus one. When the numbers are equal the design is called saturated design. When run size less than the number of factors is called super saturated design. Supersaturated design- a factorial design with n observations and m factors with m > n - 1.

Example:Supersaturated design with 14 factors and 12 runs.

1	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**
-1	**1**	**-1**	**1**	**-1**	**1**	**-1**	**1**	**-1**	**1**	**-1**	**1**	**-1**	**1**
1	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
-1	**-1**	**1**	**1**	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**1**	**1**	**-1**	**-1**
1	**1**	**1**	**-1**	**-1**	**-1**	**-1**	**1**	**1**	**1**	**1**	**-1**	**-1**	**-1**
-1	**1**	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**-1**
1	**-1**	**-1**	**-1**	**-1**	**1**	**1**	**1**	**1**	**-1**	**-1**	**-1**	**-1**	**1**
-1	**-1**	**1**	**-1**	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**-1**	**1**	**1**
1	**1**	**1**	**1**	**1**	**1**	**1**	**-1**	**-1**	**-1**	**-1**	**-1**	**-1**	**-1**
-1	**1**	**-1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**-1**	**1**	**-1**	**1**	**-1**
1	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**1**

-1	**-1**	**1**	**1**	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**-1**	**1**	**1**

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 **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 1s.

2. Optimality Criteria for supersaturated designs

Consider experiments with p − 1 two-level factors and an a priori model that contains the main effects and an intercept term. Use the notation **X** to denote the design, as well as the model matrix. **X**is a n × p matrix with entries −1 or 1 with the first column consisting of 1's. Assume p > n and rank (**X**) = n.

Let $\mathbf{S = X'X}$denote the information matrix and $s_{ij}$the elementsof S. If s_{ij}= 0, then factors i and j are orthogonal. Adesign for which this condition holds for all i and j (i ≠ j) isan orthogonal design, and for this design the intercept and allmain effects are estimated with maximal efficiency. A necessarycondition for the existence of an orthogonal design is n = 2 orn ≡ 0(mod 4) and n ≥ p. Sincep > n in supersaturated design's, orthogonaldesigns do not exist.

A measure of efficiency of two level supersaturated design's (SSD)therefore, is the departure from orthogonality or amount of non-orthogonality present in the design.

2.1$E(S^2)$ criterion *(Booth and Cox, 1962)*

Booth and Cox (1962) proposed the $E(S^2)$ criterion for the choice of SSD by imposing condition that means of all main effects are orthogonal to intercept.

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

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

2.2 $UE(S^2)$ criterion *(Jones and Majumdar, 2014)*

Since condition means that all main effects are orthogonal to the intercept $E(S^2)$-optimality may be viewed as *conditional* optimality. Jones and Majumdar (2014) explore the *unconditional* version of this optimality criterion.

Let

$\boldsymbol{O(X)} = \sum_{i\neq j=1}^{p}\sum \boldsymbol{s^2}_{\boldsymbol{ij}}$**…(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 call 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.

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

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

This formula can be expressed as

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

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

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

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

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

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

3. Methods of construction of $UE(S^2)$-optimal designs and Lower bounds for $UE(S^2)$designs .

3.1 Method 1 for p = 0(mod 4), 2 ≤ n ≤ p − 1.

- Start with a NormalizedHadamard matrix of order p ($\mathbf{H_p}$).

- Let $\mathbf{X_0}$ be the n × p matrix formed by any n rows of $\mathbf{H_p}$.
- The resultant matrix will be super saturated design.
- Then find $\mathbf{R_0}$=$\mathbf{X_0}\mathbf{X_0}'= \boldsymbol{p}\ \boldsymbol{I_n}$. A design $\mathbf{X_0}$ in this case will be called a type $\mathbf{T_0}$ design.

Example 3.1: Letp=16 and n=10 so take 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

- X_0 be the 10 × 16 matrix formed by any 10 rows of $\mathbf{H_{16}}$.

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

- So it is a supersaturated design$\mathbf{X_0}$ withp=16and n=10.

- $\mathbf{R_0}$=$\mathbf{X_0 X_0{'}}$

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**	**0**
0	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**16**

- $\mathbf{R_0}$ **=** $16\mathbf{I_{10}}$hence design$\mathbf{X_0}$ called a type $\mathbf{T_0}$design.

  By using 2.3 Calculated $UE(S^2) = 4$

- Lower bound for $UE(S^2)$If $p = 0$ (mod 4),

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

...(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

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

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

We know that$\boldsymbol{R = XX' = pI_n}$

So

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

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

Hence proved.

The minimum in (3.1) is attained whenever $\boldsymbol{R} = \boldsymbol{p}\,\boldsymbol{I_n}$ hencetype T_0 designs are $UE(S^2)$-optimal.

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

- Start with a Normalized Hadamard matrix of order p-1 ($\mathbf{H_{p-1}}$).
- Let **V**be the n × (p-1)matrix formed by any n rows of $\mathbf{H_{p-1}}$.
- Let **ϕ** be the n × 1vector with entries 1 or -1.
- Let $\mathbf{X_0} = (\mathbf{V}, \boldsymbol{\phi})$
- The$\mathbf{X_0}$ matrix will be super saturated design.
- Then $\mathbf{R_0}=\mathbf{X_0}\mathbf{X_0}' = (\boldsymbol{p}-\mathbf{1})\boldsymbol{I_n} + \boldsymbol{\phi}\,\boldsymbol{\phi}'$,a matrix with diagonal entries p and off diagonal entries 1 or −1. A design $\mathbf{X_0}$ in this case will be called a type $\boldsymbol{T_1}$ design.

Example 3.2:

- Letp=9 and n=7 and p-1=8
- Take Hadamard matrix of order 8($\mathbf{H_8}$).

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

- Let **V** be the 7 × 8 matrix formed by any 7 rows of $\mathbf{H_8}$

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 × 1vector with entries -1

❖ **X_0= (V, ϕ)**oforder 7×9

1	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**-1**
1	**-1**	**1**	**-1**	**1**	**-1**	**1**	**-1**	**-1**
1	**1**	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**-1**
1	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**1**	**-1**
1	**1**	**1**	**1**	**-1**	**-1**	**-1**	**-1**	**-1**
1	**-1**	**1**	**-1**	**-1**	**1**	**-1**	**1**	**-1**
1	**1**	**-1**	**-1**	**-1**	**-1**	**1**	**1**	**-1**

❖ So it is a supersaturated design **X_0** withp=10 and n=7.

❖ **R_0**=$\boldsymbol{X_0 X_0}'$oforder 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**

❖ **R_0** = 8 **I_n**+ **ϕ ϕ** ' hence design**X_0** called a type **T_1** design .
By using 2.3 Calculated $UE(S^2) = 2.33$

➢ Lower bound for $UE(S^2)$If $p = 1$ (mod 4),

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

…(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

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

And hence

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

The minimum in (3.2) is attained whenever R is a matrix with diagonal entries p andoff-diagonal entries either 1 or −1.Hencetype 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* = 2*m*.**

- Start with a Normalized Hadamard matrix of order p-2 ($\mathbf{H}_{p-2}$).
- Let **X*** be the n × (p-2) matrix formed by any n rows of $\mathbf{H}_{p-2}$.
- Let $\mathbf{U_1}$ be the n × 2matrix 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).
- Let $\boldsymbol{X_0} = (\mathbf{X^*}, \mathbf{U_1})$
- The$\boldsymbol{X_0}$ matrix will be super saturated design.
- $\mathbf{R_0} = \boldsymbol{X_0}\boldsymbol{X_0}'$has the block diagonal structure:
  - $\begin{pmatrix} S_m O_{m,m} \\ O_{m,m} S_m \end{pmatrix}$
- Where the notation $\mathbf{O}_{m,m}$ denotes a $m\times m$ matrix with entries 0,and $S_m$denotes a $m\times m$ matrix with diagonal entries p and off-diagonal entries either 2 or −2.
- Then $\boldsymbol{X_0}$is called type T_2 design

Example 3.3(1):

- ❖ Letp=18 and n=10 (even) m=5 and p-2=16
- ❖ Take Hadamard matrix of order 16($\mathbf{H_{16}}$).

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

- Let **X*** be the 10 × 16matrix formed by any n rows of $\mathbf{H_{16}}$.

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

- Let $\mathbf{U_1}$ be the 10 × 2matrix with each of the first *5* rows (1, 1) and each of the last *5* rows (1,−1)

- $\boldsymbol{X_0}$ **= (X*,$\mathbf{U_1}$)** will be

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

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

- ❖ So it is a supersaturated design $\mathbf{X_0}$ withp=18 and n=10.

- ❖ Then $\mathbf{R_0} = \boldsymbol{X_0 X_0}'$

By using 2.3

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**

Calculated $UE(S^2)$ of$\boldsymbol{X_0}$= 5.88

- ➢ Lower bound for $UE(S^2)$If p = 2 (mod 4) and n is even, then

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

…[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 either0 or even. This means that for i ≠ j , $|r_{ij}| = 2$ whenever $r_{ij} \neq 0$.

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 areno 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 acomplete 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

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

And hence

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

The minimum in [3.3(1)] is attained whenever the rows of ***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*.**

- Start with a Normalized Hadamard matrix of order p-2 ($\mathbf{H_{p-2}}$).
- Let **X*** be the n × (p-2) matrix formed by any n rows of $\mathbf{H_{p-2}}$.
- Let $\mathbf{U_2}$ be the n × 2matrix 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).
- Let $\boldsymbol{X_0}$ **= (X*,U**$_2$ **)**

- The $\boldsymbol{X_0}$ matrix will be super saturated design.
- **R_0=** $\boldsymbol{X_0 X_0}'$has the block diagonal structure:
  - $\begin{pmatrix} S_m O_{m,m+1} \\ O_{m+1,m} S_{m+1} \end{pmatrix}$

- A design $\boldsymbol{X_0}$ in Case 1 and case 2 will be called a type T_2 design

Example 3.3(2):

- ❖ Letp=10 and n=7 (odd) m=3 and p-2=8
- ❖ Take Hadamard matrix of order 8($\mathbf{H_8}$).

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**

❖ Let **X*** be the 7 × 8matrix formed by any n rows of $\mathbf{H_8}$.

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 $\mathbf{U_2}$ be the 7 × 2matrix with each of the first *3* rows (-1,- 1) and each of the last *4* rows (1,−1)

❖ $\boldsymbol{X_0}$ **= (X*,$\mathbf{U_2}$)** will be

1	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**-1**	**-1**
1	**-1**	**1**	**-1**	**1**	**-1**	**1**	**-1**	**-1**	**-1**
1	**1**	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**-1**	**-1**

1	**-1**	**-1**	**1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
1	**1**	**1**	**1**	**-1**	**-1**	**-1**	**-1**	**1**	**-1**
1	**-1**	**1**	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**
1	**1**	**-1**	**-1**	**-1**	**-1**	**1**	**1**	**1**	**-1**

- So it is a supersaturated design $\mathbf{X_0}$ withp=10 and n=7.
- Then $\mathbf{R_0} = \boldsymbol{X_0 X_0}'$

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 (2.3) Calculated $UE(S^2)$ of $\boldsymbol{X_0}$ = 3.133

- Lower bound for $UE(S^2)$If p = 2 (mod 4) and n is even, then

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

…[3.3(2)**]**

Proof

It is similar to it is proved for **[3.3**(1)**]**

When n is odd, $n = 2m + 1$, 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 $N(n) = 2m(m + 1)$.

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

And hence

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

The minimum in (2.9) 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 T2 designs possess this property hence they are $UE(S^2)$-optimal.

3.4 Method 4 for p = 3(mod 4), $2 \le n \le p - 1$.

- Start with a Normalized Hadamard matrix of order p+1 ($\mathbf{H_{p+1}}$).
- Let **X*** be the n × (p+1) matrix formed by any n rows of $\mathbf{H_{p+1}}$.
- Suppose the last column of **X***is denoted by$\boldsymbol{\phi}$and $\mathbf{X}^* = (X_0, \boldsymbol{\phi})$
- The X_0 matrix will be super saturated design.
- Then $\mathbf{R_0} = X_0 X_0' = (p+1)I_n - \boldsymbol{\phi}\,\boldsymbol{\phi}'$,a matrix with diagonal entries p and off diagonal entries 1 or −1. A designX_0 in this case will be called a type T_3 design.

Example 3.2:

- ❖ Letp=15 and n=10 and p+1=16
- ❖ Take Hadamard matrix of order 16($\mathbf{H_{16}}$).

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

- ❖ X^* be the 10 × 16 matrix formed by any 10 rows of $\mathbf{H_{16}}$.

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 $\boldsymbol{X}^{*}$ is denoted by $\boldsymbol{\phi}$

- $\boldsymbol{X_0}$ matrix is given by

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

- $\mathbf{R_0}=\boldsymbol{X_0}\boldsymbol{X_0}'$

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**

- $\boldsymbol{\phi}\,\boldsymbol{\phi}'$ matrix is

1	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**-1**	**1**
-1	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
-1	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
1	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**-1**	**1**
-1	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
1	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**-1**	**1**
1	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**-1**	**1**
-1	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
-1	**1**	**1**	**-1**	**1**	**-1**	**-1**	**1**	**1**	**-1**
1	**-1**	**-1**	**1**	**-1**	**1**	**1**	**-1**	**-1**	**1**

- $\mathbf{R_0} = 16\mathbf{I_{10}} - \boldsymbol{\phi}\,\boldsymbol{\phi}'$ hence it is T_3 type design

  By using (2.3) Calculated $UE(S^2)$ of **Xo** = 4

- Lower bound for $UE(S^2)$If p = 3(mod 4),

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

…(3.4)

Proof is similar given for **(3.2)**

The minimum in (3.4) is attained whenever R is a matrix withdiagonal entries p and off-diagonal entries either 1 or −1. Hence type T3 designs 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. Through an exploration of various design criteria such as $E(S^2)$optimality and $UE(S^2)$optimality, the study highlights the importance of balancing efficiency and resource utilization in experimental design. The utilization of Hadamard matrices in constructing optimal supersaturated designs further enhances the understanding of design methodologies. By bridging theory 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.

References

Booth, K. H., & Cox, D. R. (1962). Some systematic supersaturated designs. *Technometrics*, **4(4)**, 489-495.

Bulutoglu, D. A., and Cheng, C. S. (2004). Construction of $E(S^2)$-optimal supersaturated designs. *The Annals of Statistics*, **32(4)**, 1662-1678.

Chai, F. S., Chatterjee, K., Das, A., and Midha, C. (2012). Optimal Supersaturated Designs for s m Factorials in N≢ 0 (mod s) Runs. *Journal of Statistical Theory and Practice*, **6(1)**, 169-177.

Eskridge, K. M., Gilmour, S. G., Mead, R., Butler, N. A., and Travnicek, D. A. (2004). Large supersaturated designs. *Journal of Statistical Computation and Simulation*, **74(7)**, 525-542.

Jones, B., and Majumdar, D. (2014). Optimal supersaturated designs. *Journal of the American Statistical Association*, **109(508)**, 1592-1600.

Kole, B., Gangwani, J., Gupta, V. K., and Parsad, R. (2010). Two-level supersaturated designs: a review. *Journal of Statistical Theory and Practice*, **4(4)**, 589-608.

Lin, D. K. (1993). A new class of supersaturated designs. *Technometrics*, **35(1)**, 28-31.

Ryan, K. J., and Bulutoglu, D. A. (2007). $E(S^2)$--optimal supersaturated designs with good minimax properties. *Journal of Statistical Planning and Inference*, **137(7)**, 2250-2262.

Tang, B., and Wu, C. F. J. (1997). A method for constructing supersaturated designs and its Es2 optimality. *Canadian Journal of Statistics*, **25(2)**, 191-201.

Wu, C. F. J. (1993). Construction of supersaturated designs through partially aliased interactions. *Biometrika*, **80(3)**, 661-669.

Youden, W. J., Kempthorne, O., Tukey, J. W., Box, G. E. P., and Hunter, J. S. (1959). Discussion of the papers of Messrs. Satterthwaite and Budne. *Technometrics*, **1(2)**, 157-184