Technical Report 2015
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2nd February 2015

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Abstract

A popular measure to assess two-level supersaturated designs is the $E(s^2)$ criteria. Recently, Jones and Majumdar (2014) introduced the $UE(s^2)$ criteria and obtained optimal designs under the criteria. Effect-sparsity principle states that only a very small proportion of the factors have effects that are large. These factors with large effects are called *active* factors. Therefore, the basis of using a supersaturated design is the inherent assumption that there are very few active factors which one has to identify. Though there are only a few active factors, it is not known a priori what these active factors are. The identification of the active factors, say k in number, is based on model building regression diagnostics (e.g. forward selection method) wherein one has to desirably use a supersaturated design which on an average estimates the model parameters optimally during the sequential introduction of factors in the model building process. Accordingly, to overcome possible lacuna on existing criteria of measuring the goodness of a supersaturated design, we meaningfully define the $ave(s_k^2)$ and $ave(s^2)_\rho$ criteria, where ρ is the maximum number of active factors. We obtain superior $UE(s^2)$-optimal designs in $\mathcal{D}_U(m,n)$ and compare them against $E(s^2)$-optimal designs under the more meaningful criteria of $ave(s_k^2)$ and $ave(s^2)_\rho$. It is seen that $E(s^2)$-optimal designs perform fairly well or better even against superior $UE(s^2)$-optimal designs with respect to $ave(s_k^2)$ and $ave_d(s^2)_\rho$ criteria.

Key words and phrases: Effect sparsity; Hadamard matrices; lower bound; screening designs; active factors.

1. Introduction

Supersaturated designs and their application in factor screening experiments have received considerable attention in the recent past. In a factorial experiment involving m two-level factors and n runs, n is required to be at least $m+1$ for the estimability of all main effects and the general mean. A design is called supersaturated if $n < m+1$. Under the assumption of effect sparsity that only a small number of factors are active, a supersaturated design can provide considerable cost saving in factor screening.

We represent an n-run supersaturated design d for m two-level factors by an $n \times m$ matrix X_d of 1's and -1's. We assume that $n > 2$ and that for any two columns $u = (u_1, \ldots, u_n)'$ and $v = (v_1, \ldots, v_n)'$ of X_d, $u \neq \pm v$ and $u \neq 1_n$ where $1_n = [1, 1, \ldots, 1]'$. We call such a X_d to have *distinct* columns. The number of possible factors m that can be accommodated in d is at most M, where $M = 2^{n-1} - 1$. Thus we have $n \leq m \leq M$.

Throughout this paper, for the given supersaturated design d, we use the linear main effects model,

$$y = [1_n \vdots X_d]\beta + \epsilon, \;\; \epsilon \sim N_n(0_n, \sigma^2 I_n),$$

where y is the $n \times 1$ response vector and $\beta = [\beta_0, \beta_1, \ldots, \beta_m]'$ is the parameter vector representing the general mean effect and the m main effects. Here, $[1_n \vdots X_d]$ is the $n \times (m+1)$ model matrix. Let $X_d = [x_{d1}, \ldots, x_{dm}]$ where $x_{dl} = [x_{d1l}, x_{d2l}, \ldots, x_{dnl}]', l = 1, 2, \ldots, m$. Then, x_{dl} represents the main effect contrast of factor l corresponding to $\beta_l, l = 1, 2, \ldots, m$. Also, 1_n represents the general mean effect vector corresponding to β_0. The experimental error is denoted by ϵ and is assumed to be i.i.d. multi-variate normal with dimension n, mean vector 0_n and a variance matrix $\sigma^2 I_n$, where I_n is the identity matrix of order n and 0_n a zero column vector of order n.

For a supersaturated design d, let $Y_d = [1_n \vdots X_d]$ denote the model matrix. Then, the information matrix under d for the parameter vector β is $\mathcal{I}_d = v^{-1} Y_d' Y_d = v^{-1} S_d$ where $v = 2^m$ and $S_d = ((s_{dij}))$. Also, for $X_d = ((x_{dul}))$ $(1 \leq u \leq n,\ 1 \leq l \leq m)$ the quantity x_{dul} equals 1 if the lth factor appears at level 1 in the uth run of d and equals -1 otherwise. Then for d, the information matrix $\mathcal{I}_d = v^{-1} S_d$, of order $(m+1)$, satisfies,

$$\begin{array}{ll} s_{dii} = n & 0 \leq i \leq m, \\ s_{dij} = \sum_{u=1}^{n} x_{dui} x_{duj} & 0 \leq i \neq j \leq m. \end{array}$$

Since $m + 1 > n$ the matrix $Y_d' Y_d$ is singular and thus not invertible. As a result the coefficients β cannot be estimated by the well-known least squares estimator: $\hat{\beta} = (Y_d' Y_d)^{-1} Y_d' y$. High correlations in the model matrix Y_d and the departure from orthogonality have its influence for efficient detection of the true active factors. Had s_{dij} been zero for every $i \neq j$, then $\mathcal{I}_d$ would have equaled $(n/v) I_{m+1}$ and a universal optimality result on d could have been claimed. Although the fact that $n < m+1$ rules out such a possibility, the design d may be anticipated to perform well in detecting the active main effects provided the quantities s_{dij},$i \neq j$, are small in magnitude. From this consideration, Booth and Cox (1962), under the restriction $s_{di0} = s_{d0i} = 0$ for $i = 1, 2, \ldots, m$, proposed the criteria

$$E_d(s^2) = \frac{1}{m(m-1)} \sum_{1 \leq i < j \leq m} s_{dij}^2 \tag{1.1}$$

as a performance characteristic of a supersaturated design d.

Given m and n, all supersaturated designs X_d, with

$$s_{di0} = s_{d0i} = \begin{cases} 0 & \text{for } n \text{ even}, \\ \pm 1 & \text{for } n \text{ odd}, \end{cases} \tag{1.2}$$

for $i = 1, 2, \ldots, m$, constitute a restricted class of supersaturated designs and is denoted by $\mathcal{D}_R(m, n)$. A supersaturated design d^* is said to be $E(s^2)$-optimal if $E_{d^*}(s^2) \leq E_d(s^2)$ for any $d \in \mathcal{D}_R(m, n)$. Henceforth for a design d, we denote by $E_d(s^2)_U$ the measure $E_d(s^2)$ without the restriction (1.2).

In the literature, the problem of identifying efficient two-level supersaturated designs has concentrated around finding $E(s^2)$-optimal designs in $\mathcal{D}_R(m, n)$. Prima facie it appears that there is no need to impose the restriction of balance or near balance while identifying a good supersaturated design so long as it minimizes the overall nonorthogonality among the main effects and the general mean. Accordingly, Marley and Woods (2010) extended the definition of $E_d(s^2)$ to include the inner product of first column with every other column of Y_d. For given m and n, all supersaturated designs X_d, *without any restriction* as in (1.2) constitute a unrestricted class of supersaturated designs and is denoted by $\mathcal{D}_U(m, n)$. Recently, Jones and Majumdar (2014) also introduced the criteria

$$UE_d(s^2) = \frac{1}{m(m+1)} \sum_{0 \le i < j \le m} s^2_{dij} \tag{1.3}$$

denoting a performance characteristic of a supersaturated design under $\mathcal{D}_U(m, n)$. A supersaturated design $d^* \in \mathcal{D}_U(m, n)$ is said to be $UE(s^2)$-optimal if $UE_{d^*}(s^2) \le UE_d(s^2)$ for any $d \in \mathcal{D}_U(m, n)$. Jones and Majumdar (2014) obtain $UE(s^2)$-optimal supersaturated designs in $\mathcal{D}_U(m, n)$.

In what follows, in Section 2 we first explicitly list down the sharpest bounds available for both $E(s^2)$ and $UE(s^2)$. We also make a brief note on available constructions on $E(s^2)$- and $UE(s^2)$-optimal designs. A more suitable criteria $ave(s^2_k)$ in the context of supersaturated designs having a small number of active factors k is introduced and then it is shown that the criteria $E(s^2)$ and $UE(s^2)$ are special cases of our criteria. Similarly, we define $ave(s^2)_\rho$ criteria, where ρ is the maximum number of active factors. Section 3 provides new constructions of $UE(s^2)$-optimal designs (called superior $UE(s^2)$-optimal designs) which are $ave(s^2_k)$-better than the general constructions given in Jones and Majumdar (2014). We also provide an additional $UE(s^2)$-optimal design construction for $m + 1 \equiv 2 \pmod 4$ and $n = m$, which seems to be missing in Jones and Majumdar (2014). In Section 4 we show how $E(s^2)$-optimal or even nearly $E(s^2)$-optimal designs are almost always better than even the superior $UE(s^2)$-optimal designs under effect-sparsity. Finally, a Discussion section is provided.

2. $E(s^2)$- and $UE(s^2)$-optimality and a new optimality criteria

In most of the industrial experimentation, even though the number of available factors is very large, it is usually seen that only very few of these factors are active. An ideal situation would be where active factors can be identified in much lesser number of observations than the number of factors in the experiment. This would reduce cost and time for the experimentation. Accordingly, supersaturated designs are used for identification of the few active factors. Substantial work has been done on finding $E(s^2)$-optimal designs in $\mathcal{D}_R(m, n)$. Recently work has also been done on finding $UE(s^2)$-optimal designs under the broader class $\mathcal{D}_U(m, n)$. For $d \in \mathcal{D}_R(m, n)$, it follows from (1.2) that,

$$\begin{aligned} UE_d(s^2) &= \tfrac{m-1}{m+1} E_d(s^2) && \text{for } n \text{ even}, \\ UE_d(s^2) &= \tfrac{m-1}{m+1} E_d(s^2) + \tfrac{2}{m+1} && \text{for } n \text{ odd}. \end{aligned} \tag{2.1}$$

We now summarize the available lower bounds for $E_d(s^2)$ and $UE_d(s^2)$ and constructions of supersaturated designs attaining such bounds.

Lower bounds for $E_d(s^2)$ and constructions for $d \in \mathcal{D}_R(m,n)$:

$E(s^2)$-optimal designs in $\mathcal{D}_R(m,n)$ have been obtained, for n even, by Butler *et al.* (2001), Bulutoglu and Cheng (2004), Ryan and Bulutoglu (2007) and, for n odd, by Nguyen and Cheng (2008) and Bulutoglu and Ryan (2008). Das *et al.* (2008), for n even, and Suen and Das (2010), for n odd provided the sharpest available bound known today. Georgiou (2014) present a comprehensive review of supersaturated designs till date.

When n is even, let $m = q(n-1) \pm r$ (q positive, $0 \le r < \frac{n}{2}$). Then,

(1) When $n \equiv 0 (\text{mod } 4)$,

$$E_d(s^2) \ge \frac{n^2(m-n+1)}{(n-1)(m-1)} + \frac{n}{m(m-1)}\left\{D(n,r) - \frac{r^2}{n-1}\right\}, \tag{2.2}$$

where

$$D(n,r) = \begin{cases} n+2r-3 & \text{for } r \equiv 1 \text{ (mod 4)} \\ 2n-4 & \text{for } r \equiv 2 \text{ (mod 4)} \\ n+2r+1 & \text{for } r \equiv 3 \text{ (mod 4)} \\ 4r & \text{for } r \equiv 0 \text{ (mod 4)}. \end{cases}$$

(2) When $n \equiv 2$ (mod 4),

$$E_d(s^2) \ge \max\left\{\frac{n^2(m-n+1)}{(n-1)(m-1)} + \frac{n}{m(m-1)}\left\{D(n,r) - \frac{r^2}{n-1}\right\}, 4\right\}, \tag{2.3}$$

where

$$D(n,r) = \begin{cases} n+2r-3+x/n & \text{for } r \equiv 1 \text{ (mod 4) and } q \text{ even} \\ 2r-8r/n+n-16/n+9 & \text{for } r \equiv 1 \text{ (mod 4) and } q \text{ odd} \\ 2n-4+8/n & \text{for } r \equiv 2 \text{ (mod 4) and } q \text{ even} \\ 4r-8r/n-8/n+8 & \text{for } r \equiv 2 \text{ (mod 4) and } q \text{ odd} \\ n+2r+1 & \text{for } r \equiv 3 \text{ (mod 4) and } q \text{ even} \\ 2r+n+8/n-3 & \text{for } r \equiv 3 \text{ (mod 4) and } q \text{ odd} \\ 4r & \text{for } r \equiv 0 \text{ (mod 4) and } q \text{ even} \\ 2n-4+x/n & \text{for } r \equiv 0 \text{ (mod 4) and } q \text{ odd.} \end{cases}$$

and $x = 32$ if $\left\{\frac{m-1-2i}{4} + [\frac{m+(1+2i)(n-1)}{4(n-1)}]\right\} \equiv (1-i)$ (mod 2), for $i = 0$ or 1; else $x = 0$. Here, $[z]$ denotes the largest integer less than or equal to z.

When n is odd, for $m \ge n$, let t be the integer such that $m + t \equiv 2$ (mod 4) and $-2n \le tn - m \le 2n$, and let $g(t) = n(m+t)^2 - 2mt - (m+t^2)n^2$. Also, let $p^* = \lceil\{n - \sqrt{(|tn-m| - n)(n-1) + n}\}/2\rceil$, $\alpha = 4p^*(n-p^*) - (2n - |tn-m|)(n-1)$, and $\alpha^* = 4(n+1-2p^*)$, where $\lceil z \rceil$ stands for the smallest integer greater or equal to z and $|z|$ stands for the absolute value of z. Then,

(3) When $|tn - m| \leq n - 1$,

$$E_d(s^2) \geq \frac{1}{m(m-1)}\{2(n-1)^2 + g(t)\}. \tag{2.4}$$

(4) When $|tn - m| > n - 1$ and $\alpha \leq \alpha^*/2$

$$E_d(s^2) \geq \frac{1}{m(m-1)}\{4(n-1)(|tn-m| - n) + 8p^*(n-p^*) + g(t)\}. \tag{2.5}$$

(5) When $|tn - m| > n - 1$ and $\alpha > \alpha^*/2$

$$E_d(s^2) \geq \frac{1}{m(m-1)}\{4n(n-1) - 8(p^*-1)(n-p^*+1) + g(t)\}. \tag{2.6}$$

Constructions of $E(s^2)$-optimal designs in $d \in \mathcal{D}_R(m, n)$ have been researched extensively over the years starting with Booth and Cox (1962) who gave the first systematic constructions using computer search. Despite strong contributions by several authors, construction of $E(s^2)$-optimal designs in $\mathcal{D}_R(m, n)$ remains a difficult problem in general and the goal of obtaining a complete catalog appears hard to attain. However, one can refer to the review paper Georgiou (2014) for detailed standpoint on constructions of such designs.

Lower bounds for $UE_d(s^2)$ and constructions for $d \in \mathcal{D}_U(m, n)$:

As indicated in Section 1, the lower bounds for $UE_d(s^2)$ under $\mathcal{D}_U(m, n)$ have been recently provided by Jones and Majumdar (2014). The bounds are

$$UE_d(s^2) \geq \left(\frac{n(m+1-n)}{m} + \frac{B}{m(m+1)}\right) \tag{2.7}$$

where

$$B = \begin{cases} 0 & \text{for } m+1 \equiv 0 \pmod 4, \\ 2n(n-2) & \text{for } m+1 \equiv 2 \pmod 4 \text{ and } n \text{ even}, \\ 2\{n(n-2)+1\} & \text{for } m+1 \equiv 2 \pmod 4 \text{ and } n \text{ odd}, \\ n(n-1) & \text{for } m+1 \equiv 1 \pmod 4 \text{ or } m+1 \equiv 3 \pmod 4. \end{cases}$$

Let $H_{p,q}$ be a matrix of elements ± 1 such that $H_{p,q}H'_{p,q} = qI_p$. When $p = q = N$, $H_{N,N}$ is said to be a Hadamard matrix of order N. A necessary condition for the existence of $H_{N,N}$ is that $N \equiv 0 \pmod 4$. Furthermore, $H_{N,N}$ with its first row and first column of all 1's is said to be a normal $H_{N,N}$. Such a normal $H_{N,N}$ can easily be obtained from $H_{N,N}$. It is also noted that ignoring the first row of normal $H_{N,N}$, the residual matrix of order $(N-1) \times N$ with columns as runs, forms an orthogonal array $OA(N, 2^{N-1}, 2)$. (An orthogonal array $OA(N, 2^n, g)$, having N columns, $n(\geq 2)$ rows and strength $g(\leq n)$, is an $n \times N$ array having all possible 2^g combinations of symbols appearing equally often as columns in every $g \times N$ subarray.

Jones and Majumdar (2014) also provided general constructions for $UE(s^2)$-optimal designs using Hadamard matrices for all cases except when $m+1 \equiv 2 \pmod 4$ and $n = m$. Their construction of Y_d employ adding columns to or deleting columns from a $H_{N,N}$. They provide four sets of constructions based on the values of m.

i) For $m+1 \equiv 0 \pmod 4$, $2 \leq n \leq m$, any n rows from a normal Hadamard matrix of order $m+1$ is retained (rest of the rows deleted) to get Y_d;

ii) For $m+1 \equiv 1 \pmod 4$, $2 \leq n \leq m$, any n rows from a normal Hadamard matrix of order m is retained and then any column of ± 1 is added to get Y_d;

iii) For $m+1 \equiv 2 \pmod 4$, $2 \leq n \leq m-1$, any n rows from a normal Hadamard matrix of order $m-1$ is retained and then two columns are added such that half of the rows are either (1,1) or (-1, -1) and another half of the rows are either (1,-1) or (-1,1) to get Y_d;

iv) For $m+1 \equiv 3 \pmod 4$, $2 \leq n \leq m$, any n rows from a normal Hadamard matrix of order $m+2$ is retained and then the last column is deleted to get Y_d.

However, their constructions have a caveat while retaining any n rows. Their method requires that the retained n rows of $H_{N,N}$ are such that no two columns are identical or negative of the other. The moment one imposes this requirement, the deletion of any rows of $H_{N,N}$ to get Y_d may not hold. We address this question in Section 3.

Now that we have given the lower bounds for the respective classes of designs $\mathcal{D}_R$ and $\mathcal{D}_U$, and also their constructions, we now illustrate the precise relation between these two lower bounds. As noted in Jones and Majumdar (2014), for any $d_1 \in \mathcal{D}_U$ and any $d_2 \in \mathcal{D}_R$,

$$min_{d_1 \in \mathcal{D_U}} UE_{d_1}(s^2) \leq \frac{(m-1)}{(m+1)} min_{d_2 \in \mathcal{D_R}} E_{d_2}(s^2). \tag{2.8}$$

Additionally, for given m, n and with n even, it is possible to have $UE(s^2)$-optimal design and a $E(s^2)$-optimal design such that $min_{d_1 \in \mathcal{D_U}} UE_{d_1}(s^2) = \frac{(m-1)}{(m+1)} min_{d_2 \in \mathcal{D_R}} E_{d_2}(s^2)$. Such an equality holds if and only if the following parametric relations are satisfied:

<u>For $n \equiv 0 \pmod 4$</u>

a) $r \equiv 0 (\text{mod } 4)$ and $m \equiv 2 \pmod 4$ and $m = 2n-2$

b) $r \equiv 1 \pmod 4$ and $m \equiv 0 \pmod 4$ and $\left[\frac{m}{(n-1)}\right] = 1$

c) $r \equiv 1 \pmod 4$ and $m \equiv 1 \pmod 4$ and $\left[\frac{m}{(n-1)}\right] = 1$

d) $r \equiv 2 \pmod 4$ and $m \equiv 1 \pmod 4$ and $\left[\frac{m}{(n-1)}\right] = 1$

<u>For $n \equiv 2 \pmod 4$</u>

a) $r \equiv 0 \pmod 4$ and $m \equiv 1 \pmod 4$ and odd q and $\left[\frac{m}{(n-1)}\right] = 1$ and $x = 0$

b) $r \equiv 0 \pmod 4$ and $m \equiv 2 \pmod 4$ and even q and $m = 2n - 2$

c) $r \equiv 1 \pmod 4$ and $m \equiv 1 \pmod 4$ and even q and $\left[\frac{m}{(n-1)}\right] = 1$ and $x = 0$

Similarly, for given m, n and with n odd, it is possible to have $UE(s^2)$-optimal design and a $E(s^2)$-optimal design such that $min_{d_1 \in \mathcal{D}_{\mathcal{U}}} UE_{d_1}(s^2) = \frac{2}{m+1} + \frac{(m-1)}{(m+1)} min_{d_2 \in \mathcal{D}_{\mathcal{R}}} E_{d_2}(s^2)$. Such an equality holds if the following parametric relations are satisfied:

For $n \equiv 1 \pmod 4$

a) $m \equiv 1 \pmod 4$ and $m \leq 2n - 1$

For $n \equiv 3 \pmod 4$

a) $m \equiv 0 \pmod 4$ and $m = n + 1$
b) $m \equiv 1 \pmod 4$ and $m \leq 2n - 1$
c) $m \equiv 3 \pmod 4$ and $m = n$

The literature on optimal supersaturated designs had mostly concentrated on $E(s^2)$-optimal designs and now recently on $UE(s^2)$-optimal designs. The objective of supersaturated design is to identify very few active factors. Such identification is usually based on the forward selection method of model building involving say, k active factors. Thus, one has to desirably use a supersaturated design which on an average estimates the model parameters optimally during the model building process. Accordingly, we now define a criteria $ave(s_k^2)$, based on k active factors. For a supersaturated design d, having k active factors, we define

$$ave_d(s_k^2) = \frac{1}{\binom{m}{k}} \sum_{t=1}^{\binom{m}{k}} UE_d(s_k^2)_t \tag{2.9}$$

where $UE_d(s_k^2)_t$ is the value of $UE_d(s^2)$ corresponding to the tth sub-matrix of $Y_d'Y_d$ involving mean effect and k main effects; there being a total of $\binom{m}{k}$ such sub-matrices of order $k+1$. In other words, the criteria $UE_d(s_k^2)_t$ is the sum of squares of off-diagonal elements of $Y_d'Y_d$ involving only k factors which is a criteria equivalent to the MS-optimality criteria involving k factors in n runs. For given k, a supersaturated design $d^* \in \mathcal{D}_U(m,n)$ is said to be $ave(s_k^2)$-optimal if $ave_{d^*}(s_k^2) \leq ave_d(s_k^2)$ for any $d \in \mathcal{D}_U(m,n)$.

We now give the following simplified expression of $ave_d(s_k^2)$ in terms of the $UE_d(s^2)$ and $E_d(s^2)_U$.

Lemma 2.1 For a supersaturated design d,

$$ave_d(s_k^2) = \frac{m+1}{k+1} \left\{ UE_d(s^2) - \frac{m-k}{m+1} E_d(s^2)_U \right\}. \tag{2.10}$$

Proof Let the set $(\gamma_1, \gamma_2, \ldots, \gamma_k)$ represent the k out of m factors where $\gamma_i < \gamma_j$, $\gamma_i \in \{1, 2, \ldots, m\}$ and $\gamma_0 = 0$. Thus, $UE_d(s_k^2)_t = \frac{1}{k(k+1)} \sum_{i=0}^{k} \sum_{j=0, j\neq i}^{k} s^2_{d\gamma_i\gamma_j}$.

Summing over all such possible $\binom{m}{k}$ combinations, we get

$$\sum_{t=1}^{\binom{m}{k}} UE_d(s_k^2)_t = \frac{1}{k(k+1)} \sum_{t=1}^{\binom{m}{k}} \sum_{i=0}^{k} \sum_{j=0, j\neq i}^{k} s^2_{d\gamma_i\gamma_j}. \tag{2.11}$$

From (2.11), one can see that the terms $s^2_{d\gamma_0\gamma_j}$ and $s^2_{d\gamma_i\gamma_0}$ each appear $\binom{m-1}{k-1}$ times for each γ_i, γ_j, $i, j = 1, 2, \ldots, m$. Also, the terms $s^2_{d\gamma_i\gamma_j}$ appear $\binom{m-2}{k-2}$ times for each $\gamma_i \neq \gamma_j$, $i, j = 1, 2, \ldots, m$ in (2.11). Therefore, from (2.9) and (2.11),

$$ave_d(s_k^2) = \frac{1}{k(k+1)\binom{m}{k}} \left\{ \binom{m-1}{k-1} \sum_{i=1}^{m} (s^2_{d0\gamma_j} + s^2_{d\gamma_i 0}) + \binom{m-2}{k-2} \sum_{i=1}^{m} \sum_{j=1, j\neq i}^{m} s^2_{\gamma_i\gamma_j} \right\} \tag{2.12}$$

$$\begin{aligned}
ave_d(s_k^2) &= \tfrac{1}{k(k+1)\binom{m}{k}} \left\{ \tfrac{k}{m}\binom{m}{k} \textstyle\sum_{i=1}^{m} (s^2_{d0\gamma_j} + s^2_{d\gamma_i 0}) + \tfrac{k(k-1)}{m(m-1)} \binom{m}{k} \sum_{i=1}^{m} \sum_{j=1, j\neq i}^{m} s^2_{d\gamma_i\gamma_j} \right\} \\
&= \tfrac{1}{(k+1)} \left\{ \tfrac{1}{m} \textstyle\sum_{i=1}^{m} (s^2_{d0\gamma_j} + s^2_{d\gamma_i 0}) + \tfrac{(k-1)}{m(m-1)} \sum_{i=1}^{m} \sum_{j=1, j\neq i}^{m} s^2_{d\gamma_i\gamma_j} \right\} \\
&= \tfrac{1}{(k+1)} \left\{ (m+1)\, UE_d(s^2) - (m-1) E_d(s^2)_U + (k-1) E_d(s^2)_U \right\} \\
&= \tfrac{1}{(k+1)} \left\{ (m+1)\, UE_d(s^2) - (m-k) E_d(s^2)_U \right\} \\
&= \tfrac{m+1}{k+1} \left\{ UE_d(s^2) - \tfrac{(m-k)}{(m+1)} E_d(s^2)_U \right\}.
\end{aligned}$$

■

Now in the absence of the knowledge of the precise number of active factors, which are few in number, we define a criteria, $ave(s^2)_\rho$, which is a function of the maximum number of active factors. With ρ being the maximum number of active factors, for a supersaturated design d,

$$ave_d(s^2)_\rho = \frac{\sum_{k=1}^{\rho} \binom{m}{k} ave_d(s_k^2)}{\sum_{k=1}^{\rho} \binom{m}{k}}. \tag{2.13}$$

For given ρ, a supersaturated design $d^* \in \mathcal{D}_{\mathcal{U}}(m, n)$ is said to be $ave(s^2)_\rho$-optimal if $ave_{d^*}(s^2)_\rho \leq ave_d(s^2)_\rho$ for any $d \in \mathcal{D}_U(m, n)$.

We now give the following simplified expression of $ave_d(s^2)_\rho$ in terms of the $UE_d(s^2)$ and $E_d(s^2)_U$.

Lemma 2.2 For a supersaturated design d,

$$ave_d(s^2)_\rho = \frac{UE_d(s^2)\sum_{k=1}^{\rho}\binom{m+1}{k+1} - E_d(s^2)_U\sum_{k=1}^{\rho}\binom{m}{k+1}}{\sum_{k=1}^{\rho}\binom{m}{k}}. \tag{2.14}$$

Proof From (2.10) and (2.13) we get,

$$\begin{aligned}
ave_d(s^2)_\rho &= \frac{\sum_{k=1}^{\rho}\binom{m}{k}\frac{m+1}{k+1}\left\{UE_d(s^2) - \frac{m-k}{m+1}E_d(s^2)_U\right\}}{\sum_{k=1}^{\rho}\binom{m}{k}} \\
&= \frac{\sum_{k=1}^{\rho}\binom{m+1}{k+1}\left\{UE_d(s^2) - \frac{m-k}{m+1}E_d(s^2)_U\right\}}{\sum_{k=1}^{\rho}\binom{m}{k}} \\
&= \frac{\sum_{k=1}^{\rho}\binom{m+1}{k+1}UE_d(s^2) - \sum_{k=1}^{\rho}\binom{m+1}{k+1}\frac{m-k}{m+1}E_d(s^2)_U}{\sum_{k=1}^{\rho}\binom{m}{k}} \\
&= \frac{\sum_{k=1}^{\rho}\binom{m+1}{k+1}UE_d(s^2) - \sum_{k=1}^{\rho}\binom{m}{k+1}E_d(s^2)_U}{\sum_{k=1}^{\rho}\binom{m}{k}} \\
&= \frac{UE_d(s^2)\sum_{k=1}^{\rho}\binom{m+1}{k+1} - E_d(s^2)_U\sum_{k=1}^{\rho}\binom{m}{k+1}}{\sum_{k=1}^{\rho}\binom{m}{k}}. \quad \blacksquare
\end{aligned}$$

The ideal optimization problem in a supersaturated design would be to identify a $ave(s_k^2)$-optimal or a $ave(s^2)_\rho$-optimal design. Later in Section 4, we show that an $E(s^2)$-optimal design is always $ave(s_k^2)$-better than a $UE(s^2)$-optimal design when $k = 1, 2$. We also show that an $E(s^2)$-optimal design is $ave(s^2)_\rho$-better than a $UE(s^2)$-optimal design whenever $\rho = 1, 2$ and for $\rho = 3, 4$ for most of the parameter pairs (m, n).

Let $\mathcal{D}_\mathcal{U}^*$ be the class of $UE(s^2)$-optimal designs. For a supersaturated design $d \in \mathcal{D}_\mathcal{U}$ with k active factors, it follows from (2.10) that a *two-step minimization* of $ave_d(s_k^2)$ would yield a design $d^* \in \mathcal{D}_\mathcal{U}^*$ such that $E_{d^*}(s^2) \geq E_d(s^2)$ for any $d \in \mathcal{D}_\mathcal{U}^*$. Such a design d^* need not always be $ave(s_k^2)$-optimal in $\mathcal{D}_\mathcal{U}$ but is $ave(s_k^2)$-better among $UE(s^2)$-optimal designs $d \in \mathcal{D}_\mathcal{U}^*$. Therefore, this *two-step minimization* of $ave_d(s_k^2)$ (over $d \in \mathcal{D}_\mathcal{U}^*$) is an improvement over $UE(s^2)$-optimal designs proposed by Jones and Majumdar (2014). We call such designs superior $UE(s^2)$-optimal designs. These designs satisfy the secondary criteria proposed in Jones and Majumdar (2014).

Again for a supersaturated design $d \in \mathcal{D}_\mathcal{U}$ with k active factors, it follows from (2.12) that an *alternate two-step minimization* of $ave_d(s_k^2)$ would yield a design $d^* \in \mathcal{D}_\mathcal{R}$ such that $E_{d^*}(s^2) \leq E_d(s^2)$ for any $d \in \mathcal{D}_\mathcal{R}$. $E(s^2)$ criteria is therefore a special case of the $ave(s_k^2)$ criteria under *alternate two-step minimization* of $ave_d(s_k^2)$.

From above it follows that *two-step minimization* can be viewed as minimizing the first term of (2.10) and then maximizing the second term within the class of designs $\mathcal{D}_\mathcal{U}^*$. Such a criteria is an improvement over the $UE(s^2)$ criteria. Similarly, the *alternate two-step minimization* can be viewed as minimizing the first term of (2.12) and then minimizing the second term within the class of designs $\mathcal{D}_{\mathcal{R}}$. Such a *alternate two-step minimization* of $ave_d(s_k^2)$ is thus equivalent to the traditional $E(s^2)$ criteria.

It follows from the above discussion that in order to get a superior $UE(s^2)$-optimal design, while constructing $UE(s^2)$-optimal designs in $\mathcal{D}_U(m,n)$, we need to additionally ensure that the design matrix X_d is constructed in a way such that $E_d(s^2)_U$ is maximum for $d \in \mathcal{D}^*_{\mathcal{U}}$. Constructions provided in Jones and Majumdar (2014) do not necessarily maximize $E_d(s^2)_U$ for designs $d \in \mathcal{D}^*_{\mathcal{U}}$. In the next section, we provide constructions of superior $UE(s^2)$-optimal designs improving over the constructions provided by Jones and Majumdar (2014).

3. Construction of superior $UE(s^2)$-optimal designs

In this section, we improve upon the constructions provided by Jones and Majumdar (2014). As seen from Lemma 2.1, one way to minimize $ave_d(s_k^2)$ is to additionally maximize $E_d(s^2)_U$ under the class of all designs $d \in \mathcal{D}^*_{\mathcal{U}}$.

As mentioned in Section 2, we look at the caveat imposed in the constructions provided in Jones and Majumdar (2014). Their method requires that n rows of the supersaturated design are such that no two columns are identical or negative of the other. The moment one imposes this requirement, the deletion of *any* rows of $H_{N,N}$, as suggested in their construction, to get Y_d, may not hold.

For every $n \le N$, deleting any $N-n$ rows of $H_{N,N}$ we get $H_{n,N}$ such that $H_{n,N}H'_{n,N} = NI_n$. In our endeavour to construct a superior $UE(s^2)$-optimal design, we first address the above caveat and evaluate the number of rows $(N-n)$ that can be deleted from a $H_{N,N}$ such that the N columns in the resultant matrix of order $n \times N$ are *distinct*. We show that for $N \equiv 0 \pmod 4$, starting from $H_{N,N}$ one can randomly delete upto $N/2-1$ rows resulting in $H_{n,N}$ (=Y_0, say) with $n > N/2$, such that no two columns of Y_0 have an inner product equal to $\pm n$ i.e., all columns are *distinct*. However, for deleting $N/2$ or more rows, one would need to carefully delete rows so as to ensure that all columns are *distinct*. Henceforth we always consider normal $H_{N,N}$.

Lemma 3.1 When *any* $N-n$ rows of a Hadamard matrix $H_{N,N}$ are deleted to obtain Y_0, the columns of Y_0 are *distinct* if and only if $n > N/2$.

Proof Interchanging the rows of $H_{N,N}$ retains the Hadamard property of $H_{N,N}$. Therefore, without loss of generality let,

$$H_{N,N} = \begin{pmatrix} H_{N-n,N} \\ Y_0 \end{pmatrix}. \tag{3.1}$$

Therefore,

$$Y_0'Y_0 + H'_{N-n,N}H_{N-n,N} = H'_{N,N}H_{N,N} = NI_N. \tag{3.2}$$

Let $Y_0'Y_0 = ((u_{ij}))$ and $H'_{N-n,N}H_{N-n,N} = ((w_{ij}))$. Then from (3.2), it follows that

$$u_{ij} + w_{ij} = 0 \text{ or } |u_{ij}| = |w_{ij}| \tag{3.3}$$

and

$$|u_{ij}| \leq n \text{ and } |w_{ij}| \leq N - n. \tag{3.4}$$

Only if condition : Let Y_0 has *distinct* columns. Then, for $i \neq j$, $|u_{ij}| < n$. Thus from (3.3) $|w_{ij}| < n$, or from (3.4) $N - n < n$, i.e., $n > N/2$.

If condition : Let $n > N/2$. If possible let $|u_{ij}| = n$ for some (i, j), say (i_0, j_0). Then from (3.3) and (3.4) $|u_{i_0 j_0}| = n = |w_{i_0 j_0}| \leq N - n$. Thus $n \leq N - n$, or, $n \leq N/2$, which is not possible. Therefore, $|u_{ij}| < n$ for all (i, j), and hence the columns of Y_0 are *distinct*. ■

Remark 3.2 Let w be an integer. Then, for $N = 2^w$, we can always obtain $H_{w,N}$ directly by listing all possible 2^w combinations as columns. Here, to get *distinct* columns, number of rows $n \geq w = log_2 N$. When $2^w < N < 2^{w+1}$, N *distinct* columns can be obtained provided $n \geq [log_2 N] + 1$.

Remark 3.3 We also did a complete enumeration on $H_{N,N}$, $4 \leq N \leq 128$, to find out the the least number of rows n required so as to have N *distinct* columns in $H_{n,N}$. Results showed that,
(A) for $N = 2^w$,
a) For $N = 4$, 8, 16, 32 and 64: $n \geq [log_2 N] + 1$,
b) For $N = 128$: $n \geq [log_2 N] + 2$,
and
(B) for $N \neq 2^w$
c) For $N \leq 44$ (except $N = 12, 24$ and 28) or $N = 80$ and 88: $n \geq [log_2 N] + 2$,
d) For $48 \leq N \leq 96$ (except $N = 80$ and 88) or $N = 12, 24$ and 28: $n \geq [log_2 N] + 3$
e) For $100 \leq N \leq 124$: $n \geq [log_2 N] + 4$.

The following theorem shows that choice of the deleted rows in a Hadamard matrix do not affect the value of $E_d(s^2)_U$.

Theorem 3.4 For $m + 1 \equiv 0 \pmod 4$, the design that maximizes $E_d(s^2)_U$ under the class of all designs in $\mathcal{D}^*_{\mathcal{U}}(m, n)$, is independent of which $m + 1 - n$ rows are deleted of a $H_{m+1,m+1}$ to get Y_d.

Proof Let d be the design obtained by deleting any $m + 1 - n$ rows of a $H_{m+1,m+1}$ to get Y_d. Then, it is easy to see that,

$$trace(Y_d' Y_d)^2 = (m + 1)n^2 + \sum_{i=0}^{m} \sum_{j(\neq i)=0}^{m} s_{dij}^2, \tag{3.5}$$

and,

$$trace(Y_d Y_d')^2 = n(m + 1)^2 + \sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t_{dij}^2. \tag{3.6}$$

where t_{dij} is the (i, j)-th entry of $Y_d Y_d'$ or $Y_d Y_d' = ((t_{dij}))$.

From (3.5) and (3.6),

$$UE_d(s^2) = \frac{1}{m(m+1)} \left\{ n(m+1)(m+1-n) + \sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t_{dij}^2 \right\}. \tag{3.7}$$

Similarly, the equations analogous to (3.5), (3.6) and (3.7) can be obtained for X_d. Therefore, from (3.7) and its analogous equation, it follows that for all Y_d, $UE_d(s^2) = f(m,n) + \sum_{i=1}^{n}\sum_{j(\neq i)=1}^{n} t_{dij}^2$ and $E_d(s^2)_U = g(m,n) + \sum_{i=1}^{n}\sum_{j(\neq i)=1}^{n}(t_{dij}-1)^2$. Thus, it follows that $UE_d(s^2)$ is minimized only when $\sum_{i=1}^{n}\sum_{j(\neq i)=1}^{n} t_{dij}^2$ is minimized and $E_d(s^2)_U$ is maximized only when $\sum_{i=1}^{n}\sum_{j(\neq i)=1}^{n}(t_{dij}-1)^2$ is maximized. We also know that $Y_dY_d' = (m+1)I_n = 11' + X_dX_d'$. Therefore, independent of which $m+1-n$ rows are deleted, $UE_d(s^2)$ is minimum since off-diagonal elements of Y_dY_d' are 0. This also implies that, independent of which $m+1-n$ rows are deleted, the off-diagonal elements of X_dX_d' are -1 which also gives the maximum value of $E_d(s^2)_U$. Thus $E_d(s^2)_U$ gets maximized independent of the choice of rows which are deleted. ■

Using Lemma 3.1 and Theorem 3.4, we now provide constructions for superior $UE(s^2)$-optimal designs.

Theorem 3.5 The constructions for a superior $UE(s^2)$-optimal design with model matrix Y_d, $d \in \mathcal{D}_{\mathcal{U}}(m,n)$ are

i) For $n \leq m$ and $m+1 \equiv 0 \pmod 4$, delete any $m+1-n$ rows of $H_{m+1,m+1}$ to obtain a $n \times (m+1)$ model matrix $Y_d = Y_0$.

ii) For $n \leq m$ and $m+1 \equiv 1 \pmod 4$, we obtain $n \times m$ model matrix Y_0 from Construction (i) and then add any column with (nearly) equal number of ± 1 which is also distinct to the existing columns in Y_0, to get Y_d.

iii) For $n \leq m-1$ and $m+1 \equiv 2 \pmod 4$, we obtain $n \times (m-1)$ model matrix Y_0 from Construction (i) and then add two columns which are distinct to the existing columns in Y_0 such that the frequencies of (1,1), (-1,-1), (1,-1) and (-1, 1) in the rows of the two added columns is (nearly) equal, to get Y_d.

iv) For $n \leq m$ and $m+1 \equiv 3 \pmod 4$, we obtain $n \times (m+2)$ model matrix Y_0 from Construction (i) and then delete the column with maximum column sum, to get Y_d.

Proof We take up the four cases one by one.

i) This result directly follows from Lemma 3.1 and Theorem 4.3.

ii) For $n \leq m$ and $m+1 \equiv 1 \pmod 4$, Jones and Majumdar (2014) proposed adding any column with elements $+1$ and -1 to $n \times m$ model matrix Y_0 obtained from Construction (i). To obtain the $ave(s_k^2)$-optimal design, we should add a column to Y_0 such that this column is as orthogonal to mean as possible. Thus, any column with (nearly) equal number of ± 1 which is also distinct to the existing columns in Y_0 is added to get Y_d.

iii) For $n \leq m-1$ and $m+1 \equiv 2 \pmod 4$, Jones and Majumdar (2014) proposed adding any two columns such that their inner product with each other is atmost one, to $n \times (m-1)$ model matrix Y_0 obtained from Construction (i). Such a construction attains $UE(s^2)$-optimality bound. To additionally minimize $ave(s_k^2)$ criteria, we add two columns to Y_0 such that these columns are as orthogonal to mean as possible. Thus, we add columns such that the frequencies of (1,1), (-1,-1), (1,-1) and (-1,1) are (nearly) equal and they are also distinct to the existing columns of Y_0, to get Y_d.

iv) For $n \leq m$ and $m+1 \equiv 3 \pmod 4$, Jones and Majumdar (2014) proposed deleting any column from $n \times (m+2)$ model matrix Y_0 obtained from Construction (i). To additionally minimize $ave(s_k^2)$ criteria, we delete a column such that which had maximum non-orthogonality with mean. Thus, the column with maximum column sum is deleted from Y_0, to get Y_d. ■

The construction of $UE(s^2)$-optimal design for $m+1 \equiv 2 \pmod 4$ and $n = m$ had not been provided by Jones and Majumdar (2014). The following result gives a construction of superior $UE(s^2)$-optimal design for this case.

Theorem 3.6 For $n = m$ and $m+1 \equiv 2 \pmod 4$, a superior $UE(s^2)$-optimal design with model matrix Y_d, $d \in \mathcal{D}_{\mathcal{U}}(m, n)$ is obtained by first obtaining Y_0 of order $n \times (m+3)$ from Construction (i) of Theorem 3.5 and then deleting two columns from Y_0 such that the column sum of one column is ± 3 and another is ± 1.

Proof After getting $n \times (m+3)$ model matrix Y_0 from Construction (i) of Theorem 3.5, in order to arrive at a $UE(s^2)$-optimal design X_d, we delete two columns of Y_0 such that $Y_d Y_d'$ has maximum number of 0's in its off-diagonal positions. This is achieved when the difference between the frequencies of rows of type {(1,1), (-1,-1)} and rows of type {(1,-1), (-1,1)} in the deleted two columns is ± 1.

In the above described construction of $UE(s^2)$-optimal design there always exist the required two columns in Y_0 which are deleted to get Y_d. The existence follows since in the three deleted rows there would always be at least two columns such that their inner product is ± 1. This is true because the columns of the deleted matrix forms an orthogonal array $OA(m+3, 2^3, 2)$.

Additionally, to get a superior $UE(s^2)$-optimal design, we need to minimize the sum of squares of the inner product of the columns of X_d, $d \in \mathcal{D}_{\mathcal{U}}^*$ with 1_n or equivalently, maximize the sum of squares of the inner product of the deleted columns with 1_n (deleted columns being the columns deleted to arrive at X_d, $d \in \mathcal{D}_{\mathcal{U}}^*$). Theoretically, such a maximum of the sum of squares of the inner product of the deleted columns with 1_n is achieved when each of the column sums are ± 3 or equivalently, each of the column sums of the corresponding columns in the three deleted rows are ± 3 leading to their inner product being ± 3. This is not achievable for $d \in \mathcal{D}_{\mathcal{U}}^*$. Therefore, the next best is to delete two columns with column sums of deleted row being ± 3 and ± 1.

For some w, if $m+3 = 2^w$ with $H_{2^w,2^w} = \otimes_{i=1}^{w} H_{2,2}$ and $H_{2,2} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, the 5th and 6th column sums of the last three rows is ± 3 and ± 1 respectively and thus, one can delete the last three rows and 5th and 6th column of $H_{m+3,m+3}$ to arrive at the superior $UE(s^2)$-optimal design X_d.

For some w, if $m+3 \neq 2^w$ and $m+3$ is not a multiple of 8, then existence of such two columns in the deleted rows is guaranteed because Cheng (1995) showed that if $m+3$ is not a multiple of 2^3, then the projection of an $\text{OA}(m+3, 2^{m+2}, 2)$ with $m+2 \geq 4$ onto any 3 factors must contain at least one complete 2^3 factorial. Thus, one can delete any three rows and then delete two columns such that their column sums are ± 3 and ± 1.

For some w, if $m+3 \neq 2^w$ and $m+3$ is a multiple of 8, from Lemma 2.2 of Cheng (1995), there would always exist at least one set of three rows in $H_{m+3,m+3}$ such that it has at least two columns with respective sums being ± 3 and ± 1. Thus, one can always delete some three rows and then delete two columns such that their column sums are ± 3 and ± 1. ■

We now give a result on the upper bound of $E_d(s^2)_U$ for $d \in \mathcal{D}^*_{\mathcal{U}}$, proof of which is given in the Appendix.

Theorem 3.7 An upper bound to $E_d(s^2)_U$ for $d \in \mathcal{D}^*_{\mathcal{U}}$ is given by

$$E_d(s^2)_U \leq \frac{1}{m(m-1)} \{nm(m-n) + T\} \tag{3.8}$$

where

$$T = \begin{cases} n(n-1) & \text{for } m+1 \equiv 0 \pmod 4 \\ 2n^2 & \text{for } m+1 \equiv 1 \pmod 4 \text{ and } n \text{ even} \\ 2(n^2-1) & \text{for } m+1 \equiv 1 \pmod 4 \text{ and } n \text{ odd} \\ n(3n-1) & \text{for } m+1 \equiv 2 \pmod 4 \text{ and } n \equiv 0 \pmod 4 \\ 3n^2-n-8 & \text{for } m+1 \equiv 2 \pmod 4 \text{ and } n \equiv 2 \pmod 4 \\ 3n^2-n-2 & \text{for } m+1 \equiv 2 \pmod 4 \text{ and } m \neq n \equiv 1 \text{ or } 3 \pmod 4 \\ 3(n^2-9n+22) & \text{for } m+1 \equiv 2 \pmod 4 \text{ and } n = m \\ 4(n-1)(n-2) & \text{for } m+1 \equiv 3 \pmod 4 \text{ and } n \leq (m+2)/2 \\ m(m+2)+(2n-m-2)(2n-m-4) & \text{for } m+1 \equiv 3 \pmod 4 \text{ and } n > (m+2)/2. \end{cases}$$

4. Comparison of $E(s^2)$- and $UE(s^2)$-optimal designs

Box and Meyer (1986) was the first to introduce the principle of effect-sparsity. Effect-sparsity principle states that only a very small proportion of the factors have effects that are large. These factors with large effects are called *active* factors, and the rest are called *inert* factors. Therefore, the basis of using a supersaturated design is the inherent assumption that there are very few active factors which one has to identify.

The concept of supersaturated designs depend critically on effect sparsity in the form of the supposition that only a few of the m factors are actually active. The objective of a supersaturated design is to optimally identify the very few active factors which are not known a priori. Accordingly, in Section 2 we have defined the $ave(s_k^2)$ and $ave(s^2)_\rho$ criteria, where ρ is the maximum number of active factors.

In Section 3, we have obtained a superior $UE(s^2)$-optimal designs in $\mathcal{D}_U(m,n)$. We now investigate how good these superior $UE(s^2)$-optimal designs are as against $E(s^2)$-optimal designs using the criteria of $ave_d(s_k^2)$ and $ave_d(s^2)_\rho$.

The following result shows that $E(s^2)$-optimal designs perform fairly well or better as against superior $UE(s^2)$-optimal designs with respect to $ave(s_k^2)$ and $ave_d(s^2)_\rho$ criteria.

Theorem 4.1 For k active factors or atmost ρ active factors, let d_1 be a $E(s^2)$-optimal design attaining the bounds (2.2)-(2.6) and d_2 be a superior $UE(s^2)$-optimal design where $d_1 \in \mathcal{D}_\mathcal{R}$ and $d_2 \in \mathcal{D}_\mathcal{U}$. Then,

A) For k active factors,

1. For $k=1$, $ave_{d_2}(s_k^2) \geq ave_{d_1}(s_k^2) = 0$ for n even, and $ave_{d_2}(s_k^2) \geq ave_{d_1}(s_k^2) = 1$ for n odd.
2. For $k=2$, $ave_{d_2}(s_k^2) \geq ave_{d_1}(s_k^2)$.
3. For $k=3$, $ave_{d_2}(s_k^2) \geq ave_{d_1}(s_k^2)$ unless (i) $n=m$ and $m \equiv 2 \pmod 4$, or (ii) $n=m-1$ and $m \equiv 3 \pmod 4$.
4. For $k=4$, $ave_{d_2}(s_k^2) \geq ave_{d_1}(s_k^2)$ unless (i) $n=m$ and $m \equiv 2 \pmod 4$, or (ii) $n=m-1$ and $m \equiv 3 \pmod 4$, or (iii) $n=5$ and $m=7$.

B) For atmost ρ active factors,

1. For $\rho=1$, $ave_{d_2}(s^2)_\rho \geq ave_{d_1}(s^2)_\rho = 0$ for n even, and $ave_{d_2}(s^2)_\rho \geq ave_{d_1}(s^2)_\rho = 1$ for n odd.
2. For $\rho=2$, $ave_{d_2}(s^2)_\rho \geq ave_{d_1}(s^2)_\rho$.
3. For $\rho=3$, $ave_{d_2}(s^2)_\rho \geq ave_{d_1}(s^2)_\rho$ unless $n=m$ and $m \equiv 2 \pmod 4$.
4. For $\rho=4$, $ave_{d_2}(s^2)_\rho \geq ave_{d_1}(s^2)_\rho$ unless (i) $n=m$ and $m \equiv 2 \pmod 4$, or (ii) $n=m-1$ and $m \equiv 3 \pmod 4$.

Proof For $k=\rho=1$ and any $d \in \mathcal{D}_\mathcal{U}$, $ave_d(s_k^2) = ave_d(s^2)_\rho$. Also, for $d \in \mathcal{D}_\mathcal{R}$, $ave_d(s_k^2) = 0$ (for n even) and $ave_d(s_k^2) = 1$ (for n odd). Furthermore, for $d' \in \mathcal{D}_\mathcal{U}$, $ave_{d'}(s_k^2) \geq ave_d(s_k^2)$.

For $k \geq 2$, from Lemma 2.1, it follows that $d_1 \in \mathcal{D}_\mathcal{R}(m,n)$ is $ave(s_k^2)$-better than $d_2 \in \mathcal{D}_\mathcal{U}^*$ if the following condition holds

for even n,

$$(k-1)E_{d_1}(s^2) \leq (m+1)\,UE_{d_2}(s^2) - (m-k)E_{d_2}(s^2)_U, \tag{4.1}$$

and for odd n,

$$(k-1)E_{d_1}(s^2) \leq (m+1)\,UE_{d_2}(s^2) - (m-k)E_{d_2}(s^2)_U - 2. \tag{4.2}$$

Similarly for $\rho \geq 2$, from Lemma 2.2, it follows that $d_1 \in \mathcal{D}_{\mathcal{R}}(m,n)$ is $ave(s^2)_\rho$-better than $d_2 \in \mathcal{D}^*_{\mathcal{U}}$ if the following condition holds
for even n,

$$E_{d_1}(s^2)\sum_{k=1}^{\rho}\left\{\binom{m}{k+1}\frac{k-1}{m-k}\right\} \leq UE_{d_2}(s^2)\sum_{k=1}^{\rho}\binom{m+1}{k+1} - E_{d_2}(s^2)_U\sum_{k=1}^{\rho}\binom{m}{k+1}, \tag{4.3}$$

and for odd n,

$$E_{d_1}(s^2)\sum_{k=1}^{\rho}\left\{\binom{m}{k+1}\frac{k-1}{m-k}\right\} \leq \left(UE_{d_2}(s^2) - \frac{2}{m+1}\right)\sum_{k=1}^{\rho}\binom{m+1}{k+1} - E_{d_2}(s^2)_U\sum_{k=1}^{\rho}\binom{m}{k+1}. \tag{4.4}$$

Using the bounds (2.2)-(2.6) for the design d_1 and the bounds (2.7) and (3.8) for the design d_2, and working out (4.1)-(4.4) for $k = 2, 3, 4$ and for $\rho = 2, 3, 4$, the conditions (A) for k active factors and conditions (B) for atmost ρ active factors follows. ■

Usually, we have $\min_{d_1 \in \mathcal{D}_{\mathcal{R}}} ave_{d_1}(s^2)_\rho \leq \min_{d_2 \in \mathcal{D}^*_{\mathcal{U}}} ave_{d_2}(s^2)_\rho$ for smaller values of ρ. However, as ρ increases, the inequality may reverse its direction. Under the effect-sparsity principle, since in a supersaturated design we have imposed only a relaxed condition of *distinctness* among factors, it becomes increasingly difficult to guarantee estimation of larger number of factors than a very few number of active factors at the time of model building. Thus, one can reasonably assume that $\rho \leq 4$.

Though Jones and Majumdar (2014) indicates that as a secondary criteria one could maximize the number of level-balanced factors, we have shown that such a maximization mostly does not perform better than a $E(s^2)$-optimal design. We now take up few examples to compare superior $UE(s^2)$-optimal designs vis-a-vis $E(s^2)$-optimal designs based on our criteria of $ave(s^2)_\rho$ for $\rho = 1, 2, 3, 4$.

Analogous to the definition of $ave_d(s^2)_\rho$ in (2.13), we can define $ave_d(D)_\rho$ where instead of taking $UE_d(s_k^2)_t$ in (2.9), we take $\{\det(Y_d'Y_d)_k\}_t^{1/(k+1)}$. Here $\{\det(Y_d'Y_d)_k\}_t$ is the value of $\det(Y_d'Y_d)_k$ corresponding to the tth sub-matrix of $Y_d'Y_d$ involving mean effect and k main effects. For given ρ, a supersaturated design $d^* \in \mathcal{D}_{\mathcal{U}}(m,n)$ is said to be $ave(D)_\rho$-optimal if $ave_{d^*}(D)_\rho \geq ave_d(D)_\rho$ for any $d \in \mathcal{D}_U(m,n)$. For the examples that follows, we also provide the measures of $ave_d(D)_\rho$ values for the designs.

Example 4.1 Let $m = 14$ and $n = 12$. Jones and Majumdar (2014) has provided two designs $d_1 \in \mathcal{D}_{\mathcal{R}}(m,n)$ and $d_2 \in \mathcal{D}_{\mathcal{U}}(m,n)$ where d_1 is $E(s^2)$-optimal and d_2 is $UE(s^2)$-optimal. Corresponding to d_2, we provide superior $UE(s^2)$-optimal design $d_3 \in \mathcal{D}_{\mathcal{U}}(m,n)$. Specifically, d_1, d_2, d_3 are

$$
d_1 = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\
-1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\
1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & -1 & 1 \\
1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 \\
-1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\
-1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 \\
-1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\
-1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 \\
1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\
1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1
\end{pmatrix}
$$

$$
d_2 = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 \\
-1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\
1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\
-1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1
\end{pmatrix}
$$

$$
d_3 = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 \\
1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 \\
-1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\
1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 \\
-1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\
1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\
-1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & -1
\end{pmatrix}.
$$

For d_1, d_2 and d_3, $E_{d_1}(s^2) = 4.22$, $E_{d_2}(s^2)_U = 3.17$ and $E_{d_3}(s^2)_U = 3.34$. Moreover, $UE_{d_1}(s^2) = 3.66$, $UE_{d_2}(s^2) = 3.20$ and $UE_{d_3}(s^2) = 3.20$. Table 1 provide the values of $ave_d(s^2)_\rho$ and $ave_d(D)_\rho$ for designs d_1, d_2, d_3 and for $\rho = 1, 2, 3, 4$. We see that d_1 has the best performance.

Table 1: The $ave(s^2)_\rho$ and $ave(D)_\rho$ values for d_1, d_2 and d_3 with $m = 14$, $n = 12$

ρ	$ave_{d_1}(s^2)_\rho$	$ave_{d_2}(s^2)_\rho$	$ave_{d_3}(s^2)_\rho$	$ave_{d_1}(D)_\rho$	$ave_{d_2}(D)_\rho$	$ave_{d_3}(D)_\rho$
1	0	3.43	2.29	12.00	11.85	11.90
2	1.41	3.35	2.64	11.89	11.71	11.78
3	1.91	3.31	2.76	11.75	11.54	11.65
4	2.33	3.28	2.87	11.59	11.32	11.48

Therefore, Example 4.1 shows that $E(s^2)$-optimal design d_1 is $ave(s^2)_\rho$-better and $ave(D)_\rho$-better than the superior $UE(s^2)$-optimal design d_3 for $\rho = 1, 2, 3, 4$.

Example 4.2 Let $m = 11$ and $n = 8$. Let $d_1 \in \mathcal{D}_{\mathcal{R}}(m, n)$ be a design (as below) which is not $E(s^2)$-optimal but has a $E_{d_1}(s^2)$-efficiency of 0.94, where $E_{d_1}(s^2)$-efficiency $= \frac{min_{d \in \mathcal{D}_{\mathcal{R}}} E_d(s^2)}{E_{d_1}(s^2)}$. (Note that, $E_{d_1}(s^2) = 4.95$ and from (2.2), $E_d(s^2) \geq 4.65$.) Also, let $d_2 \in \mathcal{D}_{\mathcal{U}}(m, n)$ be a superior $UE(s^2)$-optimal design. The designs d_1 and d_2 are

$$d_1 = \begin{pmatrix} -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 \end{pmatrix}$$

$$d_2 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\ -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \end{pmatrix}.$$

For d_1, d_2, $E_{d_1}(s^2) = 4.95$ and $E_{d_2}(s^2)_U = 2.91$. Moreover, $UE_{d_1}(s^2) = 4.12$ and $UE_{d_2}(s^2) = 2.91$. Table 2 provide the values of $ave_d(s^2)_\rho$ and $ave_d(D)_\rho$ for d_1, d_2 and for $\rho = 1, 2, 3, 4$. We see that d_1 is better than d_2.

Table 2: The $ave(s^2)_\rho$ and $ave(D)_\rho$ values for d_1 and d_2 with $m = 11$, $n = 8$

ρ	$ave_{d_1}(s^2)_\rho$	$ave_{d_2}(s^2)_\rho$	$ave_{d_1}(D)_\rho$	$ave_{d_2}(D)_\rho$
1	0	2.91	8.00	7.82
2	1.38	2.91	7.81	7.63
3	2.16	2.91	7.56	7.41
4	2.63	2.91	7.26	7.17

Therefore, Example 4.2 shows that even though d_1 is not $E(s^2)$-optimal, d_1 is $ave(s^2)_\rho$-better and $ave(D)_\rho$-better than the superior $UE(s^2)$-optimal design d_2 for $\rho = 1, 2, 3, 4$.

5. Discussion

Jones and Majumdar (2014) indicate that unless estimation of the intercept is a major goal of the experiment, $UE(s^2)$-optimality is the preferred criterion due to the higher efficiency of main effect estimation, connection to D-optimality and availability of a complete catalog of optimal designs. However, there is a significant impact of mean effect or the intercept term not being an integral part of the model. This is so since if we consider a simple problem where two models are fit – one with intercept along with factor effects and another with only factor effects, apart from extreme situations, model with intercept and factor effects have better predictive power than the model without intercept. Intercept ensures that the model is unbiased, i.e., the mean of the residuals will be exactly zero.

The basis of using a supersaturated design is the inherent assumption that there are very few active factors which one has to identify even though it is not known a priori what these active factors are. The identification of the active factors is usually based on the forward selection method of model building involving k active factors where one has to desirably use a supersaturated design which on an average estimates the model parameters optimally during the model building process. Accordingly, in Section 2, we have defined the more meaningful criteria $ave(s_k^2)$ and $ave(s^2)_\rho$ criteria, where ρ is the maximum number of active factors.

In order to ensure that all active factors can be properly estimated after the projection onto the k factors, we have to carefully select the supersaturated design. Suppose, for example, it is known that there are at most four active factors among all the factors. To ensure identifiability, we need to select a supersaturated design such that any four columns of the design are linearly independent. Hence, the estimability of the effects of these factors depends on whether or not the projected design has full rank. Under the effect-sparsity principle, since in a supersaturated design we have imposed only a relaxed condition of *distinctness* among factors, it becomes increasingly difficult to guarantee estimation of larger number of factors than a very few active factors at the time of model building. Thus, one can reasonably assume that $\rho \leq 4$ as considered in our paper.

In this connection, we have obtained superior $UE(s^2)$-optimal designs in $\mathcal{D}_U(m,n)$ and compared them against $E(s^2)$-optimal designs under the more meaningful criteria of $ave(s_k^2)$ and $ave(s^2)_\rho$. Usually for $d_1 \in \mathcal{D}_\mathcal{R}$ and $d_2 \in \mathcal{D}_\mathcal{U}^*$, we have $\min_{d_1 \in \mathcal{D}_\mathcal{R}} \; ave_{d_1}(s^2)_\rho \leq \min_{d_2 \in \mathcal{D}_\mathcal{U}^*} \; ave_{d_2}(s^2)_\rho$ for smaller values of ρ. It has been shown that $E(s^2)$-optimal designs perform fairly well or better even against superior $UE(s^2)$-optimal designs with respect to $ave(s_k^2)$ and $ave_d(s^2)_\rho$ criteria. However, as ρ increases, the inequality may reverse its direction.

Also, though Jones and Majumdar (2014) have established the D-optimality of $UE(s^2)$-optimal designs, it is seen that for $\rho = 1, 2$, the $E(s^2)$-optimal designs are $ave(D)_\rho$-better than the superior $UE(s^2)$-optimal designs.

Thus, it seems that the only advantage of the superior $UE(s^2)$-optimal designs is the ease of available constructions when $E(s^2)$-optimal designs are not readily available. However, as seen in Example 4.2, even though we have a design which is *not* $E(s^2)$-optimal, it is $ave(s^2)_\rho$-better and $ave(D)_\rho$-better than a superior $UE(s^2)$-optimal design for $\rho = 1, 2, 3, 4$. This calls for a study of $E(s^2)$-efficient designs (in the absence of available $E(s^2)$-optimal designs) which are $ave(s^2)_\rho$-better and $ave(D)_\rho$-better than the superior $UE(s^2)$-optimal designs.

Acknowledgment

The work is partially supported by DST project Grant 14DST007.

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Appendix

Proof for Theorem 3.7 Let X_d be a $n \times m$ design matrix with $d \in \mathcal{D}^*_{\mathcal{U}}$. It can be seen that,

$$trace(X'_d X_d)^2 = mn^2 + \sum_{i=1}^{m} \sum_{j(\neq i)=1}^{m} s^2_{dij}, \tag{1}$$

and,

$$trace(X_d X'_d)^2 = nm^2 + \sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t^2_{dij}. \tag{2}$$

where t_{dij} is the (i,j)-th entry of $X_d X'_d$ or $X_d X'_d = ((t_{dij}))$.

From (1) and (2),

$$E_d(s^2)_U = \frac{1}{m(m-1)} \left\{ nm(m-n) + \sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t^2_{dij} \right\}. \tag{3}$$

In what follows, we obtain an upper bound to $\sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t^2_{dij}$ in the class of designs $d \in \mathcal{D}^*_{\mathcal{U}}$ and then substituting that bound value in (3), we get the upper bound of $E_d(s^2)_U$.

We consider the cases based on the values of m.

Case 1: $m+1 \equiv 0 \pmod 4$: As seen in Theorem 3.5, for a design d to be in $\mathcal{D}^*_{\mathcal{U}}$, the $n \times (m+1)$ matrix Y_d should be such that $Y_d Y'_d = (m+1)I_n$, i.e., the inner product of any two rows of Y_d is 0. X_d is thus obtained by deleting a column of all 1's from Y_d. Therefore, it follows that the inner product of any two rows of X_d is -1, i.e., each of the $n(n-1)$ off-diagonal elements of $X_d X'_d$ are -1. Hence, the upper bound for $\sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t^2_{ij} \leq n(n-1)$.

Case 2: $m+1 \equiv 1 \pmod 4$: Again, as seen in Theorem 3.5, for a design d to be superior $UE(s^2)$-optimal, a column with equal (or nearly equal) number of ± 1's is added to Y_d. When a column of all 1's is deleted from Y_d to arrive at X_d, the off-diagonal entries of $X_d X'_d$ are 0 or -2. However, the pattern of the added column guarantees maximum number of -2's, i.e., $n^2/2$ (for n even) or $(n^2-1)/2$ (for n odd) number of -2's. Thus, for n even, $\sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t^2_{ij} \leq 2n^2$ and for n odd, $\sum_{i=1}^{n} \sum_{j(\neq i)=1}^{n} t^2_{ij} \leq 2(n^2-1)$.

Case 3: $m+1 \equiv 2 \pmod 4$, $n < m$: Again, as seen in Theorem 3.5, for a design d to be superior $UE(s^2)$-optimal, two columns are added such that frequencies of the two types of rows (1,1) and (-1,-1) in the added columns are equal (or nearly equal) and the frequencies of the two types of rows (1,-1) and (-1,1) in the added columns are also equal (or nearly equal). Furthermore, the frequencies of the row types {(1,1),(-1,-1)} and of the types {(1,-1),(-1,1)} are equal (or nearly equal). The upper bound varies as per n and are as follows,

a) For, $n \equiv 0 \pmod 4$, $(n^2/4)$ entries are -3 in off-diagonal position of $X_d X_d'$ and rest $3n^2/4 - n$ entries are ± 1. Thus, $\sum_{i=1}^n \sum_{j(\neq i)=1}^n t_{ij}^2 \leq 9n^2/4 + 3n^2/4 - n \leq n(3n-1)$.

b) For, $n \equiv 2 \pmod 4$, $((n^2-4)/4)$ entries are -3 in off-diagonal position of $X_d X_d'$ and rest $((3n^2+4)/4) - n$ entries are ± 1. Thus, $\sum_{i=1}^n \sum_{j(\neq i)=1}^n t_{ij}^2 \leq 9(n^2-4)/4 + (3n^2+4)/4 - n \leq 3n^2 - n - 8$.

c) For, $n \equiv 1 \pmod 4$, $(n^2-1)/4$ entries are -3 in off-diagonal position of $X_d X_d'$ and rest $(3n^2+1)/4 - n$ entries are ± 1. Thus, $\sum_{i=1}^n \sum_{j(\neq i)=1}^n t_{ij}^2 \leq 9(n^2-1)/4 + (3n^2+1)/4 - n \leq 3n^2 - n - 2$.

Case 4: $m+1 \equiv 3 \pmod 4$: Again, as seen in Theorem 3.5, a column with maximum column sum is deleted from $H_{n,m+2}$ to get a superior $UE(s^2)$-optimal design d. Since we are deleting from a Hadamard matrix and we know that each row and each column of $H_{n,m+2}$ can have at most $(m+2)/2$ +1's or -1's, therefore if $n \leq (m+2)/2$, there can at most be $(n-1)$ elements of one type and 1 element of other type (else, the deleted column would be same as ± 1). Thus, the nonzero off-diagonal entries of $X_d X_d'$ are ± 2 with frequency $2\binom{n-1}{2}$. However, if $n > (m+2)/2$, the nonzero off-diagonal entries of $X_d X_d'$ are ± 2 with frequency $2\{\binom{(m+2)/2}{2} + \binom{n-(m+2)/2}{2}\}$. Thus, if $n \leq (m+2)/2$, $\sum_{i=1}^n \sum_{j(\neq i)=1}^n t_{ij}^2 \leq 4(n-1)(n-2)$ and if $n > (m+2)/2$, then $\sum_{i=1}^n \sum_{j(\neq i)=1}^n t_{ij}^2 \leq m(m+2) + (2n-m-2)(2n-m-4)$.

Case 5: $m+1 \equiv 2 \pmod 4$ and $n = m$: As seen in Theorem 3.6, two columns are deleted from $H_{m,m+3}$ to get a superior $UE(s^2)$-optimal design d such that difference between the frequencies of rows of the type {(1,1), (-1,-1)} and the rows of the type {(1,-1), (-1,1)}, in the deleted columns, is ± 1. Furthermore, the column sums of the deleted columns are ± 3 and ± 1 respectively. For column sums to be that, we should pick columns which maximize the frequencies of same type of rows. Since, we are deleting from Hadamard matrix, we know that maximum frequency of each of the four sets can be $(m+3)/4$ and thus, the frequency of -3's in the off-diagonal position of $X_d X_d'$ is $2\left(\binom{(m+3)/4}{2} + \binom{(m-1)/4}{2} + \binom{(m+3)/4}{2} + \binom{(m-5)/4}{2}\right) = (m^2 - 4m + 11)/2$. The remaining off-diagonal elements of $X_d X_d'$ are ± 1. Thus, $\sum_{i=1}^n \sum_{j(\neq i)=1}^n t_{ij}^2 \leq (9(n^2 - 4n + 11)/4) + ((3n^2 - 11)/4) = 3(n^2 - 9n + 22)$. ■