

$E(s^2)$ -Optimal supersaturated designs with good minimax properties

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Abstract

An improved $E(s^2)$ lower bound is derived for two-level supersaturated designs. This improved bound is used to prove $E(s^2)$ -optimality of the best designs obtained via algorithmic search in all cases with $N = 10, 12, 14$, and 16 runs (except the $N = 14$ run, $m = 16$ factor case). New exchange algorithms which generalize the NOA algorithm of Nguyen [1996. An algorithmic approach to constructing supersaturated designs. *Technometrics* 38, 69–73] and which tend to find $E(s^2)$ -optimal designs with better minimax properties are proposed. Row swapping algorithms are used to find $E(s^2)$ -optimal designs when the number of factors is large. $E(s^2)$ -optimal designs found via algorithmic search are compared to cyclicly constructed $E(s^2)$ -optimal designs using the minimax criterion.

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1. Introduction

A factorial design that does not have enough runs to estimate all main effects is called a supersaturated design (SSD). First introduced by Booth and Cox (1962), SSDs have received increased attention since Lin (1993a, 1995) and Wu (1993) because of their potential use in factor screening experiments. For example, Nguyen (1996) discussed an SSD application involving a passenger-impact crash test where there are a large number of factors while only a small number of runs are affordable.

A two-level SSD with N runs and m factors is represented by an $N \times m$ matrix X , where each entry is ± 1 , the frequency of $+1$ in each column is $N/2$, and no two columns of X are completely aliased. The j th column of X contains factor levels for the j th factor, and each row of X is a particular combination of factor levels at which an observation of the response is to be collected. If an SSD is normalized (by multiplying a subset of columns by -1) to have an all $+1$ s row, then there are $N - 1$ remaining rows in which $N/2 - 1$ more $+1$ s must be chosen per column. Hence,

$$N - 1 < m \leq \binom{N - 1}{\frac{N}{2} - 1} = \frac{1}{2} \binom{N}{\frac{N}{2}} =: m_F,$$

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where m_F is the maximum number of factors for an N run SSD. A design with $m = N - 1$ factors but which satisfies all other properties of an SSD is called a saturated design (SD).

The $E(s^2)$ value of an SSD (or SD) is

$$E(s^2) = \frac{\sum_{i < j} s_{ij}^2}{\binom{m}{2}},$$

where s_{ij} is the dot product between the i th and j th columns of X . Due to their balance, SSDs estimate an effect optimally when only one factor is active. When two or more factors are active, $E(s^2)$ approximates various criteria for estimating main effects; see Booth and Cox (1962).

Achievable lower bounds for $E(s^2)$ must be derived to prove $E(s^2)$ -optimality. The $E(s^2)$ achievable lower bound is the largest lower bound; thus, it is desirable to increase an $E(s^2)$ lower bound as much as possible. Nguyen (1996) and Tang and Wu (1997) independently proved that

$$E(s^2) \geq \frac{m - N + 1}{(m - 1)(N - 1)} N^2 \tag{1}$$

for any SSD. Bound (1) can be achieved only if $m = q(N - 1)$ and $N \equiv 0 \pmod{4}$ or if $m = 2q(N - 1)$ and $N \equiv 2 \pmod{2}$ for some positive integer q . Bound (1) was independently improved by Butler et al. (2001) and Bulutoglu and Cheng (2004). These improved lower bounds are equal when they both apply. Unlike the bound of Butler et al. (2001), the more general bound of Bulutoglu and Cheng (2004) is applicable for all possible N and m . Section 2 presents an improvement to the Bulutoglu and Cheng (2004) bound.

The minimax criterion was also proposed by Booth and Cox (1962) for selecting SSDs. Tang and Wu (1997) investigated this criterion when $m = q(N - 1)$ for some integer $q > 0$. The minimax criterion order designs by

$$s_{\max} = \max_{i < j} |s_{ij}|$$

and then by the frequency of s_{\max}

$$f_{s_{\max}} = \sum_{i < j} I_{s_{\max}}(|s_{ij}|),$$

where indicator $I_a(b) = 1$ if $a = b$ and is 0 otherwise. (Equivalently, one may replace frequency $f_{s_{\max}}$ with proportion $p_{s_{\max}} = 2f_{s_{\max}} / (m(m - 1))$.) Bounds for s_{\max} are also provided in Section 2. The minimax criterion is a secondary criterion to compare designs having the same $E(s^2)$ value.

Algorithms for finding $E(s^2)$ -optimal, minimax optimal, SSDs are presented in Section 3. The bounds from Section 2 prove optimality. Defined in Section 3.1, the NOA_k algorithms, which generalize the NOA algorithm of Nguyen (1996), tend to find $E(s^2)$ -optimal SSDs with better minimax properties than those found by the NOA algorithm. Two row swapping algorithms (defined in Section 3.2) concatenate the columns of two $E(s^2)$ -optimal SSDs to produce an $E(s^2)$ -optimal SSD. The NOA_k algorithms can be used to find the smaller designs needed by the row swapping algorithms. Together, these algorithms successfully found $E(s^2)$ -optimal SSDs for every case with $N = 10, 12, 14$, and 16 runs (except the $N = 14$ run, $m = 16$ factor case). This is a sizable continuation of Cheng (1997) who constructed $E(s^2)$ -optimal SSDs for each case with $N = 8$ runs. The fact that the problem of finding $E(s^2)$ -optimal SSDs was solved in all cases with $N \leq 16$ runs except one suggests that the new bound in Section 2 is close to the largest lower bound. A fundamental question is whether our bound is achievable when $N > 16$.

There is a vast literature on other ways of obtaining $E(s^2)$ -optimal SSDs. Li and Wu (1997) used columnwise–pairwise algorithms. Others constructed $E(s^2)$ -optimal SSDs when m is a multiple of $N - 1$; see Bulutoglu (2006), Bulutoglu and Cheng (2004), Eskridge et al. (2004), Liu and Dean (2004), and Liu and Zhang (2000). A comparison of construction methods to our algorithmically located SSDs is in Section 4. These comparisons support our algorithms. The following are used throughout this paper.

- $\text{SS}(M)$ denotes the sum of the squared entries of a matrix M .
- For any $x \in \mathbb{R}$, $\lfloor x \rfloor^+ = \max\{0, \lfloor x \rfloor\}$, and $\lceil x \rceil^+ = \max\{0, \lceil x \rceil\}$, where $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ are the floor and ceiling functions, respectively.
- Two SSDs are called *isomorphic* if one can be obtained from the other via run permutations and/or column permutations and/or a multiplication of a subset of columns by -1 .

2. Lower bounds for $E(s^2)$ and s_{\max}

While using Section 3.1 algorithms, we noticed that in several $N \equiv 2 \pmod{4}$ cases that we were getting SSDs with $E(s^2)$ values slightly above the Bulutoglu and Cheng (2004) bound. This observation led us to believe that the Bulutoglu and Cheng (2004) bound could be improved. The following theorem improves the $E(s^2)$ lower bound for SSDs derived by Bulutoglu and Cheng (2004) when $N \equiv 2 \pmod{4}$. (The Bulutoglu and Cheng, 2004 lower bound is obtained if “ \lceil ” and “ \lceil^+ ” are removed from Eq. (2).) The proof uses discreteness.

Theorem 1. *Let m be a positive integer such that $m > N - 1$. Then there exists a unique positive integer q (which depends on N and m) such that $-2N + 2 < m - q(N - 1) < 2N - 2$ and $(m + q) \equiv 2 \pmod{4}$. Define $g = (m + q)^2 N - q^2 N^2 - mN^2$.*

(1) *If $N \equiv 0 \pmod{4}$, then*

$$E(s^2) \geq \begin{cases} \frac{g + 2N^2 - 4N}{m(m - 1)} & \text{if } |m - q(N - 1)| < N - 1, \\ \frac{g - 2N^2 + 4N + 4N|m - q(N - 1)|}{m(m - 1)} & \text{if } N - 1 < |m - q(N - 1)| \leq \frac{3}{2}N - 2, \\ \frac{g + 4N^2 - 4N}{m(m - 1)} & \text{if } |m - q(N - 1)| > \frac{3}{2}N - 2. \end{cases}$$

(2) *If $N \equiv 2 \pmod{4}$, then*

$$E(s^2) \geq 4 + 64 \frac{\lceil m(m - 1)(h - 4)/64 \rceil^+}{m(m - 1)}, \tag{2}$$

where for even q

$$h = \begin{cases} \frac{g + 2N^2 - 4N + 8}{m(m - 1)} & \text{if } |m - q(N - 1)| < N - 1, \\ \frac{g - 2N^2 + 20N + (4N - 8)|m - q(N - 1)| - 24}{m(m - 1)} & \text{if } N - 1 < |m - q(N - 1)| \leq \frac{3}{2}N - 3, \\ \frac{g + 4N^2 - 4N}{m(m - 1)} & \text{if } |m - q(N - 1)| > \frac{3}{2}N - 3 \end{cases}$$

and for odd q

$$h = \begin{cases} \frac{g + 2N^2 - 4N}{m(m - 1)} & \text{if } |m - q(N - 1)| < N - 1, \\ \frac{g - 2N^2 + 4N + 4N|m - q(N - 1)|}{m(m - 1)} & \text{if } N - 1 < |m - q(N - 1)| \leq \frac{3}{2}N - 1, \\ \frac{g + 4N^2 - 12N + 8|m - q(N - 1)| + 8}{m(m - 1)} & \text{if } |m - q(N - 1)| > \frac{3}{2}N - 1. \end{cases}$$

Proof. The $E(s^2)$ value of an SSD X with N runs and m factors is $E(s^2) = [SS(X^T X) - mN^2]/[m(m - 1)]$ which is equal to the average of the squared lower diagonal entries of $X^T X$.

Using previous notation, let s_{ij} be the (i, j) th entry of $X^T X$, and suppose that $N \equiv 2 \pmod{4}$. Therefore, $s_{ij} \equiv 2 \pmod{4}$, so $s_{ij} = 4t_{ij} + 2$ for some integer t_{ij} . Since $t_{ij}^2 + t_{ij}$ is even and

$$(4t_{ij} + 2)^2 = 16(t_{ij}^2 + t_{ij}) + 4,$$

it follows that $(4t_{ij} + 2)^2 \equiv 4 \pmod{32}$. Hence,

$$E(s^2) = \frac{4m(m-1)/2 + 32K}{m(m-1)/2} = 4 + \frac{64K}{m(m-1)} \quad \text{for some } K \in \mathbb{Z}^+.$$

So by Theorem 3.1 of Bulutoglu and Cheng (2004),

$$E(s^2) = 4 + \frac{64K}{m(m-1)} \geq \max(h, 4)$$

which implies that

$$E(s^2) \geq 4 + 64 \frac{\lceil m(m-1)(h-4)/64 \rceil^+}{m(m-1)}. \quad \square$$

Remark 2. If $N \equiv 0 \pmod{4}$, then the $s_{ij} \equiv 0 \pmod{4}$ implying that the square of any off diagonal entry of $X^T X$ is a multiple of 16 and that the sum of all squared lower diagonal entries of $X^T X$ is a multiple of 16. Hence,

$$E(s^2) = \frac{16K}{m(m-1)/2} = \frac{32K}{m(m-1)} \quad \text{for some } K \in \mathbb{Z}^+.$$

Unlike the $N \equiv 2 \pmod{4}$ case, this observation does not help improve the $E(s^2)$ lower bound since $m(m-1)$ multiplied by the $E(s^2)$ lower bound is a multiple of 32 when $N \equiv 0 \pmod{4}$.

The following definition helps begin a discussion about the minimax criterion.

Definition 3. An SSD is called *minimax optimal* if no other SSD with the same number of runs and factors has a lower s_{\max} or the same s_{\max} with a lower $f_{s_{\max}}$.

Whether or not an $E(s^2)$ -optimal, minimax optimal SSD can be found (for a given number of runs and factors) is an interesting question. Lin (1993b) proved that $s_{ij} \equiv N \pmod{4}$ and discussed bounds for s_{\max} based on this fact. The following theorem demonstrates that $E(s^2)$ -optimality is a sufficient condition for minimax optimality if s_{\max} attains certain values.

Theorem 4. Let X be an N run, m factor $E(s^2)$ -optimal SSD.

- (1) If $N \equiv 0 \pmod{4}$ and $s_{\max} = 4$, then X is minimax optimal.
- (2) If $N \equiv 2 \pmod{4}$ and $s_{\max} \in \{2, 6\}$, then X is minimax optimal.

Proof.

- (1) Each entry of $X^T X$ is a multiple of 4. Since X is an SSD, $X^T X$ has non-zero off-diagonal entries. Therefore, $s_{\max} \geq 4$.
- (2) Each entry of $X^T X$ is congruent to 2 (mod 4), so if $s_{\max} = 2$, then X is clearly minimax optimal. If X is $E(s^2)$ -optimal and $s_{\max} = 6$ on the other hand, $f_{s_{\max}}$ cannot be reduced (while maintaining $s_{\max} \leq 6$) without reducing $E(s^2)$. Therefore, X is again minimax optimal. \square

Butler et al. (2001) describe a theoretical construction for optimal SSDs. Their construction yields designs with an equal number of +1s and -1s in each column and with $E(s^2)$ values that achieve the lower bound in this paper, but it does not always yield designs with no aliased columns. When their construction applies, it is based on an $N/2 \times m_0$ optimal SSD X_0 and an $N/2 \times m_1$ matrix X_1 , where each element of X_1 is ± 1 and the rows of X_1 are orthogonal. (The values m_0 and m_1 depend on N and m .) The design

$$X = \begin{pmatrix} X_0 & X_1 \\ X_0 & -X_1 \end{pmatrix}$$

Table 1
Properties of $E(s^2)$ -optimal SSDs constructed by Theorem 3.1 and Corollary 3.2 Bulutoglu and Cheng (2003)

N	m	$E(s^2)$	s_{\max}	$f_{s_{\max}}$	$P_{s_{\max}}$	s_{\max} Upper bound	Method
12	55	10.6667	4	990	0.6667	12	Thm. 3.1
12	66	11.0769	4	1485	0.6923	12	Cor. 3.2
20	171	18.8235	12	684	0.0471	12	Thm. 3.1
20	190	19.0476	12	855	0.0476	12	Cor. 3.2
24	253	22.8571	8	11,385	0.3571	8	Thm. 3.1
24	276	23.0400	8	13,662	0.3600	8	Cor. 3.2
28	351	26.8800	12	6318	0.1029	12	Thm. 3.1
28	378	27.0345	12	7371	0.1034	12	Cor. 3.2
32	465	30.8966	8	52,080	0.4828	16	Thm. 3.1
32	496	31.0303	8	59,520	0.4848	16	Cor. 3.2
44	903	42.9268	12	90,300	0.2217	12	Thm. 3.1
44	946	43.0222	12	99,330	0.2222	12	Cor. 3.2
48	1081	46.9333	16	35,673	0.0611	16	Thm. 3.1
48	1128	47.0204	16	38,916	0.0612	16	Cor. 3.2

is an $E(s^2)$ -optimal SSD with N runs and $m = m_0 + m_1$ factors. See Theorem 3 of Butler et al. (2001) for details. Generalizing earlier notation, let $s_{\max}(\mathbf{D})$ be the s_{\max} value of some SSD \mathbf{D} . It is clear that $s_{\max}(\mathbf{X}) \geq 2s_{\max}(\mathbf{X}_0)$. Therefore, $s_{\max}(\mathbf{X}) \geq 8$ as $s_{\max}(\mathbf{X}_0) \geq 4$. These inequalities can be used to compare designs from the construction of Butler et al. (2001) to designs found using the algorithms in Section 3. The algorithms tend to find $E(s^2)$ -optimal designs with better minimax properties.

A way to show that a family of SSDs is well-behaved with respect to the minimax criterion is to find an upper bound for s_{\max} . It is sometimes possible to derive s_{\max} upper bounds for a family of $E(s^2)$ -optimal SSDs. For example, by Theorem 2.1 and Lemma 2.4 Bulutoglu and Cheng (2003), the upper bound

$$s_{\max} \leq \begin{cases} \lfloor 6 + 2\sqrt{N-1} \rfloor_{8k+4} & \text{if } N/4 \text{ is odd,} \\ \lfloor 6 + 2\sqrt{N-1} \rfloor_{8k} & \text{if } N/4 \text{ is even,} \end{cases} \tag{3}$$

where $\lfloor m \rfloor_{8k+4}$ is the largest integer smaller than m of the form $8k + 4$ for some $k \in \mathbb{Z}$ and $\lfloor m \rfloor_{8k}$ is the largest integer smaller than m of the form $8k$ for some $k \in \mathbb{Z}$, applies to the resulting $E(s^2)$ -optimal SSDs when Theorem 3.1 or Corollary 3.2 Bulutoglu and Cheng (2003) is applied to Paley matrices. Table 1 contains s_{\max} and $f_{s_{\max}}$ values of $E(s^2)$ -optimal SSDs from Theorem 3.1 or Corollary 3.2 Bulutoglu and Cheng (2003). The s_{\max} upper bounds (3) are not achieved by these $E(s^2)$ -optimal SSDs in several cases, so $E(s^2)$ -optimal SSDs in this family are often better than the guarantee of bound (3). \square

3. Algorithms for finding optimal supersaturated designs

3.1. Generalizations of the NOA algorithm

Designs that are both $E(s^2)$ -optimal and minimax optimal for several cases of N and m were found by modifying the search criterion of the Nguyen (1996) NOA algorithm. The following generalization of the $E(s^2)$ criterion was used.

Definition 5. Let \mathbf{X} be an $N \times m$ SSD. Define

$$f^k(\mathbf{X}) = \sum_{i < j} |s_{ij}|^k$$

for some fixed $k \in \mathbb{R}$.

Note that $E(s^2) = f^2(\mathbf{X}) / \binom{m}{2}$. Under a fixed level of experimental effort N and m , there can exist $E(s^2)$ -optimal SSDs at various levels of the minimax criterion. The near orthogonal array k (NOA $_k$) algorithm below uses criteria f^k to search for $E(s^2)$ -optimal SSDs with desirable minimax properties.

Algorithm 1 (NOA_k). (1) Randomly generate an $N \times m$ matrix X with elements ± 1 such that each column has an equal number of $+1$ s and -1 s. Compute $X^T X$, set $j = 1$, and set count = 0.
 (2) For the $(N/2)^2$ sign swaps in column j of X , compute the change in f^k . If at least one of these swaps reduces $f^k(X)$, update X and $X^T X$ with a swap that reduces $f^k(X)$ the most and set count = 0; else increment count = count + 1.
 (3) If count < m , set $j = \max\{(j + 1) \bmod (m + 1), 1\}$ and GOTO Step (2).
 (4) When this step is reached, the algorithm has found an f^k local optimum. Compute $E(s^2)$, s_{\max} , and $f_{s_{\max}}$ from $X^T X$. If $E(s^2)$ attains the Theorem 1 lower bound and if $s_{\max} < N$ such that s_{\max} and $f_{s_{\max}}$ are at desired levels, exit; else GOTO Step (1) and try to find a better design.

NOA_k optimizes f^k of a pseudo-random balanced design by swapping $+1$, -1 pairs in columns of X . In some cases when $E(s^2)$ is optimized (i.e., $k = 2$), the probability of obtaining an $E(s^2)$ -optimal design with $s_{\max} = N$ is high. By altering the search criterion to $k > 2$, the objective function becomes a compromise between $E(s^2)$ and $(s_{\max}, f_{s_{\max}})$, and the probability of obtaining $E(s^2)$ -optimal SSDs with good minimax properties is increased. The NOA_k algorithm can be programmed to avoid unnecessary arithmetic operations and increase speed; note the following.

- A local optimum is found when count = m as no swaps reducing f^k exist.
- Only compute and update elements of $X^T X$ on one side of the diagonal.
- Nguyen (1996) presents formulas for updating the j th row and j th column of $X^T X$ when a single swap is performed in the j th column of X . These formulas can be used to efficiently update $X^T X$ and compute changes in f^k ; recalculating $X^T X$ after each single swap is wasteful.

NOA_k was run for $k = 2, 4$, and 8 when $N = 12$ and for $k = 2$ and 4 when $N = 14$ and 16 . (For example, when $(N, k) = (16, 8)$, N^k exceeds the largest available integer on our computer, so $k = 8$ was not tested with $N = 14$ and 16 . Also, k was restricted to powers of 2 because integer arithmetic greatly speeds up the algorithm and because powers of 2 require less operations.) Each (N, m, k) triple was run for 2 days CPU or until a minimax optimal, $E(s^2)$ -optimal SSD was found. All jobs were processed by an Athlon 3000 + 2.1 GHz CPU with 1 GB memory.

The characteristic $s_{\max} + p_{s_{\max}}$ orders SSDs by the minimax criterion. Fig. 1 contains plots of $s_{\max} + p_{s_{\max}}$ against m for $E(s^2)$ -optimal SSDs with $N = 12$ runs found by NOA_k ($k = 2, 4$, and 8). NOA_2 did not find $E(s^2)$ -optimal, minimax optimal SSDs when $m > 22$, while NOA_4 and NOA_8 found $E(s^2)$ -optimal, minimax optimal SSDs for most cases when $22 \leq m \leq 66$. NOA_2 did not find $E(s^2)$ -optimal SSDs for cases when $m > 142$, and NOA_4 found $E(s^2)$ -optimal SSDs for less than half the cases when $m > 208$. NOA_8 found an $E(s^2)$ -optimal SSD for each case when $m \leq 240$. For cases when $m \approx 100$, NOA_2 found $E(s^2)$ -optimal SSDs where $p_{s_{\max}}$ is about 0.02 higher than that of NOA_4 or NOA_8 . Although not visible in Fig. 1(c), NOA_8 did tend to locate $E(s^2)$ -optimal SSDs with smaller $f_{s_{\max}}$ than NOA_4 .

Plots like those in Fig. 1 were constructed for $N = 14$ and 16 . These plots were omitted because they were similar to Fig. 1 with one exception; less cases were solved in the allotted 2 day CPU time limit because the search space is larger with increased N and/or because the lower bounds (of $E(s^2)$ -optimal SSDs) for s_{\max} in the proof of Theorem 4 can be improved.

Consider first $N = 14$ cases. NOA_2 did not find $E(s^2)$ -optimal, minimax optimal SSDs when $m > 45$. NOA_4 found $E(s^2)$ -optimal, minimax optimal SSDs when $m \leq 87$, except 5 cases. Neither NOA_2 nor NOA_4 found an SSD which could be proven to be $E(s^2)$ -optimal in the $N = 14$ and $m = 16$ case which deserves special attention because it is the only unsolved case with $N = 10, 12, 14$, or 16 . (All other cases not solved with NOA_k algorithms were eventually solved with row swapping algorithms and by taking complements which are discussed in Section 3.2.) The best SSD found for this troublesome case (from any reviewed source) had $s_{\max} = 6$ and $f_{s_{\max}} = 2$ implying $E(s^2) \approx 4.53$. Furthermore, the Theorem 1 bound $E(s^2) \geq 4$ is trivial as all $s_{ij} \equiv 2 \pmod{4}$. We believe that the obtained $E(s^2) \approx 4.53$ SSD is $E(s^2)$ -optimal (and hence minimax optimal) and that the Theorem 1 bound can be increased in this case because NOA_k was so successful at quickly solving neighboring cases.

Consider now $N = 16$ cases. NOA_2 found $E(s^2)$ -optimal, minimax optimal SSDs up to $m = 24$ and $E(s^2)$ -optimal, $s_{\max} = 8$ SSDs when $25 \leq m \leq 27$. NOA_4 found $E(s^2)$ -optimal, minimax optimal SSDs up to $m = 24$ and when $m = 28$. As for the $25 \leq m \leq 27$, NOA_4 did not find $E(s^2)$ -optimal SSDs in the allotted time. However, the best SSDs found by NOA_4 for these cases had $s_{\max} = 4$ and an $E(s^2)$ value about 2% higher than the Theorem 1 bound. Based on this information, it may not be possible to optimize both $E(s^2)$ and minimax simultaneously in the $m = 25, 26$, and 27 cases. Table 2 lists all cases where the best obtained $E(s^2)$ -optimal SSD is minimax optimal.

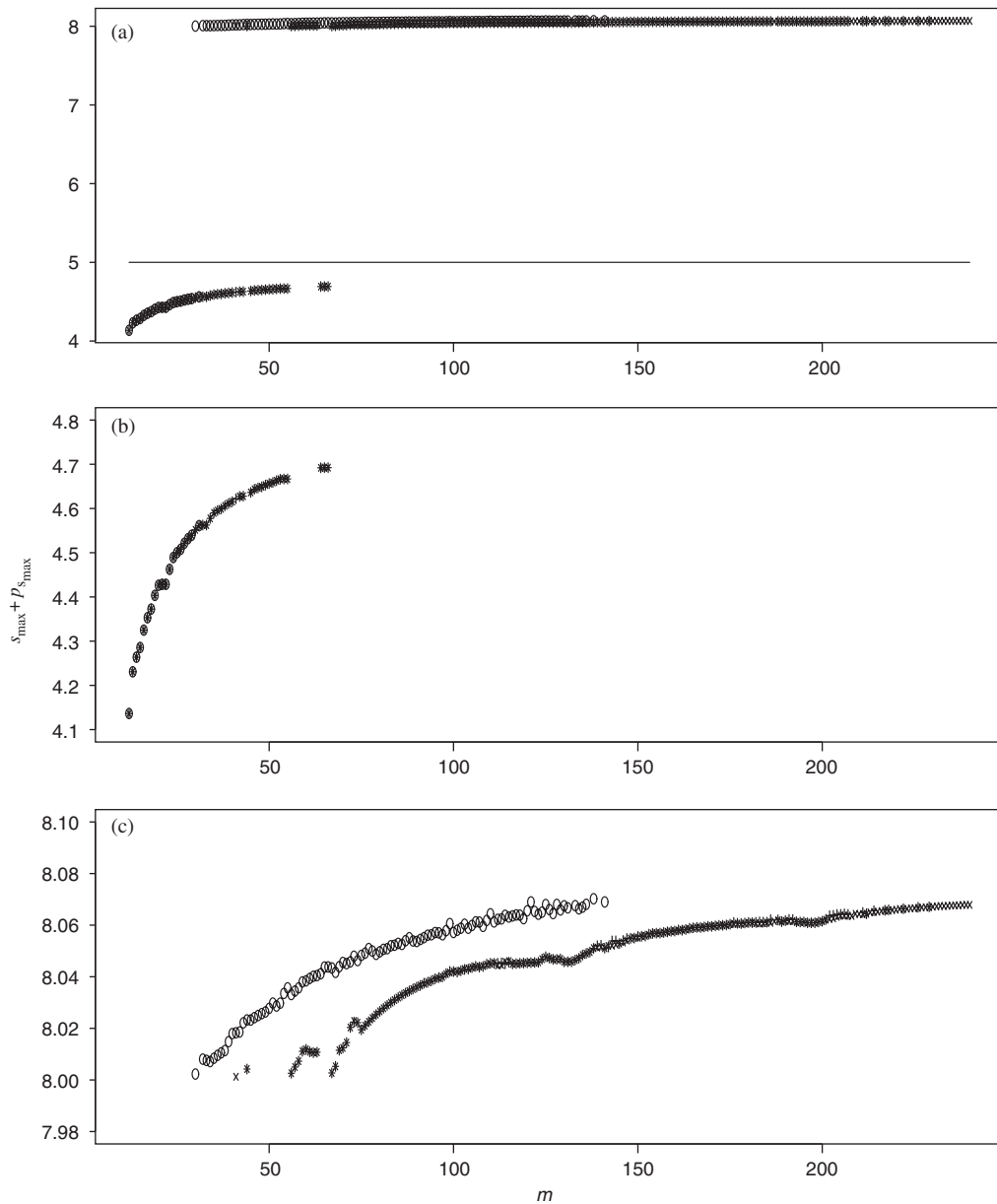


Fig. 1. Plots of $s_{\max} + P_{s_{\max}}$ versus number of factors m for $E(s^2)$ -optimal SSDs with $N = 12$ runs. Circles denote characteristics of SSDs found via NOA_2 , crosses via NOA_4 , and X's via NOA_8 . (a) Circles, crosses, or X's below the horizontal line at 5 correspond to SSDs that are also minimax optimal by Theorem 4. (b) A plot of the minimax optimal SSDs from (a). (c) A plot of the non-minimax optimal designs from (a).

Table 2
 $E(s^2)$ -optimal, minimax optimal SSDs found by NOA_k

N	m
10	10–126
12	12–43, 45–55, 64–66
14	14, 15, 17–76, 80, 81, 83–87
16	16–24, 28
18	18, 19, 21, 22

3.2. Row swapping algorithms

It is sometimes possible to concatenate the columns of two N run $E(s^2)$ -optimal SDs or SSDs into a new N run $E(s^2)$ -optimal SSD. The following theorem, restated from Butler et al. (2001), provides a sufficient condition for when such concatenations produce $E(s^2)$ -optimal SSDs. This theorem provides the theoretical justification for the row swapping algorithms in this section.

Theorem 6. *Let X_0 be an $E(s^2)$ -optimal SD or SSD with N runs and m_0 factors, and let X be an $E(s^2)$ -optimal design with N runs and $q(N - 1)$ factors, where q is some positive integer if $N \equiv 0 \pmod{4}$ and q is some positive, even integer if $N \equiv 2 \pmod{4}$. Then the design*

$$X_1 = [X_0 : X]$$

is an $E(s^2)$ -optimal SSD with N runs and $m = m_0 + q(N - 1)$ factors provided that no two columns of X_1 are aliased.

Taking complements is another method for constructing SSDs.

Theorem 7. *Let X_F be the SSD with N runs and $m_F = \binom{N-1}{N/2-1}$ factors, let X be an $E(s^2)$ -optimal SSD with N runs and m factors satisfying*

$$m_F - m > N - 1,$$

and let the columns of X_c be the columns of X_F that are not aliased with any column of X . Then X_c is an $E(s^2)$ -optimal SSD with N runs and $m_F - m$ factors.

Before proving this theorem, an important identity for any SSD X is stated:

$$SS(X^T X) = \text{tr}[X^T X X^T X] = \text{tr}[X X^T X X^T] = SS(X X^T). \tag{4}$$

Therefore, $E(s^2)$ is minimized if and only if $SS(X X^T)$ is minimized.

Proof. Let m_c be the number of columns of X_c . Since each column of X is aliased with one column of X_F , $m_c = m_F - m$. Observe that the SSD X_F with m_F factors is unique up to isomorphism. Isomorphic SSDs have the same $E(s^2)$ value; thus, X_F is $E(s^2)$ -optimal. Also, the entries of $X_F X_F^T$ do not change when a subset of factors are multiplied by -1 , so WLOG, suppose that the first row of X_F is all $+1$ s. Note that

$$m_F = \binom{N-1}{N/2-1} = \binom{N-2}{N/2-2} + \binom{N-2}{N/2-1},$$

so the frequency of $+1$ and -1 in each row of X_F (except the first) is $\binom{N-2}{N/2-2}$ and $\binom{N-2}{N/2-1}$, respectively. Hence, the full SSD satisfies

$$X_F X_F^T = (m_F + q)I_N - qJ_N,$$

where $q = \binom{N-2}{N/2-1} - \binom{N-2}{N/2-2} = m_F / (N - 1)$, I_N is the $N \times N$ identity matrix, and J_N is the $N \times N$ matrix of $+1$ s. Thus,

$$X_F X_F^T = X X^T + X_c X_c^T;$$

$$X_c X_c^T = -X X^T + [(m_F + q)I_N - qJ_N].$$

Since all columns of X sum to 0, all rows of XX^T sum to 0. Therefore,

$$SS(X_c X_c^T) = SS(XX^T) + N(m_F + q)^2 + N^2 q^2 - 2N(m_F + q)(m + q),$$

and $SS(X_c X_c^T)$ is minimized if and only if $SS(XX^T)$ is minimized. The fact after identity (4) completes the proof. \square

Before describing some row swapping algorithms, a definition is needed.

Definition 8. If X_0 is an $E(s^2)$ -optimal SD or SSD with N runs and m_0 factors satisfying

- $N - 1 \leq m_0 < 2(N - 1)$ if $N \equiv 0 \pmod{4}$ or
- $2(N - 1) \leq m_0 < 4(N - 1)$ if $N \equiv 2 \pmod{4}$,

then X_0 is called an *initial design*.

Row swap random (RSR) searches for $E(s^2)$ -optimal SSDs using Theorem 6.

Algorithm 2 (RSR). Let $\alpha = N \pmod{4}$. Inputs: An initial design X_0 having N runs and m_0 factors and a Hadamard matrix X from which an all +1s column is deleted if $N \equiv 0 \pmod{4}$ or an $E(s^2)$ -optimal SSD X with N runs and $2(N - 1)$ factors if $N \equiv 2 \pmod{4}$.

(1) Set $i = 1$, and compute

$$\theta = \left\lfloor \frac{\binom{N-1}{N/2-1} - 2m_0}{(\alpha+2)(N-1)} \right\rfloor^+,$$

i.e., the largest positive integer satisfying

$$m_0 + \left(\frac{\alpha}{2} + 1\right)\theta(N-1) \leq \frac{1}{2} \binom{N-1}{N/2-1}.$$

(2) Randomly permute the rows of X until $X_i = [X_{i-1} : X]$ has no aliased columns.

(3) Increment $i = i + 1$, and repeat the last step if $i \leq \theta$.

Output: An N run, $m_0 + \theta(N - 1)$ factor $E(s^2)$ -optimal SSD whose first $m_0 + i(\alpha/2 + 1)(N - 1)$ columns form an $E(s^2)$ -optimal SSD for each $i = 1, 2, \dots, \theta$.

Row swap 4 (RS₄) is another row swapping algorithm that searches for optimal SSDs using Theorem 6. Before outlining algorithm RS₄, a definition is needed.

Definition 9. Let X_1 and X_2 be two N run SSDs, and let i and j be distinct elements of $\{1, 2, \dots, N\}$. Define

$$\Delta f^k(X_1, X_2, i, j) = f^k([X_1 : X_2]) - f^k([X_1 : X_2^*]),$$

where X_2^* is the N run SSD formed by swapping the i th and j th rows of X_2 .

Algorithm 3 (RS₄). Inputs: An N run, m factor $E(s^2)$ -optimal SSD X_0 and an $E(s^2)$ -optimal SSD X with N runs and $q(N - 1)$ factors (where $q \in \mathbb{Z}^+$ if $N \equiv 0 \pmod{4}$ or $q \in 2\mathbb{Z}^+$ if $N \equiv 2 \pmod{4}$).

- (1) Randomly permute the rows of X .
- (2) Compute $[X_0 : X]^T [X_0 : X]$.
- (3) Calculate $\Delta f^4(X_0, X, i, j)$, for each of the $\binom{N}{2}$ pairwise row swaps of X (i.e., for each $i, j \in \mathbb{Z}$ such that $1 \leq i < j \leq N$).
- (4) Update X with a row swap that reduces $f^4([X_0 : X])$ the most.

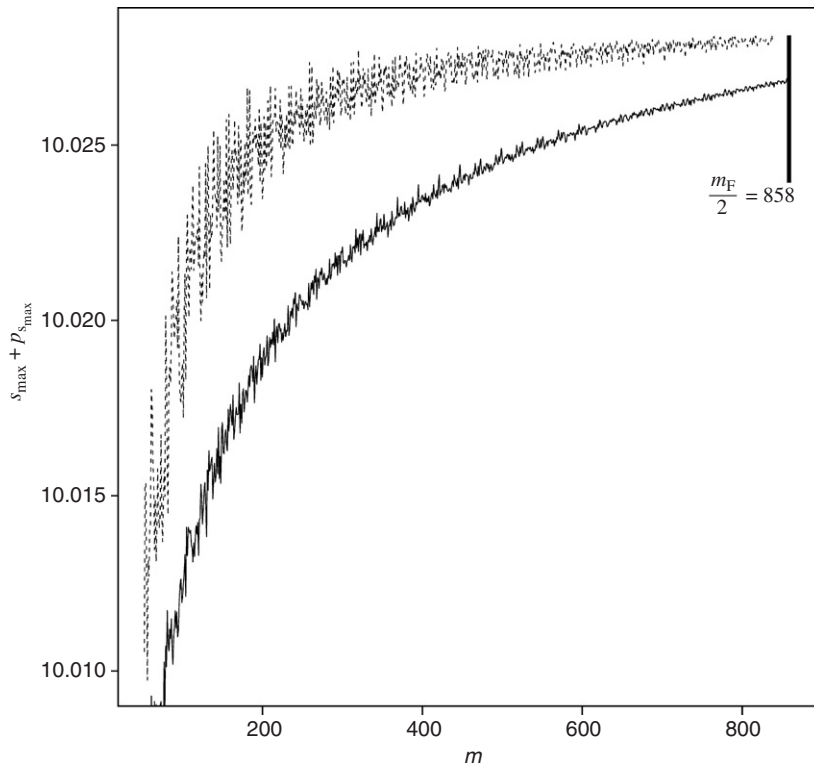


Fig. 2. A plot of $s_{\max} + p_{s_{\max}}$ versus number of factors m for $E(s^2)$ -optimal SSDs with $N = 14$ runs. Dashed line connects the design characteristic of SSDs found via RSR; solid line via SRS_4 .

- (5) GOTO Step (3) until no further reduction in $f^4([X_0 : X])$ is possible.
- (6) If $[X_0 : X]$ has aliased columns, GOTO Step (1); else, return $[X_0 : X]$.

Output: An N run, $m + q(N - 1)$ factor $E(s^2)$ -optimal SSD.

To efficiently implement algorithm RS_4 , there are several issues to consider. For example, evaluation of $f^4([X_0 : X])$ is never needed, and Step 2 is the only step requiring matrix multiplication. The updating formulas of Nguyen (1996) efficiently update $[X_0 : X]^T [X_0 : X]$ from which $\Delta f^4(X_0, X, i, j)$ is calculated. These updating formulas drastically reduce computation time. Given all initial designs with N runs, the algorithm sequential row swap 4 (SRS_4) below calls algorithm RS_4 to construct an $E(s^2)$ -optimal SSD for each case with N runs using Theorems 6 and 7.

Algorithm 4 (SRS_4). Inputs: X_0, X , and θ as defined in Algorithm 2.

- (1) Initialize $i = 1$.
- (2) Compute X_i using algorithm RS_4 with inputs X_{i-1} and X .
- (3) Increment $i = i + 1$, and repeat the last step if $i \leq \theta$.

Output: Same output as Algorithm 2.

To assess the gain of optimizing (i.e., SRS_4) over a random search (i.e., RSR), the best SSDs found with NOA_k algorithms for $N = 14$ and 16 runs (with the exception of the $N = 14$ and $m = 16$ case) were used as initial designs, and RSR and SRS_4 were run on the processor mentioned earlier. When $N = 14$, RSR and SRS_4 concatenate an initial design having 26 columns to an $E(s^2)$ -optimal SSD to produce another $E(s^2)$ -optimal SSD, so RSR and SRS_4 each consist of 26 sequences of $E(s^2)$ -optimal SSDs. Each SRS_4 sequence finished in less than 12 CPU hours. All but one of the RSR sequences, on the other hand, did not finish after a 2 day CPU limit. Fig. 2 is a plot of $s_{\max} + p_{s_{\max}}$ against

m for $E(s^2)$ -optimal SSDs found via algorithms RSR and SRS_4 . The proportion $p_{s_{\max}}$ was about 0.005 higher for RSR, and, more importantly, RSR could not find $E(s^2)$ -optimal SSDs for most $820 < m \leq 858$. SRS_4 found all $E(s^2)$ -optimal SSDs up to $m_F/2 = 858$.

A plot similar to that in Fig. 2 was constructed when $N = 16$, but was not included as the results were similar. The function $s_{\max} + p_{s_{\max}}$ was uniformly lower for SRS_4 compared to RSR, and all (none) of the 15 SRS_4 (RSR) sequences finished up to $m_F/2 = 3217$ within 12 CPU hours.

4. SSDs based on balanced incomplete block designs

When m is a multiple of $N - 1$, Bulutoglu and Cheng (2004) presented a method based on balanced incomplete block designs for constructing $E(s^2)$ -optimal SSDs. Bulutoglu (2006) generalized theorems in Bulutoglu and Cheng (2004) and provided a method for finding the set of all m for which the construction of Bulutoglu and Cheng (2004) yields an $E(s^2)$ -optimal SSD. Table 3 lists $E(s^2)$ -optimal SSDs with the best minimax properties found by NOA_k algorithms, constructed by Bulutoglu and Cheng (2004, Theorem 2.2) or Bulutoglu (2006, Remark 1), and constructed by Bulutoglu and Cheng (2004, Theorem 2.3) or Bulutoglu (2006, Remark 2). The letter h denotes that a design was constructed by the second part of Remark 1 of Bulutoglu (2006) or by applying Bulutoglu (2006, Remark 2) to two designs constructed by the second part of Remark 1 of Bulutoglu (2006). The designs needed to compute the last two sets of columns in Table 3 were constructed using GAP (The GAP Group, 2002).

The NOA_k columns in Table 3 have missing values for two reasons. First, the number of SSDs increases with increased N or m making a search more difficult. Second, (as observed in Section 3.1) increased k tends to restrict the search to designs having small s_{\max} . Although a design with a small s_{\max} can be $E(s^2)$ -optimal, there is no guarantee that this has to be the case as designs with small s_{\max} may have too many non-zero entries in $X^T X$ to be $E(s^2)$ -optimal. Unfortunately, with increased N or m , there is a breaking point after which NOA_k did not find optimal SSDs in a reasonably short span of time. However, NOA_k found optimal SSDs for all (or most) consecutive cases up to this breaking point (which depends on k and corresponds to smaller values of N with increased k).

The $E(s^2)$ -optimal SSDs reported in Table 3 found by NOA_8 have better minimax properties than those constructed theoretically. By Bulutoglu (2006, Theorem 6), the $E(s^2)$ -optimal SSDs constructed by Bulutoglu and Cheng (2004, Theorem 2.2) or Bulutoglu (2006, Remark 1) have a structure. SSDs having this structure may not have the best minimax properties. This helps provide an explanation of the pattern in Table 3 as SSDs found via NOA_8 do not necessarily have this structure. Nonetheless, the theoretically constructed SSDs reported in Table 3 have decent minimax properties.

Bulutoglu and Cheng (2004), Eskridge et al. (2004), Liu and Dean (2004), and Liu and Zhang (2000) constructed $E(s^2)$ -optimal SSDs with $m = q(N - 1)$ (for some positive integer q) by cyclically shifting rows or columns. For $N \leq 14$, we were able to find $E(s^2)$ -optimal, minimax optimal SSDs; see Table 2. For $N \leq 14$, best $E(s^2)$ -optimal SSDs found by NOA_k are better than or at least as good as those constructed by Eskridge et al. (2004), Liu and Dean (2004), and Liu and Zhang (2000) with respect to the minimax criterion. Furthermore, the $E(s^2)$ -optimal SSDs found by NOA_k are equally as good as those that are in this literature only if such SSDs are minimax optimal.

SRS_4 found $E(s^2)$ -optimal SSDs with $m = q(N - 1)$ for even $q \geq 4$ if $N \equiv 2 \pmod{4}$ and for integer $q \geq 2$ if $N \equiv 0 \pmod{4}$. Even though SRS_4 did not find $E(s^2)$ -optimal SSDs with better minimax properties than NOA_k (in cases solved by both), SRS_4 still found $E(s^2)$ -optimal SSDs which are at least as good or better than those reported in the construction literature except when compared to Bulutoglu and Cheng (2004). The input designs for SRS_4 should be obtained from NOA_k if possible; if not, the reader can use the available constructions.

5. Summary

SSD bounds for $E(s^2)$ and s_{\max} were derived. By generalizing the NOA search criterion, algorithms NOA_k were defined. Algorithms NOA_k tend to search a restricted space of SSDs with desirable minimax properties (when k is large). As m is increased, NOA_k algorithms did not quickly find optimal SSDs given our computing capabilities; fortunately, row-swapping algorithms like SRS_4 did. Using algorithms NOA_k and SRS_4 (along with the improved $E(s^2)$ lower bound and Theorem 7), we found an $E(s^2)$ -optimal SSD for each case with $N = 10, 12, 14$, and 16 runs (except the $N = 14, m = 16$ case and its complement). This is a large number of cases—8685 in all—suggesting that

Table 3
 Properties of $E(s^2)$ -optimal SSDs constructed by NOA_k algorithms, Theorems 2.2 and 2.3 of Bulutoglu and Cheng (2004), and Remarks 1 and 2 of Bulutoglu (2006)

N	m	$E(s^2)$	NOA_2		NOA_4		NOA_8		Bulutoglu and Cheng (2004, Thm. 2.2) or Bulutoglu (2006, R1)			Bulutoglu and Cheng (2004, Thm. 2.3) or Bulutoglu (2006, R2)		
			s_{max}	$f_{s_{max}}$	s_{max}	$f_{s_{max}}$	s_{max}	$f_{s_{max}}$	s_{max}	$f_{s_{max}}$	h	s_{max}	$f_{s_{max}}$	h
10	18	5.8824	6	9	6	9	6	9	6	9		—	—	
10	36	8.5714	6	90	6	90	6	90	6	90	h	—	—	
10	72	9.8592	6	468	6	468	6	468	6	468		—	—	
12	22	6.8571	4	99	4	99	4	99	8	11		—	—	
12	55	10.6667	8	53	4	990	4	990	4	990	h	—	—	
12	66	11.0769	8	96	4	1485	4	1485	—	—		8	55	h
12	110	11.8899	8	372	8	273	8	270	8	275		8	275	
12	132	12.0916	—	—	8	396	8	396	—	—		8	396	
12	220	12.4932	—	—	—	—	8	1589	—	—		8	1650	
14	13	4.0000	2	78	2	78	2	78	—	—		—	—	
14	26	7.8400	6	39	6	39	6	39	6	39	h	—	—	
14	52	11.5294	10	9	6	312	6	312	10	26		—	—	
14	78	12.7273	10	35	—	—	—	—	6	819	h	10	39	
14	104	13.3204	10	91	—	—	—	—	—	—		6	1560	h
14	130	13.6744	10	165	—	—	—	—	—	—		10	65	
14	156	13.9097	10	263	—	—	—	—	10	156		10	52	
14	182	14.0774	—	—	—	—	—	—	—	—		10	325	
14	208	14.2029	—	—	—	—	—	—	—	—		10	260	
14	234	14.3004	—	—	—	—	—	—	—	—		10	351	
14	312	14.4952	—	—	—	—	—	—	—	—		10	858	
18	34	9.8182	—	—	—	—	—	—	14	17		—	—	
18	68	14.5075	—	—	—	—	—	—	14	34		—	—	
18	102	16.0396	—	—	—	—	—	—	—	—		14	51	
18	136	16.8000	—	—	—	—	—	—	6	3672	h	—	—	
18	170	17.2544	—	—	—	—	—	—	—	—		14	17	
18	204	17.5567	—	—	—	—	—	—	—	—		14	34	
18	272	17.9336	—	—	—	—	—	—	10	1496		10	1054	h
18	306	18.0590	—	—	—	—	—	—	—	—		14	17	
18	340	18.1593	—	—	—	—	—	—	—	—		14	34	
18	408	18.3100	—	—	—	—	—	—	—	—		10	3400	
18	544	18.4972	—	—	—	—	—	—	—	—		10	7072	
20	38	10.8108	—	—	—	—	—	—	16	19		—	—	
20	57	14.2857	—	—	—	—	—	—	8	95	h	—	—	
20	76	16.0000	—	—	—	—	—	—	—	—		8	304	h
20	114	17.6991	—	—	—	—	—	—	8	1083		8	1083	h
20	171	18.8235	—	—	—	—	—	—	8	1710	h	—	—	
20	190	19.0476	—	—	—	—	—	—	—	—		8	2394	h
20	228	19.3833	—	—	—	—	—	—	—	—		12	57	h
20	342	19.9414	—	—	—	—	—	—	12	513		12	171	h

the improved lower bound for $E(s^2)$ is close to the largest lower bound for general N and m . The bounds for s_{max} proved that 246 cases were also minimax optimal. $E(s^2)$ -optimal SSDs found via NOA_k algorithmic search were also compared to $E(s^2)$ -optimal SSDs obtained via available construction methods using the minimax criterion. The best $E(s^2)$ -optimal SSD found with algorithms NOA_k was typically better than that found via theoretical construction. In addition, available constructions do not apply to all N and m , while the algorithms do not have this shortcoming. On the other hand, NOA_k were ineffective at finding $E(s^2)$ -optimal SSDs in most $N \geq 18$ cases (assuming that the Theorem 1 bounds are achievable).

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