E(s^2)-Optimal Supersaturated Designs with Good Minimax Properties

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Outline

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  - E(s^2) Criterion
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- Lower Bounds for E(s^2) and s_{max}
- Isomorphic SSDs and E(s^2)-Optimal SSDs via Complements
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  - Row Swapping Algorithms (RSR, RS$_4$)
- SSD Search Results and Discussion

Definitions: SSDs

- A *two-level supersaturated design* (SSD) with N runs and m factors is a factorial design and is represented by an $N \times m$ matrix $\boldsymbol{X}$, where

  $N < m$,

  all entries of $\boldsymbol{X}$ are ± 1,

  every column of $\boldsymbol{X}$ has an equal number of $+1$s and -1s, and

  no pair of columns of $\boldsymbol{X}$ have a dot product of $\pm N$.

Definitions (cont.): SSD Optimality Criteria Booth and Cox (1962)

- The $\mathsf{E}(s^2)$ value of SSD $\boldsymbol{X}$ is

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

where s_{ij} is the $(i,\, j)$th entry of $\boldsymbol{X}^T\boldsymbol{X}$.

- The *minimax criterion* orders SSDs by

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

and then by

$$f_{s_{\mathsf{max}}} = \sum_{i<j} \mathrm{I}_{s_{\mathsf{max}}}(|s_{ij}|).$$

Lower Bounds for E(s^2) and s_{max}

- **Ryan and Bulutoglu (2006) Theorem 1:** Improved the Bulutoglu and Cheng (2004) lower bound for E(s^2) when $N \equiv 2 \pmod 4$; see handout.
  - When $N \equiv 2 \pmod 4$, $s_{ij} \equiv 2 \pmod 4$. The old bound was improved to account for this.

- **Ryan and Bulutoglu (2006) Theorem 2:** Let $\boldsymbol{X}$ be an N run, m factor E(s^2)-optimal SSD.
  - If $N \equiv 0 \pmod 4$ and $s_{\text{max}} = 4$, then $\boldsymbol{X}$ is minimax optimal.
  - If $N \equiv 2 \pmod 4$ and $s_{\text{max}} \in \{2, 6\}$, then $\boldsymbol{X}$ is minimax optimal.

Isomorphic SSDs

Two SSDs are *isomorphic* if one can be obtained from the other by

- permuting rows and/or
- permuting columns and/or
- multiplying a subset of columns by -1.

Isomorphic SSDs have the same $\mathrm{E}(s^2)$ value and minimax properties ($s_{\max}$, $f_{s_{\max}}$).

E(s^2)-Optimal SSDs via Complements

Ryan and Bulutoglu (2006) Theorem 4: Let $\boldsymbol{X}_F$ be the SSD with N runs and $m_F := \binom{N-1}{N/2-1}$ factors, let $\boldsymbol{X}$ be an E(s^2)-optimal SSD with N runs and m factors satisfying

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

and let the columns of $\boldsymbol{X}_c$ be the columns of $\boldsymbol{X}_F$ that are not aliased with any column of $\boldsymbol{X}$. Then $\boldsymbol{X}_c$ is an E(s^2)-optimal design with N runs and m_F factors.

A proof uses the following identity which holds for any SSD $\boldsymbol{X}$:

$$\mathrm{SS}(\boldsymbol{X}^T\boldsymbol{X}) = \mathrm{tr}[\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{X}] = \mathrm{tr}[\boldsymbol{X}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{X}^T] = \mathrm{SS}(\boldsymbol{X}\boldsymbol{X}^T),$$

where SS($\cdot$) is the sum of squared entries. Hence, E(s^2) $=$ $(\mathrm{SS}(\boldsymbol{X}^T\boldsymbol{X}) - mN^2)/(m(m-1))$ is minimized if and only if SS($\boldsymbol{X}\boldsymbol{X}^T$) is minimized.

Proof of Ryan and Bulutoglu (2006) Theorem 4

Start by finding the form of $\boldsymbol{X}_F\boldsymbol{X}_F^T$. WLOG, assume that the first row of $\boldsymbol{X}_F$ is all $+1$s and that the second row is all $+1$s up to a point followed by -1s thereafter. 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. Thus, the full SSD satisfies

$$\boldsymbol{X}_F\boldsymbol{X}_F^T = (m_F + q)\boldsymbol{I}_N - q\boldsymbol{J}_N,$$

where $q = \binom{N-2}{N/2-1} - \binom{N-2}{N/2-2} = m_F/(N-1)$, $\boldsymbol{I}_N$ is an $N \times N$ identity matrix, and $\boldsymbol{J}_N$ is an $N \times N$ matrix of $+1$s.

Theorem 4 Proof (cont.)

Because

$$\begin{aligned} \boldsymbol{X}_F \boldsymbol{X}_F^T &= \boldsymbol{X}\boldsymbol{X}^T + \boldsymbol{X}_c \boldsymbol{X}_c^T, \\ \boldsymbol{X}_c \boldsymbol{X}_c^T &= -\boldsymbol{X}\boldsymbol{X}^T + [(m_F + q)\boldsymbol{I}_N - q\boldsymbol{J}_N]. \end{aligned}$$

Since all columns of $\boldsymbol{X}$ sum to 0, all rows of $\boldsymbol{X}\boldsymbol{X}^T$ sum to 0. Therefore,

$$\text{SS}(\boldsymbol{X}_c \boldsymbol{X}_c^T) = \text{SS}(\boldsymbol{X}\boldsymbol{X}^T) + N(m_F + q)^2 + N^2 q^2 - 2N(m_F + q)(m + q). \square$$

Search Algorithms: NOA$_k$

Nguyen (1996) near orthogonal array (NOA) algorithm.

- Exchange algorithm that finds a local E(s^2)-optimal SSD from a random starting SSD.
- Use Theorem 1 lower bound to prove E(s^2)-optimality.
- To promote numerical efficiency, compute $\boldsymbol{X}^T\boldsymbol{X}$ below the diagonal and use $\boldsymbol{X}^T\boldsymbol{X}$ updating formulas by Nguyen (1996).

NOA$_k$ algorithm, a generalization of NOA, uses criteria

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

for some fixed $k \in \mathbb{R}$. (NOA and NOA$_2$ are the same algorithm.)

Search Algorithms: Row Swapping

- Butler *et al.* (2001): Sufficient condition when concatenating columns of E(s^2)-optimal SSDs yields E(s^2)-optimal design

$$\boldsymbol{X}_1 = [\boldsymbol{X}_0 : \boldsymbol{X}].$$

- **Ryan and Bulutoglu (2006):** Permute the rows of $\boldsymbol{X}$ so $\boldsymbol{X}_1$ is an E(s^2)-optimal SSD, i.e., $s_{\max} < N$.
  - Row Swap Random (RSR) randomly permutes rows of $\boldsymbol{X}$.
  - Row Swap 4 (RS_4) starts with a random permutation of $\boldsymbol{X}$'s rows and then optimizes $f^4(\boldsymbol{X}_1)$ with further row swapping of $\boldsymbol{X}$.

- E(s^2)-optimal SSDs for $m > m_F/2$ can be constructed by taking complements if one has E(s^2)-optimal designs for $m \leq m_F/2$.

Search Algorithms: Combined

To get an N run, E(s^2)-optimal SSD for each m, do the following.

1. Use NOA_2 and NOA_4 to get initial designs for small

   $m < 2(N-1)$ if $N \equiv 0 \pmod 4$ or

   $m < 4(N-1)$ if $N \equiv 2 \pmod 4$.

2. Use RSR or RS_4 with the initial designs for medium m.

3. Take complements for remaining large $m > m_F/2$ cases.

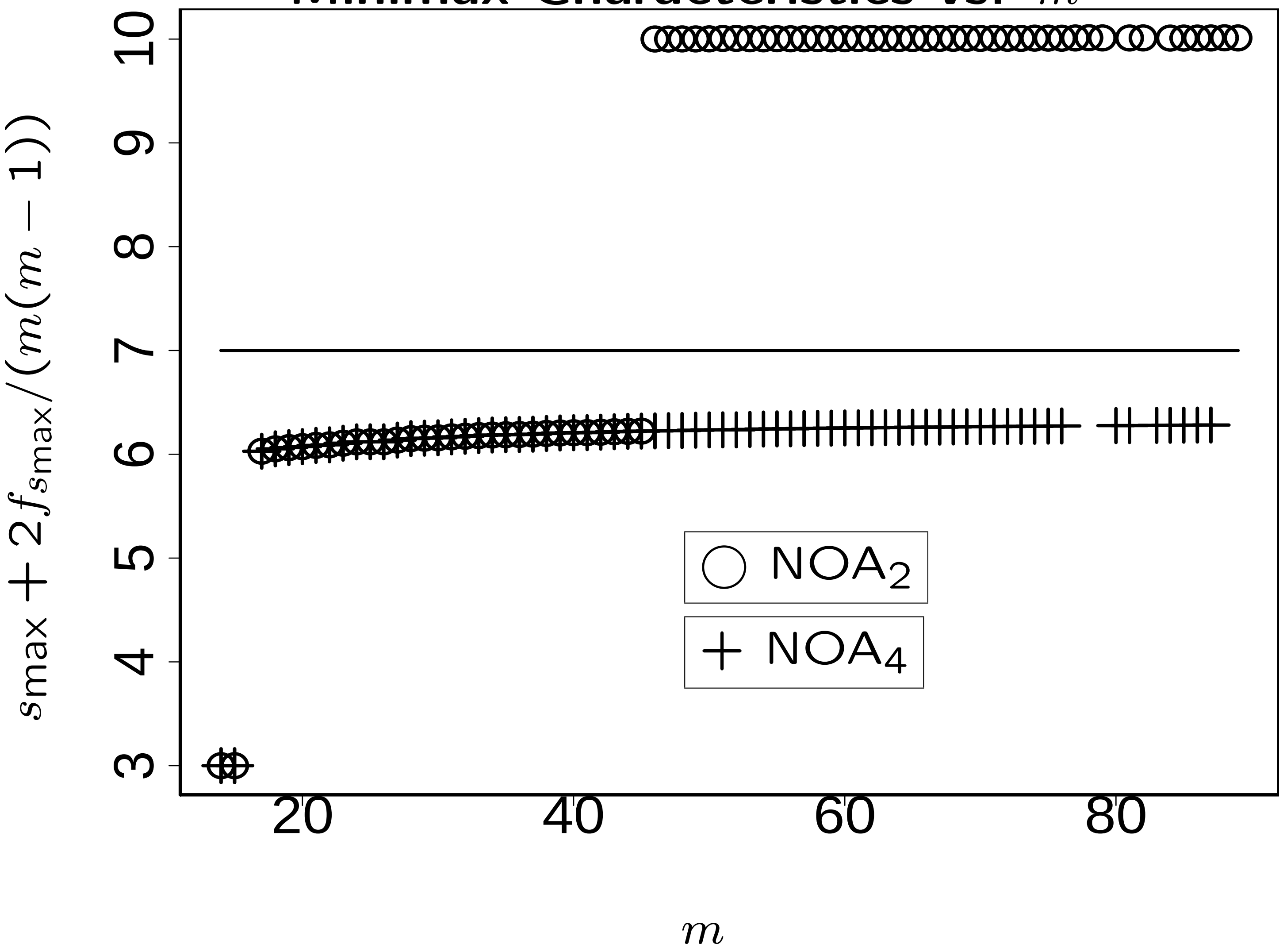
SSD Search Results

- Combined algorithm found an E(s^2)-optimal SSD with $N = 10$, 12, 14, and 16 runs for each m (except the $N = 14$, $m = 16$ case)–8,686 cases in all.

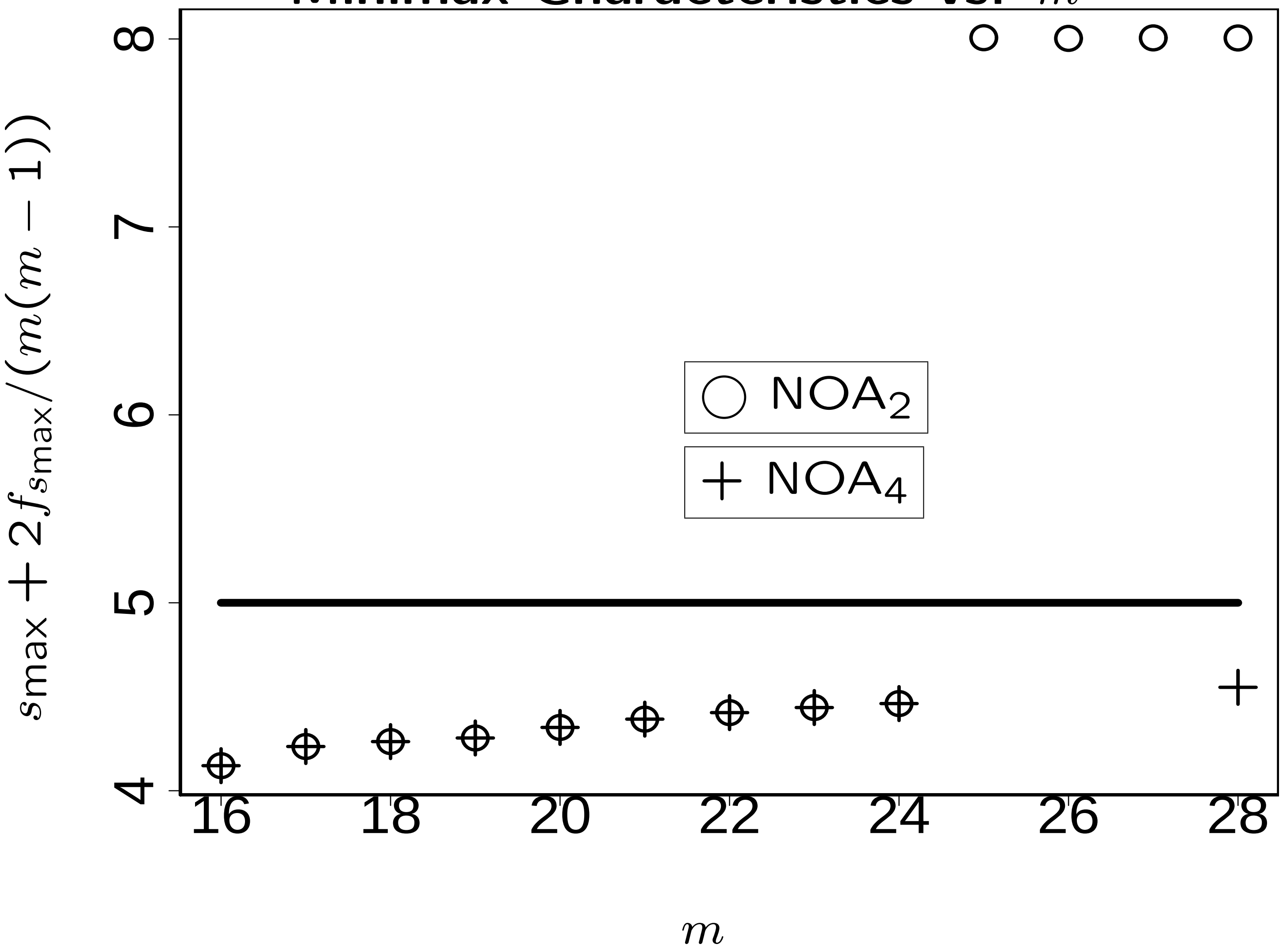
- NOA_2, NOA_4, and NOA_8 found E(s^2)-optimal, minimax optimal designs for the following cases.

N	m
10	10-126 (All cases)
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

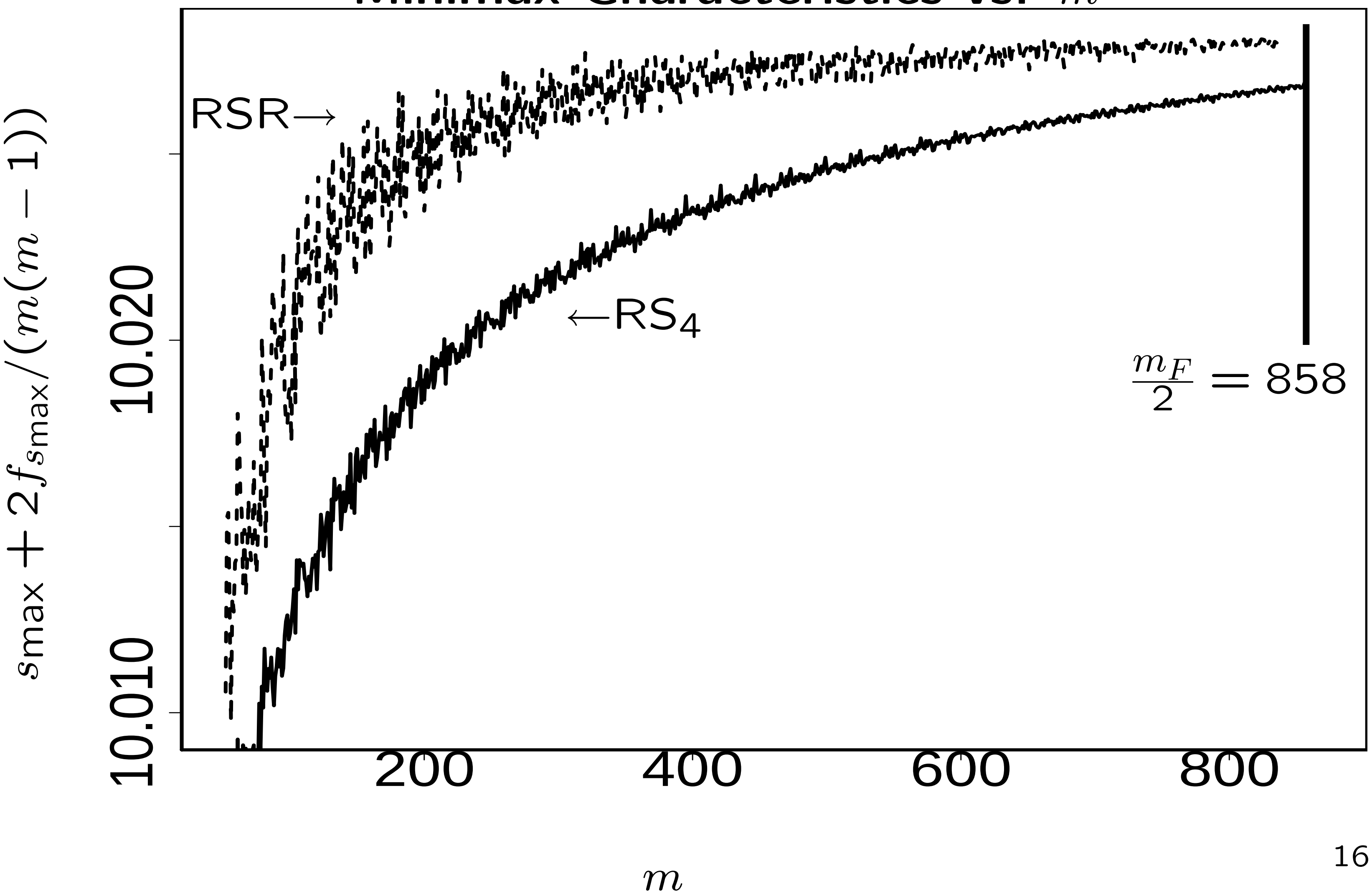
E(s^2)-Optimal SSDs with $N = 14$ Runs
Minimax Characteristics vs. m



E(s^2)-Optimal SSDs with $N = 16$ Runs
Minimax Characteristics vs. m



E(s^2)-Optimal SSDs with $N = 14$ Runs
Minimax Characteristics vs. m



Discussion

- Applications of SSDs
  - Factor Screening Experiments
  - Simple Balance Incomplete Block Designs (BIBDs)

- Why study SSDs for all m such that

$$N < m \le \binom{N-1}{N/2-2} =: m_F$$

  as SSDs with very large $m \approx m_F$ don't appear practical?
  - Theoretical Importance: Testing the bound in the Theorem 1 handout is a fundamental question.
  - Practical Importance: Complements provide an alternative way of constructing optimal SSDs with small m (and can provide a method of bound improvement).