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Non-Uniqueness of $E(s^2)$-Optimal Supersaturated Designs for $N \equiv 2 \pmod 4$ Runs with Application to the Case $N = 10$ Runs

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Abstract *In factor screening experiments with limited resources, it is common for practitioners to cut down the number of runs N and choose a supersaturated design for the experiment. In the past two decades,* $E(s^2)$*-optimality has been one of the most important criteria used to choose a supersaturated design. We show that the definition* $E(s^2)$*-optimal supersaturated designs X for* $N \equiv 2 \pmod 4$ *runs and* $m \geq N$ *factors are not unique by showing that* $XX^\top$ *allows for multiple non-isomorphic possibilities for most values of m. For* $N = 10$ *and* $12 \leq m \leq 114$ *we list all possible* $E(s^2)$*-optimal designs.*

Keywords: *Supersaturated designs,* $E(s^2)$*-optimal, Gauss-Dantzig Selector, experiments.*

1. Introduction

Supersaturated designs have gained substantial interest in the last two decades due to their ability to accommodate many more factors than saturated designs in factor screening experiments. Under the sparsity of effect principle, the experimenter may cut down the number of runs required to run a regular fractional factorial design by choosing to run a saturated design. A saturated design may be cost and time saving because it requires as many runs as factors for the experiment (see Domagni et al.

It is often easier to calculate the sum of the squares of the off-diagonal elements of $XX^\top = (t_{ij})$ instead. Since

$$\sum_{1 \leq i,j \leq m} s_{ij}^2 = \operatorname{trace} X^\top X X^\top X = \operatorname{trace} XX^\top XX^\top = \sum_{1 \leq i,j \leq N} t_{ij}^2, \tag{1}$$

$s_{ii} = m$ and $t_{ii} = N$, it follows that

$$\sum_{i \neq j} s_{ij}^2 = \sum_{i \neq j} t_{ij}^2 + mN(m-N). \tag{2}$$

Thus minimizing $\sum_{i \neq j} t_{ij}^2$ is equivalent to minimizing $\sum_{i \neq j} s_{ij}^2$.

In

2. A first example of non-isomorphic $E(s^2)$-optimal supersaturated designs

We begin this section by giving some preliminary definitions and properties

Definition 1. Two supersaturated designs X_1 and $X_2 \in \operatorname{ssd}(m,N)$ are said to be isomorphic if X_2 can be obtained by performing a series of any of these three operations on X_1.

1. Permute any two rows of the matrix X_1.

2. Permute any two columns of X_1.

3. Multiply any column of X_1 by -1.

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Recall that a permutation matrix P is a binary square matrix with each line (column or row) contains exactly one 1 and all other entries are 0. Permuting the rows of X_1 is equivalent to pre-multiplying X_1 by the appropriate permutation matrix P. Likewise, permuting the columns of X_1 and multiplying some columns of X_1 by -1 is equivalent to post-multiplying the matrix X_1 by the appropriate matrix Q, where Q is a permutation matrix where some of the non-zero entries may be -1 depending on which columns need to be multiplied by -1. Note that P has dimension N while Q has dimension m.

It follows that two supersaturated designs X_1 and $X_2 \in \mathrm{ssd}(m,N)$ are isomorphic if there exists two matrices P and Q such that $X_2 = PX_1Q$, where P is a permutation matrix and Q is a permutation matrix where the non-zero entries are 1 or -1.

The proof of the next proposition follows directly from the fact that $X_2 = PX_1Q$.

Proposition 2.1. *Suppose X_1 and X_2 are isomorphic, i.e., $X_2 = PX_1Q$, then*

$$X_2X_2^\top = PX_1X_1^\top P^\top \textit{ and } X_2^\top X_2 = Q^\top X_1^\top X_1 Q.$$

The entries of the matrix XX^T are the inner products of the rows of X while the entries of $X^\top X$ are the inner products of the columns of X.

Definition 2. Suppose $X \in \mathrm{ssd}(m,N)$ is a supersaturated designs. We say that

1. $XX^\top$ is the row Gram matrix of X and
2. $X^\top X$ is the column Gram matrix of X.

Not that if $X \in \mathrm{ssd}(m,N)$ we can always find a diagonal $\{\pm 1\}$-matrix Q such that all the entries of the first row of XQ are 1. We call such a supersaturated design normalized.

Definition 3. Suppose $X_1, X_2 \in \mathrm{ssd}(m,N)$ are two normalized supersaturated designs. We say that X_1 and X_2 are Gram isomorphic if there exist permutation matrices P and Q such that

$$X_2X_2^\top = PX_1X_1^\top P^\top \text{ and } X_2^\top X_2 = Q^\top X_1^\top X_1 Q.$$

For permutation matrices P and Q we have $P^\top = P^{-1}$ and $Q^\top = Q^{-1}$. Hence we have the following proposition.

Proposition 2.2. *Suppose $X \in ssd(m,N)$ is a normalized supersaturated design. If P is permutation matrix of dimension N and Q is a permutation matrix of dimension m, then $(PXQ)^\top(PXQ) = Q^\top X^\top XQ$ and $(PXQ)(PXQ)^\top = PXX^\top P^\top$.*

It follows immediately that if two normalized supersaturated designs $X_1, X_2 \in \mathrm{ssd}(m,N)$ are isomorphic then they are Gram isomorphic. We will use the converse to show now that there are four non-isomorphic supersaturated designs $X_1, X_2, X_3, X_4 \in \mathrm{ssd}(13,10)$ that pairwise non-isomorphic.

Consider the four normalized supersaturated designs in $\mathrm{ssd}(13,10)$.

$$X_{13,1} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix}$$

$$X_{13,2} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \end{bmatrix}$$

$$X_{13,3} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 \\ -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \end{bmatrix}$$

$$X_{13,4} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 \\ -1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}$$

They are indeed $E(s^2)$-optimal and, up to isomorphism, are the only $E(s^2)$-optimal designs in $\mathrm{ssd}(13,10)$, which follows from Proposition 3.5 below. Their row Gram matrices are

$$X_{13,1}X_{13,1}^{\top} = \left(\begin{array}{ccccc|ccccc} 13 & -3 & -3 & -3 & -3 & 3 & -1 & -1 & -1 & -1 \\ -3 & 13 & 1 & -3 & -3 & -1 & -1 & -1 & -1 & -1 \\ -3 & 1 & 13 & -3 & -3 & -1 & -1 & -1 & -1 & -1 \\ -3 & -3 & -3 & 13 & 1 & -1 & -1 & -1 & -1 & -1 \\ -3 & -3 & -3 & 1 & 13 & -1 & -1 & -1 & -1 & -1 \\ \hline 3 & -1 & -1 & -1 & -1 & 13 & -3 & -3 & -3 & -3 \\ -1 & -1 & -1 & -1 & -1 & -3 & 13 & 1 & -3 & -3 \\ -1 & -1 & -1 & -1 & -1 & -3 & 1 & 13 & -3 & -3 \\ -1 & -1 & -1 & -1 & -1 & -3 & -3 & -3 & 13 & 1 \\ -1 & -1 & -1 & -1 & -1 & -3 & -3 & -3 & 1 & 13 \end{array}\right),$$

$$X_{13,2}X_{13,2}^{\top} = \left(\begin{array}{ccccc|ccccc}
13 & -3 & -3 & 1 & 1 & -5 & -1 & -1 & -1 & -1 \\
-3 & 13 & 1 & -3 & -3 & -1 & -1 & -1 & -1 & -1 \\
-3 & 1 & 13 & -3 & -3 & -1 & -1 & -1 & -1 & -1 \\
1 & -3 & -3 & 13 & -3 & -1 & -1 & -1 & -1 & -1 \\
1 & -3 & -3 & -3 & 13 & -1 & -1 & -1 & -1 & -1 \\
\hline
-5 & -1 & -1 & -1 & -1 & 13 & 1 & -3 & 1 & -3 \\
-1 & -1 & -1 & -1 & -1 & 1 & 13 & -3 & -3 & -3 \\
-1 & -1 & -1 & -1 & -1 & -3 & -3 & 13 & -3 & 1 \\
-1 & -1 & -1 & -1 & -1 & 1 & -3 & -3 & 13 & -3 \\
-1 & -1 & -1 & -1 & -1 & -3 & -3 & 1 & -3 & 13
\end{array}\right),$$

$$X_{13,3}X_{13,3}^{\top} = \left(\begin{array}{ccccccc|ccc}
13 & 1 & -3 & -3 & -3 & -3 & 1 & -1 & -1 & -1 \\
1 & 13 & 1 & -3 & -3 & -3 & -3 & -1 & -1 & -1 \\
-3 & 1 & 13 & 1 & -3 & -3 & -3 & -1 & -1 & -1 \\
-3 & -3 & 1 & 13 & 1 & -3 & -3 & -1 & -1 & -1 \\
-3 & -3 & -3 & 1 & 13 & 1 & -3 & -1 & -1 & -1 \\
-3 & -3 & -3 & -3 & 1 & 13 & 1 & -1 & -1 & -1 \\
1 & -3 & -3 & -3 & -3 & 1 & 13 & -1 & -1 & -1 \\
\hline
-1 & -1 & -1 & -1 & -1 & -1 & -1 & 13 & -3 & -3 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1 & -3 & 13 & -3 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1 & -3 & -3 & 13
\end{array}\right),$$

$$X_{13,4}X_{13,4}^{\top} = \left(\begin{array}{ccc|ccccccc}
13 & -3 & -3 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-3 & 13 & -3 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-3 & -3 & 13 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
\hline
-1 & -1 & -1 & 13 & 1 & 1 & -3 & -3 & -3 & -3 \\
-1 & -1 & -1 & 1 & 13 & 1 & -3 & -3 & -3 & -3 \\
-1 & -1 & -1 & 1 & 1 & 13 & -3 & -3 & -3 & -3 \\
-1 & -1 & -1 & -3 & -3 & -3 & 13 & 1 & -3 & 1 \\
-1 & -1 & -1 & -3 & -3 & -3 & 1 & 13 & 1 & -3 \\
-1 & -1 & -1 & -3 & -3 & -3 & -3 & 1 & 13 & 1 \\
-1 & -1 & -1 & -3 & -3 & -3 & 1 & -3 & 1 & 13
\end{array}\right).$$

We first observe that if two normalized supersaturated designs $X_1, X_2 \in \mathrm{ssd}(m,N)$ are isomorphic then the multiset of entries of their row Gram matrices are equal and the multisets of the entries of their column Gram matrices are equal.

Note that 3 is an off-diagonal entry of $X_{13,1}X_{13,1}^{\top}$ but not an off-diagonal entry of the remaining three Gram matrices. This show that $X_{13,1}$ and $X_{13,2}$ are non-isomorphic, $X_{13,1}$ and $X_{13,3}$ are non-isomorphic, and $X_{13,1}$ and $X_{13,4}$ are non-isomorphic.

Likewise, $X_{13,2}$ is not isomorphic to the other three supersaturated designs since $X_{13,2}X_{13,2}^{\top}$ has an off-diagonal entry equal to -5 while none of the other designs have such an entry.

On the other hand, the multisets of entries of $X_{13,3}X_{13,3}^{\top}$ and $X_{13,4}X_{14,4}^{\top}$ are in fact equal. To show that $X_{13,3}$ and $X_{14,4}$ are not isomorphic we consider their column Gram matrices

$$X_{13,3}^\top X_{13,3} = \begin{pmatrix} 10 & 2 & 6 & 2 & -2 & 2 & -2 & 2 & -2 & -2 & 2 & -2 & -2 \\ 2 & 10 & 2 & 2 & 2 & -2 & 2 & -2 & 2 & -2 & 2 & -2 & -2 \\ 6 & 2 & 10 & -2 & 2 & 2 & 2 & 2 & -2 & -2 & -2 & -2 & 2 \\ 2 & 2 & -2 & 10 & 2 & 2 & 2 & 2 & 2 & -2 & 2 & -2 & 2 \\ -2 & 2 & 2 & 2 & 10 & 2 & 2 & 2 & -2 & 2 & -2 & 2 & 2 \\ 2 & -2 & 2 & 2 & 2 & 10 & 2 & -2 & 2 & -2 & -2 & 6 & 2 \\ -2 & 2 & 2 & 2 & 2 & 2 & 10 & -2 & 2 & 2 & -2 & -2 & 2 \\ 2 & -2 & 2 & 2 & 2 & -2 & -2 & 10 & 2 & 2 & -2 & -2 & 2 \\ -2 & 2 & -2 & 2 & -2 & 2 & 2 & 2 & 10 & -2 & -2 & 2 & 2 \\ -2 & -2 & -2 & -2 & 2 & -2 & 2 & 2 & -2 & 10 & 2 & 2 & -2 \\ 2 & 2 & -2 & 2 & -2 & -2 & -2 & -2 & -2 & 2 & 10 & 2 & 2 \\ -2 & -2 & -2 & -2 & 2 & 6 & -2 & -2 & 2 & 2 & 2 & 10 & 2 \\ -2 & -2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & -2 & 2 & 2 & 10 \end{pmatrix}$$

and

$$X_{13,4}^\top X_{13,4} = \begin{pmatrix} 10 & 2 & 2 & -2 & -2 & 2 & 2 & -2 & -2 & 2 & -2 & 2 & -2 \\ 2 & 10 & -2 & 2 & 2 & -2 & -2 & -2 & 2 & 2 & 2 & -2 & 2 \\ 2 & -2 & 10 & 2 & 2 & -2 & 2 & -2 & -2 & 2 & 2 & 2 & -2 \\ -2 & 2 & 2 & 10 & 2 & 2 & -2 & 2 & -2 & 2 & -2 & -2 & 2 \\ -2 & 2 & 2 & 2 & 10 & -2 & -2 & 2 & 2 & -6 & 2 & 2 & 2 \\ 2 & -2 & -2 & 2 & -2 & 10 & 2 & 2 & -2 & 2 & 2 & 2 & -2 \\ 2 & -2 & 2 & -2 & -2 & 2 & 10 & -2 & 2 & 2 & 2 & -2 & 2 \\ -2 & -2 & -2 & 2 & 2 & 2 & -2 & 10 & 6 & -2 & -2 & 2 & 2 \\ -2 & 2 & -2 & -2 & 2 & -2 & 2 & 6 & 10 & -2 & 2 & -2 & 2 \\ 2 & 2 & 2 & 2 & -6 & 2 & 2 & -2 & -2 & 10 & 2 & 2 & 2 \\ -2 & 2 & 2 & -2 & 2 & 2 & 2 & -2 & 2 & 2 & 10 & 2 & -2 \\ 2 & -2 & 2 & -2 & 2 & 2 & -2 & 2 & -2 & 2 & 2 & 10 & 2 \\ -2 & 2 & -2 & 2 & 2 & -2 & 2 & 2 & 2 & 2 & -2 & 2 & 10 \end{pmatrix}.$$

We see that $X_{13,4}^\top X_{13,4}$ has an entry equal to -6 while while $X_{13,3}^\top X_{13,3}$ has no such entry. Hence $X_{13,3}$ and $X_{13,4}$ are not isomorphic.

This finishes the proof that the four $E(s^2)$-optimal supersaturated designs $X_{13,1}, X_{13,2}, X_{13,3}, X_{13,4}$ are not isomorphic.

We comment that since for a permutation matrix P we have $P^\top = P^{-1}$ the row (column) Gram matrices of two normalized supersaturated designs are similar and hence have the same eigenvalues. An easy calculation shows that the sets of eigenvalues of the row Gram matrices of $X_{13,1}, X_{13,2}, X_{13,3}, X_{13,4}$ are distinct. This provides an alternative proof that the four designs are not isomorphic. Given the statistical significance of the off-diagonal entries the proof we gave above is more in the spirit of the subject.

In Section 3 we determine all possible structures of the row Gram matrices of $E(s^2)$-optimal supersaturated designs that achieve the best possible lower bound. In Section 4 we show that for $N = 10$ runs and all m all possible row Gram structures are realized by some $E(s^2)$-optimal supersaturated design in $\mathrm{ssd}(m, 10)$.

3. The row Gram structure of $E(s^2)$-optimal supersaturated designs

In this section we derive the structure $XX^\top$ for $E(s^2)$-optimal $X \in \mathrm{ssd}(m, N)$. The lower bounds on $E(s^2)$ proved in

The first result puts constraints on the structure of $XX^\top$. Let $R = (r_{ij}) = XX^\top + 2tJ_N = 2tI_N + P$ when b is even and $R = (r_{ij}) = XX^\top + (2t+1)J_N = 2tI_N + P + J_N$ when b is odd. We state the next result in general but apply it only in the aces $\alpha = 2t$ and $\alpha = 2t+1$.

Lemma 3.1. *Let $X \in ssd(N,m)$. Let $T = (t_{ij}) = XX^\top$ and $R = (r_{ij}) = XX^\top + \alpha J_N$. We have*

1. *$t_{ii} = m$ and $r_{ii} = m + \alpha$ for $1 \le i \le N$,*
2. *$\sum_{i=1}^N t_{ij} = 0$ and $\sum_{j=1}^N r_{ij} = \alpha N$ for $1 \le i \le N$,*
3. *$\sum_{i \ne j} r_{ij} = N((N-1)\alpha - m)$,*
4. *$\sum_{i \ne j} t_{ij}^2 = \sum_{i \ne j} r_{ij}^2 + \alpha N(2m - (N-1)\alpha)$. In particular, $\sum_{i \ne j} t_{ij}^2$ and hence $\sum_{i \ne j} s_{ij}^2$ is minimal if and only if $\sum_{i \ne j} r_{ij}^2$ is minimal.*
5. *There exists a permutation of the rows of X such that*
$$R = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} \tag{3}$$
where A is a $p \times p$ matrix, $p \ge \frac{N}{2}$, C a $(N-p) \times (N-p)$ matrix, all elements of A and C are congruent $m + \alpha$ modulo 4 and all entries of B are congruent $m + \alpha + 2$ modulo 4.
6. *Lastly, with $A = (a_{ij})$, $C = (c_{ij})$ and $B = (b_{ij})$ we have*
$$\sum_{i \ne j} c_{ij} - \sum_{k \ne l} a_{kl} = (m - \alpha(N-1))(2p - N). \tag{4}$$

Define

$$\begin{aligned} f(N,t,b) &= (2t(N-1)+b)N(2t(N-1)+b-N) \\ c(N,t,b) &= 4N(N-1) - 4N(2(N-1)+b) \\ g_0(N,t,b) &= 4Nt(t(N-1)+b) + f(N,t,b) \\ g_1(N,t,b) &= N(2t+1)((N-1)(2t-1)+2b) + f(N,t,b). \end{aligned} \tag{5}$$

Below we minimize $\sum_{i \ne j} t_{ij}^2$. The expressions $f(N,t,b)$ accounts for the added term in Equation(2). The expression $c(n,t,b)$ is used in Proposition 3.7. The expressions $g_0(N,t,b)$ respectively $g_1(N,t,b)$ account for the contribution of the term $2tJ_n$ respectively $(2t+1)J_N$ as in part 4 of Lemma 3.1 plus $f(N,t,b)$.

We start with $b \equiv 2 \pmod 4$, the easiest case.

Proposition 3.2. *Let $b = 4q+2 < N$ and let $X \in ssd(N, 2(N-1)t+b)$, $2 \le b \le N$, $t \ge 1$. Then*

$$\sum_{i \ne j} s_{ij}^2 \ge 2N^2 - 4N + 8 + g_0(N,t,b) \tag{6}$$

Furthermore, equality holds if and only if $XX^\top = 2t(NI_N - J_N) + P$ with

$$P = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} \tag{7}$$

where $A = (b-2)I_{\frac{N}{2}+1} + 2J_{\frac{N}{2}+1} - 4A(G)$, where G is a regular graph of degree $\frac{N+b}{4}$ on $\frac{N}{2}+1$ vertices, $C = (b-2)I_{\frac{N}{2}+1} + 2J_{\frac{N}{2}+1} - 4A(H)$, where H is a regular graph of degree $\frac{N+b-4}{4}$ on $\frac{N}{2}-1$ vertices, while all entries of B are 0.

When $b \equiv 0 \pmod 4$, $0 \leq b < N$, there are 2 cases to consider.

Proposition 3.3. *Let $b = 4q < N$ and let $X \in ssd(N, 2(N-1)t + b)$, $0 \leq b < N$, $t \geq 1$. Then*

1. *for $b \leq \frac{N+2}{2}$ we have*
$$\sum_{i \neq j} s_{ij}^2 \geq 4Nb + g_0(N,t,b) \tag{8}$$
Furthermore, equality holds if and only if
$$P = 4(I_N - A(G)) \tag{9}$$
where G is a regular graph of degree $\frac{b}{4}$ on N vertices.

2. *for $b \geq \frac{N+2}{2}$ we have*
$$\sum_{i \neq j} s_{ij}^2 \geq 2N^2 + 8b - 8 + g_0(N,t,b) + f(N,t,b) \tag{10}$$
Furthermore, equality holds if and only if $p = \frac{N+2}{2}$ and
$$P = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} \tag{11}$$
all entries of B have absolute value 2, A has v, off-diagonal entries equal to -4 and C has $\frac{b}{2} - v$ off-diagonal entries equal to 4 while all other off-diagonal entries of A and C are 0.

Proposition 3.4. *Let $b = 4q + 3 < N$ and let $X \in ssd(N, 2(N-1)t + b)$, $t \geq 1$. Then*

1. *for $b \leq \frac{N}{2}$ we have*
$$\sum_{i \neq j} s_{ij}^2 \geq 2N^2 + g_1(N,t,b) + f(N,t,b). \tag{12}$$
Furthermore, equality holds if and only if $p = \frac{N}{2}$ and
$$P = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} - J_N \tag{13}$$
where all diagonal entries of A and C are equal to $b+1$, all off-diagonal entries of A and C are 0 and all entries of B have absolute value 2 such that the row and column sums of B are equal to $N - b - 1$.

2. *for $b \geq \frac{N}{2}$ we have*
$$\sum_{i \neq j} s_{ij}^2 \geq 4N^2 - 4bN - 4N + 8b + g_1(N,t,b). \tag{14}$$
Furthermore, equality holds if and only if $p = N - 1$ and
$$P = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} - J_N \tag{15}$$
where B has $k = \frac{(3N-2)-(b+1)}{4}$ entries equal to 2 and $N - 1 - k$ entries equal to -2. Assuming
$$B^\top = (\underbrace{-2, \cdots, -2}_{N-1-k}, \underbrace{2, \cdots, 2}_{k}) \tag{16}$$
we have
$$A = (m+1)I_{N-1} + 4A(G) \tag{17}$$
where G is a graph with degree sequence $(d^{(N-1-k)}, (d-1)^{(k)})$ and $d = k - \frac{N-2}{2}$.

Comment: Matrices B as described in the first part of the proof exist by the Gale-Ryser Theorem

Proposition 3.5. *Let* $b = 4q+1 < N$ *and let* $X \in ssd(N, 2(N-1)t+b)$, $t \geq 1$. *Then*

1. *if* q *is even*

$$\sum_{i \neq j} s_{ij}^2 \geq 2N^2 - 4N + g_{2t+1}(N,t,b). \tag{18}$$

Furthermore, equality holds if and only if $p = \frac{N}{2}$ *and*

$$P = \begin{pmatrix} (b+1)I_{\frac{N}{2}} + 2J_{\frac{N}{2}} & 0 \\ 0 & (b+1)I_{\frac{N}{2}} + 2J_{\frac{N}{2}} \end{pmatrix} - 4A(G \cup H) - J_{10} \tag{19}$$

where G *and* H *are (disjoint) regular graphs of degree* q *on* $\frac{N}{2}$ *vertices.*

if q *is odd*

$$\sum_{i \neq j} s_{ij}^2 \geq 2N^2 - 4N + 32 + g_1(N,t,b) + f(N,t,b) \text{ if } q \text{ is odd} \tag{20}$$

Furthermore, equality holds if and only if

a.

$$P = \begin{pmatrix} (b-1)I_{\frac{N}{2}+2} + 2J_{\frac{N}{2}+2} & 0 \\ 0 & (b-1)bI_{\frac{N}{2}-2} + 2J_{\frac{N}{2}-2} \end{pmatrix} - 4A(G \cup H) - J_N \tag{21}$$

where G *is a regular graph of degree* $q+1$ *on* $\frac{N}{2}+2$ *vertices and* H *is a regular graph of degree* $q-1$ *on* $\frac{N-2}{2}$ *vertices; or*

b.

$$P = \begin{pmatrix} (b+3)I_{\frac{N}{2}} - 2J_{\frac{N}{2}} & 0 \\ 0 & (b+3)I_{\frac{N}{2}} - 2J_{\frac{N}{2}} \end{pmatrix} + 4A(G) - J_N \tag{22}$$

where G *is regular graph of degree* $d = \frac{N}{2} - 1 - q$ *on* $v_1, \cdots, v_N$ *such that the induced subgraph* G_1 *on* $v_1, \cdots, v_{\frac{N}{2}}$ *has degree sequence* $(d^{(\frac{N}{2}-1)}, d-1)$ *and the induced subgraph* G_2 *on* $v_{\frac{N}{2}+1}, \cdots, v_N)$ *has degree sequence* $(d-1, d^{(\frac{N}{2}-1)})$. *The graphs* G_1 *and* G_2 *are connected by the edge* $(v_{\frac{N}{2}}, v_{\frac{N}{2}+1})$*; or*

c.

$$P = \begin{pmatrix} (b-1)I_{\frac{N}{2}} + 2J_{\frac{N}{2}} & 0 \\ 0 & b(b-1)I_{\frac{N}{2}} + 2J_{\frac{N}{2}} \end{pmatrix} - 4A(G) - J_N \tag{23}$$

where G *is regular graph of degree* q *on* $v_1, \cdots, v_N$ *such that the induced subgraph* G_1 *on* $v_1, \cdots, v_{\frac{N}{2}}$ *has degree sequence* $(q^{(\frac{N}{2}-1)}, q-1)$ *and the induced subgraph* G_2 *on* $v_{\frac{N}{2}+1}, \cdots, v_N)$ *has degree sequence* $(q-1, q^{(\frac{N}{2}-1)})$. *The graphs* G_1 *and* G_2 *are connected by the edge* $(v_{\frac{N}{2}}, v_{\frac{N}{2}+1})$

We summarize the results of Propositions 3.2, 3.3, 3.4, and 3.5 first for the case b odd and then for the case b even.

Proposition 3.6. *Let* $X \in ssd(N, 2(N-1)t+b)$ *with* $0 \leq b < 2(N-1)$, b *odd, and* $N+2 \leq 2(N-1)+b \leq c(N)-(N+2)$. *Then*

$$\sum_{i \neq j} s_{ij}^2 \geq g_1(N,t,b) + \begin{cases} 2N^2 & \text{if} \quad b \equiv 3 \text{ (mod 4) and } b \leq \frac{N}{2} \text{ or } b \geq \frac{3N}{2} \\ 8(N-1) + (4N-8)|N-1-b| & \text{if} \quad b \equiv 3 \text{ (mod 4) and } \frac{N}{2} \leq b \leq \frac{3N}{2} \\ 2N^2 - 4N & \text{if} \quad b \equiv 1 \text{ (mod 8)} \\ 2N^2 - 4N + 32 & \text{if} \quad b \equiv 5 \text{ (mod 8)} \end{cases}$$

The result for b even follows. The proof for b even and $b \geq N$ is not complete yet and is given below.

Proposition 3.7. *Let* $X \in ssd(N, 2(N-1)t+b)$ *with* $0 \leq b < 2(N-1)$, *b even and* $N+2 \leq 2(N-1)+b \leq c(N)-(N+2)$. *Let* $b' = 2(N-1)-b$. *Then*

$$\sum_{i \neq j} s_{ij}^2 \geq g_0(N,t,b) + \begin{cases} 2N^2-4N+8 & \textit{if} \quad b \equiv 2 \textit{ (mod 4) and } b < N-1 \\ 4Nb' + c(N,t,b) & \textit{if} \quad b \equiv 2 \textit{ (mod 4) and } b \geq \frac{3N-2}{2} \\ 2N^2+8b'-8+c(N,t,b) & \textit{if} \quad b \equiv 2 \textit{ (mod 4) and } N \leq b \leq \frac{3N-2}{2} \\ 4Nb & \textit{if} \quad b \equiv 0 \textit{ (mod 4) and } b \leq \frac{N+2}{2} \\ 2N^2+8b-8 & \textit{if} \quad b \equiv 0 \textit{ (mod 4) and } \frac{N+2}{2} \leq b \leq N \\ 2N^2-4N+8+c(N,t,b) & \textit{if} \quad b \equiv 0 \textit{ (mod 4) and } b \geq N \end{cases}$$

Equality occurs for $b \geq N$ *if an only if*

$$XX^\top = 2t(NJ_N - J_N) + Q = 2t(NI_N - J_N) + 2(NI_N - J_N) - P$$

where P is as described in

1. *Proposition 3.2 when* $b \equiv 0$ *(mod 4),*
2. *Part 1 of Proposition 3.3 when* $b \equiv 2$ *(mod 4) and* $b' \leq \frac{N+2}{2}$,
3. *Part 2 of Proposition 3.3 when* $b \equiv 2$ *(mod 4) and* $b' \geq \frac{N+2}{2}$.

4. The case of $N = 10$ runs

We apply the results of the previous section to the case $N = 10$. We hope this will provide some insight into the complexities of finding all possible structures for $XX^\top$ when X is an $E(s^2)$-optimal supersaturated design for large N.

Corollary 4.1. *If* $X \in ssd(10, 18t+2)$, $t \geq 1$, *with* $\sum_{i \neq j} s_{ij}^2 = 3600t^2 - 1000t + 8$, *then* $XX^\top = 2t(10I_{10} -$

$J_{10}) + P$ with

$$P = \begin{pmatrix} 2 & 2 & 2 & -2 & -2 & -2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 2 & -2 & -2 & -2 & 0 & 0 & 0 & 0 \\ 2 & 2 & 2 & -2 & -2 & -2 & 0 & 0 & 0 & 0 \\ -2 & -2 & -2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\ -2 & -2 & -2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\ -2 & -2 & -2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 2 & 2 \end{pmatrix} \quad \textit{or} \tag{24}$$

$$P = \begin{pmatrix} 2 & 2 & -2 & -2 & -2 & 2 & 0 & 0 & 0 & 0 \\ -2 & 2 & 2 & -2 & 2 & 2 & 0 & 0 & 0 & 0 \\ -2 & -2 & 2 & 2 & 2 & -2 & 0 & 0 & 0 & 0 \\ -2 & -2 & -2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\ 2 & -2 & -2 & -2 & 2 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 2 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 2 & 2 \end{pmatrix}$$

There exist examples that realize these two Gram structures for all $1 \le t \le 7$ which we give in Section 6.

If $X \in ssd(10, 18t+6)$, $t \ge 1$, with $\sum_{i \ne j} s_{ij}^2 = 3600t^2 + 600t - 72$, then $XX^\top = 2t(10I_{10} - J_{10}) + P$ with

$$P = \begin{pmatrix} 6 & 2 & -2 & -2 & -2 & -2 & 0 & 0 & 0 & 0 \\ 2 & 6 & -2 & -2 & -2 & -2 & 0 & 0 & 0 & 0 \\ -2 & -2 & 6 & 2 & -2 & -2 & 0 & 0 & 0 & 0 \\ -2 & -2 & 2 & 6 & -2 & -2 & 0 & 0 & 0 & 0 \\ -2 & -2 & -2 & -2 & 6 & 2 & 0 & 0 & 0 & 0 \\ -2 & -2 & -2 & -2 & 2 & 6 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & -2 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & 6 & -2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 6 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & -2 & 6 \end{pmatrix} \tag{25}$$

In particular, there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for all $1 \le t \le 7$ which we give in Section 6.

If $X \in ssd(10, 18t+10)$, $t \ge 1$, with $\sum_{i \ne j} s_{ij}^2 = 3600t^2 + 2280t + 296$, then $XX^\top = (2t+1)(10I_{10} - J_{10}) - P$ with with P as in Equation (27). There exist examples that realize these four Gram structures for all $1 \le t \le 6$ which we give in Section 6.

If $X \in ssd(10, 18t+14)$, $t \ge 0$, with $\sum_{i \ne j} s_{ij}^2 = 3600t^2 + 4200t + 920$, then $XX^\top = (2t+1)(10I_{10} - J_{10}) - P$ with P as in Equation (26). In particular there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for each $1 \le t \le 6$ which we give in Section 6.

Since $s(X^2) \ge 4$ the bound of Corollary 4.1 does not apply when $m = 10$. In fact, $s(X^2) = 4$ for $E(s^2)$-optimal supersaturated designs $X \in \mathrm{ssd}(10, 10)$.

Corollary 4.2. *If $X \in ssd(10, 18t)$, $t \ge 1$, with $\sum_{i \ne j} s_{ij}^2 = 3600t^2 - 1800t$, then $XX^\top = 2t(10I_{10} - J_{10})$, i.e., $P = 0_N$.*

If $X \in ssd(10, 18t+4)$*,* $t \geq 1$*, with* $\sum_{i \neq j} s_{ij}^2 = 3600t^2 - 200t - 80$*, then* $XX^\top = 2t(10I_{10} - J_{10}) + P$ *with*

$$P = \begin{pmatrix} 4 & -4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -4 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 & -4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & -4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -4 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -4 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & -4 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4 & 4 \end{pmatrix}. \qquad (26)$$

In particular there is up to Gram isomorphism only one $E(s^2)$*-optimal supersaturated design for each* $1 \leq t \leq 7$ *which we give in Section 6.*

If $X \in ssd(10, 18t+8)$*,* $t \geq 1$*, with* $\sum_{i \neq j} s_{ij}^2 = 3600t^2 + 1400t + 96$*, then* $XX^\top = 2t(10I_{10} - J_{10}) + P$

with

$$
\begin{gathered}
P=\left(\begin{array}{cccccc|cccc}
8 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 8 & 0 & 0 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 8 & -4 & 0 & 0 & -2 & -2 & 2 & -2 \\
0 & 0 & -4 & 8 & 0 & 0 & -2 & 2 & -2 & -2 \\
0 & 0 & 0 & 0 & 8 & -4 & 2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & -4 & 8 & -2 & -2 & -2 & 2 \\
\hline
-2 & -2 & -2 & -2 & 2 & -2 & 8 & 0 & 0 & 0 \\
-2 & -2 & -2 & 2 & -2 & -2 & 0 & 8 & 0 & 0 \\
-2 & -2 & 2 & -2 & -2 & -2 & 0 & 0 & 8 & 0 \\
-2 & -2 & -2 & -2 & -2 & 2 & 0 & 0 & 0 & 8
\end{array}\right) \text{ or} \\
P=\left(\begin{array}{cccccc|cccc}
8 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 8 & 0 & 0 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 8 & 0 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 8 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 8 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 0 & 8 & -2 & -2 & -2 & -2 \\
\hline
-2 & -2 & -2 & -2 & -2 & -2 & 8 & 0 & 4 & 0 \\
-2 & -2 & -2 & -2 & -2 & -2 & 0 & 8 & 0 & 4 \\
-2 & -2 & -2 & -2 & -2 & -2 & 4 & 0 & 8 & 0 \\
-2 & -2 & -2 & -2 & -2 & -2 & 0 & 4 & 0 & 8
\end{array}\right) \text{ or} \\
P=\left(\begin{array}{cccccc|cccc}
8 & -4 & 0 & 0 & 0 & 0 & -2 & 2 & -2 & -2 \\
-4 & 8 & 0 & 0 & 0 & 0 & 2 & -2 & -2 & -2 \\
0 & 0 & 8 & 0 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 8 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 8 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 0 & 8 & -2 & -2 & -2 & -2 \\
\hline
-2 & 2 & -2 & -2 & -2 & -2 & 8 & 0 & 0 & 0 \\
2 & -2 & -2 & -2 & -2 & -2 & 0 & 8 & 0 & 0 \\
-2 & -2 & -2 & -2 & -2 & -2 & 0 & 0 & 8 & 4 \\
-2 & -2 & -2 & -2 & -2 & -2 & 0 & 0 & 4 & 8
\end{array}\right) \text{ or} \\
P=\left(\begin{array}{cccccc|cccc}
8 & -4 & -4 & 0 & 0 & 0 & 2 & 2 & -2 & -2 \\
-4 & 8 & 0 & 0 & 0 & 0 & -2 & -2 & -2 & 2 \\
-4 & 0 & 8 & 0 & 0 & 0 & -2 & -2 & 2 & -2 \\
0 & 0 & 0 & 8 & 0 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 8 & 0 & -2 & -2 & -2 & -2 \\
0 & 0 & 0 & 0 & 0 & 8 & -2 & -2 & -2 & -2 \\
\hline
2 & -2 & -2 & -2 & -2 & -2 & 8 & 0 & 0 & 0 \\
2 & -2 & -2 & -2 & -2 & -2 & 0 & 8 & 0 & 0 \\
-2 & -2 & 2 & -2 & -2 & -2 & 0 & 0 & 8 & 0 \\
-2 & 2 & -2 & -2 & -2 & -2 & 0 & 0 & 0 & 8
\end{array}\right).
\end{gathered}
\tag{27}
$$

There exist examples that realize these four Gram structures for all $1 \leq t \leq 7$ *which we give in Section 6.*

If $X \in ssd(10, 18t+12)$, $t \geq 0$, *with* $\sum_{i \neq j} s_{ij}^2 = 3600t^2 + 3240t + 528$, *then* $XX^\top = (2t+1)(10I_{10} - J_{10}) - P$ *with* P *as in Equation (25). In particular there is up to Gram isomorphism only one* $E(s^2)$*-optimal supersaturated design for each* $1 \leq t \leq 6$ *which we give in Section 6.*

If $X \in ssd(10, 18t+16)$, $t \geq 0$, with $\sum_{i \neq j} s_{ij}^2 = 3600t^2 + 5160t + 1408$, then $XX^\top = (2t+1)(10I_{10} - J_{10}) - P$ with P as in Equation (24). There exist examples that realize these two Gram structures for all $1 \leq t \leq 6$ which we give in Section 6.

Corollary 4.3. *If $X \in ssd(10, 18t+3)$, $t \geq 1$, with $\sum_{i \neq j} s_{ij}^2 = 3600t^2 - 600t - 40$, then $XX^\top = 2t(10I_{10} - J_{10}) + P$ with*

$$P = \left(\begin{array}{ccccc|ccccc}
3 & -1 & -1 & -1 & -1 & -3 & 1 & 1 & 1 & 1 \\
-1 & 3 & -1 & -1 & -1 & 1 & -3 & 1 & 1 & 1 \\
-1 & -1 & 3 & -1 & -1 & 1 & 1 & -3 & 1 & 1 \\
-1 & -1 & -1 & 3 & -1 & 1 & 1 & 1 & -3 & 1 \\
-1 & -1 & -1 & -1 & 3 & 1 & 1 & 1 & 1 & -3 \\
\hline
3 & 1 & 1 & 1 & 1 & 3 & -1 & -1 & -1 & -1 \\
1 & -3 & 1 & 1 & 1 & -1 & 3 & -1 & -1 & -1 \\
1 & 1 & -3 & 1 & 1 & -1 & -1 & 3 & -1 & -1 \\
1 & 1 & 1 & -3 & 1 & -1 & -1 & -1 & 3 & 1 \\
1 & 1 & 1 & 1 & -3 & -1 & -1 & -1 & -1 & 3
\end{array}\right). \tag{28}$$

There exist examples that realize this Gram structure. In particular there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for each $1 \leq t \leq 6$ which we give in Section 6.

If $X \in ssd(10, 18t+7)$, $t \geq 1$, with $\sum_{i \neq j} s_{ij}^2 = 3600t^2 + 1000t - 24$, then $XX^\top = 2t(10I_{10} - J_{10}) + P$ with

$$P = \left(\begin{array}{cccc|ccccc|c}
8 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \\
4 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \\
0 & 0 & 8 & 4 & 0 & 0 & 0 & 0 & 0 & -2 \\
0 & 0 & 4 & 8 & 0 & 0 & 0 & 0 & 0 & -2 \\
\hline
0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 2 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 2 \\
\hline
-2 & -2 & -2 & -2 & 2 & 2 & 2 & 2 & 2 & 8
\end{array}\right) - J_{10}. \tag{29}$$

There exist examples that realize this Gram structure. In particular, there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for each $1 \leq t \leq 6$ which we give in Section 6.

If $X \in ssd(10, 18t+11)$, $t \geq 1$, with $\sum_{i \neq j} s_{ij}^2 = 3600t^2 + 2600t + 376$, then $XX^\top = (2t+1)(10I_{10} - J_{10}) - P$ with P as in Equation (29). In particular, there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for each $1 \leq t \leq 6$ which we give in Section 6.

If $X \in ssd(10, 18t+15)$, $t \geq 0$, with $\sum_{i \neq j} s_{ij}^2 = 3600t^2 + 4680t + 1400$, then $XX^\top = (2t+1)(10I_{10} - J_{10}) - P$ with P as in Equation (28). In particular there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for each $1 \leq t \leq 6$ which we give in Section 6.

Since $s(X^2) \geq 4$ the bound of Corollary 4.3 does not apply when $m = 11$. In fact, $s(X^2) = 4$ for $E(s^2)$-optimal supersaturated designs $X \in \text{ssd}(11, 10)$.

Corollary 4.4. *If $X \in ssd(10, 18t+1)$, $t \geq 1$, with $\sum_{i \neq j} s_{ij}^2 = 3600t^2 - 1400t$, then $XX^\top = 2t(10I_{10} -$*

$J_{10})+P$ with

$$P=\left(\begin{array}{ccccc|ccccc} 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 \\ \hline -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \end{array}\right). \tag{30}$$

There exist examples that realize this Gram structure. See Section 6. In particular there is up to Gram isomorphism only one $E(s^2)$-optimal supersaturated design for each $1 \leq t \leq 7$ which we give in Section 6.

If $X \in ssd(10, 18t+5)$, $t \geq 1$, with $\sum_{i \neq j} \sum_{i \neq j} s_{ij}^2 = 3600t^2 + 200t - 48$, then $XX^\top = 2t(10I_{10} - J_{10})+$

P with

$$\begin{gathered}
P=\left(\begin{array}{ccccccc|ccc}
6 & -2 & 2 & 2 & 2 & 2 & -2 & 0 & 0 & 0\\
-2 & 6 & -2 & 2 & 2 & 2 & 2 & 0 & 0 & 0\\
2 & -2 & 6 & -2 & 2 & 2 & 2 & 0 & 0 & 0\\
2 & 2 & -2 & 6 & -2 & 2 & 2 & 0 & 0 & 0\\
2 & 2 & 2 & -2 & 6 & -2 & 2 & 0 & 0 & 0\\
2 & 2 & 2 & 2 & -2 & 6 & -2 & 0 & 0 & 0\\
-2 & 2 & 2 & 2 & 2 & -2 & 6 & 0 & 0 & 0\\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 6 & 2\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 6
\end{array}\right)-J_{10}\ \textit{or}\\
P=\left(\begin{array}{ccccccc|ccc}
6 & -2 & -2 & 2 & 2 & 2 & 2 & 0 & 0 & 0\\
-2 & 6 & -2 & 2 & 2 & 2 & 2 & 0 & 0 & 0\\
-2 & -2 & 6 & 2 & 2 & 2 & 2 & 0 & 0 & 0\\
2 & 2 & 2 & 6 & -2 & 2 & -2 & 0 & 0 & 0\\
2 & 2 & 2 & -2 & 6 & -2 & 2 & 0 & 0 & 0\\
2 & 2 & 2 & 2 & -2 & 6 & -2 & 0 & 0 & 0\\
2 & 2 & 2 & -2 & 2 & -2 & 6 & 0 & 0 & 0\\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 6 & 2\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 6
\end{array}\right)-J_{10}\ \textit{or}\\
P=\left(\begin{array}{ccccc|ccccc}
6 & -2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 0\\
-2 & 6 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 0\\
2 & 2 & 6 & 2 & -2 & 0 & 0 & 0 & 0 & 0\\
2 & 2 & 2 & 6 & -2 & 0 & 0 & 0 & 0 & 0\\
2 & 2 & -2 & -2 & 6 & 4 & 0 & 0 & 0 & 0\\
\hline
0 & 0 & 0 & 0 & 4 & 6 & -2 & -2 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & -2 & 6 & 2 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & -2 & 2 & 6 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 6 & -2\\
0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & -2 & 6
\end{array}\right)-J_{10}\ \textit{or}\\
P=\left(\begin{array}{ccccc|ccccc}
6 & -2 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 0\\
-2 & 6 & 2 & 2 & 2 & 0 & 0 & 0 & 0 & 0\\
2 & 2 & 6 & -2 & 2 & 0 & 0 & 0 & 0 & 0\\
2 & 2 & -2 & 6 & 2 & 0 & 0 & 0 & 0 & 0\\
2 & 2 & 2 & 2 & 6 & -4 & 0 & 0 & 0 & 0\\
\hline
0 & 0 & 0 & 0 & -4 & 6 & 2 & 2 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & 2 & 6 & -2 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & 2 & -2 & 6 & 2 & 2\\
0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 6 & -2\\
0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & -2 & 6
\end{array}\right)-J_{10}.
\end{gathered}\tag{31}$$

There exist examples that realize these four Gram structures for all $1\le t\le 7$ *which we give in Section 6.*

If $X\in ssd(10,18t+9)$*,* $t\ge 1$*, with* $\sum_{i\neq j}s_{ij}^2=3600t^2+1800t+160$*, then* $XX^\top=2t(10I_{10}-J_{10})+P$

with

$$P=\begin{pmatrix} 10 & 2 & -2 & -2 & 2 & 0 & 0 & 0 & 0 & 0\\ 2 & 10 & 2 & -2 & -2 & 0 & 0 & 0 & 0 & 0\\ -2 & 2 & 10 & 2 & -2 & 0 & 0 & 0 & 0 & 0\\ -2 & -2 & 2 & 10 & 2 & 0 & 0 & 0 & 0 & 0\\ 2 & -2 & -2 & 2 & 10 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 10 & 2 & -2 & -2 & 2\\ 0 & 0 & 0 & 0 & 0 & 2 & 10 & 2 & -2 & -2\\ 0 & 0 & 0 & 0 & 0 & -2 & 2 & 10 & 2 & -2\\ 0 & 0 & 0 & 0 & 0 & -2 & -2 & 2 & 10 & 2\\ 0 & 0 & 0 & 0 & 0 & 2 & -2 & -2 & 2 & 10 \end{pmatrix}-J_{10} \tag{32}$$

There exist examples that realize this Gram structure. See Section 6. In particular there is up to Gram isomorphism only one $E(s^2)$*-optimal supersaturated design for each* $1 \le t \le 6$ *which we give in Section 6.*

If $X \in ssd(10, 18t+13)$*,* $t \ge 0$*, with* $\sum_{i\neq j}\sum_{i\neq j} s_{ij}^2 = 3600t^2 + 3720t + 912$*, then* $XX^\top = 2t(10I_{10} - J_{10}) + P$ *with* P *as in Equation (31). There exist examples that realize these Gram structures for all* $1 \le t \le 6$ *which we give in Section 6.*

If $X \in ssd(10, 18t+17)$*,* $t \ge 0$*, with* $\sum_{i\neq j}\sum_{i\neq j} s_{ij}^2 = 3600t^2 + 5640t + 1920$*, then* $XX^\top = 2t(10I_{10} - J_{10}) + P$ *with* P *as in Equation (30). In particular there is up to Gram isomorphism only one* $E(s^2)$*-optimal supersaturated design for each* $1 \le t \le 6$ *which we give in Section 6.*

5. The proofs

Let $X \in \mathrm{ssd}(N, 2t(N-1)+b)$, $0 \le b < N$. We write $T = (t_{ij}) = XX^\top = 2t(NI_n - J_N) + P$, $P = (p_{ij})$. Since $t_{ii} = 2t(N-1) + b$ and $\sum_{j=1}^N t_{ij} = 0$ for $1 \le i \le N$, it follows that $p_{ii} = b$ and $\sum_{j=1}^N p_{ij} = 0$ for $1 \le i \le N$.

Proof of Lemma 3.1. The results follow by straightforward calculations from the facts that $t_{ii} = m$ and $\sum_{j=1}^N t_{ij} = 0$ for $1 \le i \le N$. □

Proof of Proposition 3.2. We use $\alpha = 2t$ and assume $R = XX^\top + 2tJ_N$ is partitioned as in Lemma 3.1 with $p \ge \frac{N}{2}$ even. Notice that $r_{ii} \equiv 2 \pmod 4$. Thus all off-diagonal entries of A and C have absolute value at least 2. Thus

$$\sum_{i\neq j} r_{ij}^2 \ge 4p(p-1) + 4(N-p)(N-p-1) = 8p(p-n) + 4n(n-1) = w(p). \tag{33}$$

Since $p \ge \frac{N}{2}$ is even $w(p)$ takes on its minimal value at $p = \frac{N}{2} + 1$. Since the row sum of A and C are 0, we find each row of A has exactly $\frac{N+b}{4}$ entries equal to -2 and each row of C has exactly $\frac{N+b-4}{4}$ entries equal to -2. This allows us to write and A and C as stated. □

Proof of Corollary 4.1.

1. If $b = 2$, Proposition 3.2 states that G is a regular graph of degree 3 on 6 vertices and H is a regular graph of degree 2 on 4 vertices. This implies that $G = K_3 \oplus K_3$ or $G = K_6 - C_6$ while $H = C_4$. This yields the two matrices for P.

2. If $b = 6$, Proposition 3.2 states that G is a regular graph of degree 4 on 6 vertices and H is a regular graph of degree 3 on 4 vertices. Hence $G = (K_2 \cup K_2 \cup K_2)^2$ and $H = K_3$. This determines P.

□

Proof of Proposition 3.3. We use $\alpha = 2t$ and assume $R = (r_{ij}) = XX^\top + 2tJ_N$ is partitioned as in Lemma 3.1 with $p \geq \frac{N}{2}$ even. Notice that all entries of B have absolute value at least 2. Furthermore, since $\sum_{i \neq j} c_{ij} - \sum_{k \neq l} a_{kl} = (2p-N)b$ and all off-diagonal entries of A and C are congruent 0 modulo 4, we have

$$\sum_{i \neq j} c_{ij}^2 + \sum_{k \neq l} a_{kl}^2 \geq 4(2p-N)b. \tag{34}$$

Thus

$$\sum_{i \neq j} r_{ij}^2 \geq 8p(N-p) + 4(2p-N)b = -8p^2 + 8(N+b)p - 4Nb = w(p). \tag{35}$$

The function $w(p)$ has a vertex at $p = \frac{N}{2} + \frac{b}{2}$. The range of p is $[\frac{N}{2}+1, N]$, which has its midpoint at $\frac{3N+2}{4}$.

If $b \leq \frac{N}{2} + 1$ the minimum of $d(p)$ occurs at the right endpoint N and we can write $XX^\top = 2t(NI_N - J_N) - 4A(G)$ where G is a regular graph of degree $\frac{b}{4}$ on N vertices.

If $b \geq \frac{N}{2} + 1$ the minimum of $d(p)$ occurs at the left endpoint N. There are several possibilities for the minimum to occur. All entries of B have absolute value 2, A has v, off-diagonal entries equal to -4 and C has $\frac{b}{2} - v$ off-diagonal entries equal to 4 while all other off-diagonal entries of A and C are 0. □

Proof of Corollary 4.2.

1. If $b = 0$, Proposition 3.3 states that $P = 0_N$.
2. If $b = 4$, Proposition 3.3 states that G is a regular graph of degree 1 on 10 vertices. Hence $G = K_2 \cup K_2 \cup K_2 \cup K_2 \cup K_2$. This determines P.
3. If $b = 8$, Proposition 3.3 states that $p = 6$ and hence C has either 0,2 or 4 entries equal to 4. Since $p = 6$ and each entry of B has absolute value 2, each row and column of C has at most one off-diagonal entry equal to 4. This leads to the four possible structures for P as listed.

□

For the case $b \equiv 3 \pmod 4$ we use Lemma 3.1 with $\alpha = 2t+1$.

Proof of Proposition 3.4. We use $\alpha = 2t+1$ and assume $R = (r_{ij}) = XX^\top + (2t+1)J_N$ is partitioned as in Lemma 3.1 with $p \geq \frac{N}{2}$ odd. Notice that all entries of B have absolute value at least 2. Furthermore, since $\sum_{i \neq j} c_{ij} - \sum_{k \neq l} a_{kl} = (2p-N)(b-N+1)$ and all off-diagonal entries of A and C are congruent 0 modulo 4, we have

$$\sum_{i \neq j} c_{ij}^2 + \sum_{k \neq l} a_{kl}^2 \geq 4(2p-N)|N-1-b| \tag{36}$$

and hence

$$\sum_{i \neq j} r_{ij}^2 \geq 8p(N-p) + 4(2p-N)|N-1-b| = w(p). \tag{37}$$

The range of p is $[\frac{N}{2}, N-1]$, which has its midpoint at $\frac{3N-2}{4}$.

If $b \leq N-1$ then $w(p)$ has a vertex at $N - \frac{b+1}{2}$. Hence, if $N - \frac{b+1}{2} \geq \frac{3N+2}{4}$, i.e., $b \leq \frac{N}{2}$, then the minimum of $f(p)$ occurs at the left endpoint $\frac{N}{2}$. In that case, all off-diagonal entries of A and C are 0 and each row and column of B has $\frac{b+1}{4}$ entries equal to -2 and $\frac{N}{2} - \frac{b+1}{4}$ entries equal to 2. It follows that $\sum_{i \neq j} r_{i,j} = 2N^2$ and hence $\sum_{i \neq j} s_{ij} = 2N^2 + g_1(N,t,b)$

Likewise, if $b \geq \frac{N}{2}$, then the minimum of $f(p)$ occurs at the right endpoint $N-1$. In that case B has $k = \frac{(3N-2)-(b+1)}{4}$ entries equal to 2 and $N-1-k$ entries equal to -2. Assuming

$$B^\top = (\underbrace{-2,\cdots,-2}_{N-1-k},\underbrace{2,\cdots,2}_{k}) \tag{38}$$

we have

$$A=(m+1)I_{N-1}+4A(G) \tag{39}$$

where G is a graph with degree sequence $(d^{(N-1-k)},(d-1)^{(k)})$ and $d=k-\frac{N-2}{2}$. The expression for $\sum_{i\neq j}s_{ij}^2$ follows.

If $b>N-1$, then $w(p)$ has a vertex at $\frac{b+1}{2}$. As above, if $b\geq\frac{3N-2}{4}$, then the minimum occurs at the left end point of the interval $[\frac{N}{2},N-1]$ and the result follows as above.

If $N-1<b\leq\frac{3N-2}{4}$, then the minimum of $w(p)$ occurs at the right endpoint $N-1$ and we proceed as above. □

Proof of Corollary 4.3.

1. If $b=3$, Proposition 3.4 implies that there is a unique solution

$$P=(4I_5-J_5)\otimes\begin{pmatrix}1&-1\\-1&1\end{pmatrix}. \tag{40}$$

2. If $b=7$, Proposition 3.4 states that $p=9$ and

$$P=\begin{pmatrix}A&B\\B^\top&C\end{pmatrix}-J_{10} \tag{41}$$

   such that B has five entries equal to 2 and four entries equal to -2 and $A=8I_9+4A(G)$ where G is a graph with degree sequence $(1,1,1,1,0,0,0,0,0)$. Thus P is a as described.

□

For the case $b\equiv 1 \pmod 4$ we use Lemma 3.1 with $\alpha=2t+1$. It splits into 2 cases, $b=8q+1$ and $b=8q+5$, the latter of which leads to 3 possibilities for the Gram structure of $XX^\top$.

Proof of Proposition 3.5. We use $\alpha=2t+1$ and assume $R=(r_{ij})=XX^\top+(2t+1)J_N$ is partitioned as in Lemma 3.1 with $p\geq\frac{N}{2}$ odd. Since all off-diagonal entries of A and C have absolute value at least 2 we have

$$\sum_{i\neq j}r_{ij}^2\geq 4p(p-1)+4(N-p)(N-p-1)=w(p). \tag{42}$$

The function $w(p)$ has a minimum at $\frac{N}{2}$.

If $b=8q+1$ then the minimum is attained by the example as stated above.

If $b=8q+5$ is odd and $p=\frac{N}{2}$, then at least one entry of B has absolute value at least 4. In that case,

$$\sum_{i\neq j}r_{ij}^2\geq 2N(N-2)+32. \tag{43}$$

This bound is achievable by the examples stated above. This bound can also be achieved for $p=\frac{N}{2}+2$ and all entries of B equal to 0, which leads to examples as stated above. □

Proof of Corollary 4.4.

1. If $b=1$, Proposition 3.5 states that G and H are regular graphs of degree 0 on 5 vertices. Thus G and H are graphs with no vertices, i.e. $A(G\cup H)$ is the zero matrix. This determines P.

2. If $b=9$, Proposition 3.5 states that G and H are regular graphs of degree 2 on 5 vertices. Thus $G=C_5=H$. This determines P.

3. If $b=5$, Proposition 3.5 states that

(a) if $p = \frac{N}{2} + 2$, then G is a regular graph of degree 2 on 7 vertices and H is a regular graph of degree 0 on 3 vertices. Thus $G = C_7$ or $G = C_3 \cup C_4$. This gives rise to the first two examples. OR

(b) G is a regular graph of degree 3 on 10 vertices such that the induced subgraph on vertices v_1, v_2, v_3, v_4, v_5 has degree sequence $(3,3,3,3,2)$ and the induced subgraph on vertices $v_6, v_7, v_8, v_9, v_{10}$ has degree sequence $(2,3,3,3,3)$. OR

(c) G is a regular graph of degree 1 on 10 vertices such that the induced subgraph on vertices v_1, v_2, v_3, v_4, v_5 has degree sequence $(1,1,1,1,0)$ and the induced subgraph on vertices $v_6, v_7, v_8, v_9, v_{10}$ has degree sequence $(0,1,1,1,1)$.

Thus P is one of the matrices listed.

□

Proof of Proposition 3.7. Write $XX^\top = 2t(NI_N - J_N) + Q = 2t(NI_N - J_N) + (2NI_N - 2J_N - P)$. Notice that

$$\begin{aligned} p_{ii} &= 2(N-1) - b, \\ \sum_{j \neq i} p_{ij} &= -2(N-1) + b, \\ \sum_{i \neq j} q_{ij}^2 &= 4N(b - (N-1)) + \sum_{i \neq j} p_{ij}^2. \end{aligned} \tag{44}$$

Thus minimizing $\sum_{i \neq j} q_{ij}^2$ is equivalent to minimizing $\sum_{i \neq j} p_{ij}^2$. Furthermore, P satisfies the conditions of Propositions 3.2, 3.3 for the respective $0 \leq b' = 2(N-1) - b < N$. □

6. The examples for $N = 10$ runs

Let $N = 2k$ and $C(2k,k)$ be the matrix whose columns are the (± 1)-vectors of length $2k$ with k entries equal to -1 and first entry equal to 1 ordered lexicographically. For example, the first column of $C(10,5)$ is $(1,1,1,1,1,-1,-1,-1,-1,-1)^\top$, the second column is $(1,1,1,1,-1,1,-1,-1,-1,-1)^\top$ and the 126th column is $(1,-1,-1,-1,-1,-1,1,1,1,1)^\top$. As such each column has an address and we list designs by the addresses of their columns. We list supersaturated designs by giving the list of column addresses. For example, we write $X_{12} = (17,20,25,31,40,57,71,76,98,105,121,124)$ for the supersaturated design with $N = 10$ runs and $m = 12$ factors whose columns are column 17 of $C(10,5)$, column 20 of $C(10,5)$ and so on.

We list the examples for values $12 \leq m \leq 63$. For $m = 10, 11$ the bounds of Propositions 3.6 and 3.7 do not apply. For $63 < m \leq 114$ we obtain $E(s^2)$-optimal supersaturated designs via complementation of $E(s^2)$-optimal supersaturated designs for $12 \leq 126 - m < 63$ factors as the next result demonstrates.

Lemma 6.1. *Let $c = |C(N,N/2)|$. Assume $X_1 \in ssd(m,N)$, $N \leq m \leq c - N$ and X_1 is $E(s^2)$-optimal. If $X_2 \in ssd(c-m,N)$ is the design formed by all columns in $C(N,N/2)$ which are not in X_1, then X_2 is $E(s^2)$-optimal.*

Proof. Let $X \in \mathrm{ssd}(m,N)$ and let $Y \in \mathrm{ssd}(b-m,N)$ be the complement of X in $B(N)$. Note that

$$XX^\top = [X,Y]\,[X,Y]^\top = XX^\top + YY^\top = sI_N - \frac{s}{N}J_N. \tag{45}$$

with $s = \frac{Nc}{(N-1)}$. Hence

$$YY^\top = sI_N - \frac{s}{N}J_N - XX^\top. \tag{46}$$

With $XX^\top = (t_{ij})$ and $YY^\top = (\tau_{ij})$ we have

$$\tau_{ij} = -\frac{c}{N-1} - t_{ij} \text{ for } i \neq j \tag{47}$$

This implies

$$\sum_{i\neq j} (\tau_{ij})^2 = \sum_{i\neq j} \left(-\frac{c}{N-1} - t_{ij} \right)^2 = \frac{cN(c-2m)}{N-1} + \sum_{i\neq j} t_{ij}^2. \tag{48}$$

Thus X is $E(s^2)$-optimal if and only if Y is $E(s^2)$-optimal. □

6.1. The examples for $b \equiv 2 \pmod 4$

$X_{14} = (2,21,25,31,44,49,57,70,76,83,98,105,110,116)$
$X_{20,1} = (7,14,16,18,21,25,27,31,45,56,59,68,69,77,86,95,107,112,120,122)$
$X_{20,2} = (3,11,14,21,24,27,38,50,54,55,65,69,76,82,95,97,111,113,117,123)$
$X_{24} = (4,16,21,25,26,31,38,39,48,49,62,64,73,75,77,78,91,93,98,103,111,118,123,125)$
$X_{28,1} = (2,18,19,21,23,31,34,39,43,45,47,52,58,61,63,67,73,79,83,89,95,106,110,111,113,117,118,123)$
$x_{28,2} = (15,16,18,20,23,28,34,36,37,44,46,48,60,64,65,67,73,76,81,88,98,100,102,109,114,115,124,125)$
$X_{28,3} = (3,6,14,19,20,25,32,35,38,39,42,43,49,51,61,64,75,76,81,82,88,93,96,104,105,111,121,124)$
$X_{28,4} = (6,12,15,17,20,29,32,36,37,38,41,46,57,59,69,75,77,78,85,88,94,98,102,104,109,121,124,125)$
$X_{32} = X_{14} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{38,1} = X_{20,1} \cup (1,12,20,32,36,40,41,50,60,63,78,83,91,93,104,109,117,118)$
$X_{38,2} = X_{20,2} \cup (1,15,17,34,35,39,43,47,59,62,81,86,88,92,107,110,115,119)$
$X_{42} = X_{24} \cup (1,13,18,32,34,37,45,52,60,65,76,85,90,95,102,109,113,121)$
$X_{46,1} = X_{28,1} \cup (3,10,13,35,36,40,41,48,57,68,81,86,88,92,99,105,119,124)$
$X_{46,2} = X_{28,2} \cup (1,13,21,27,33,39,45,53,58,69,75,82,90,99,106,107,113,119)$
$X_{46,3} = X_{28,3} \cup (1,13,18,34,36,40,41,48,60,62,80,85,90,92,106,109,117,118)$
$X_{46,4} = X_{28,4} \cup (2,8,21,31,34,39,45,49,61,63,76,83,91,95,97,110,115,123)$
$X_{50} = X_{32} \cup (6,10,16,27,29,38,43,56,59,65,74,82,90,97,100,108,114,125)$
$X_{56,1} = X_{38,1} \cup (3,15,19,22,24,46,48,54,58,71,75,79,82,105,106,110,113,119)$
$X_{56,2} = X_{38,2} \cup (4,10,18,22,30,41,48,56,63,67,74,80,84,98,101,108,112,125)$
$X_{60} = X_{42} \cup 5,11,12,24,30,41,50,55,68,69,74,80,82,92,97,106,117,126)$

6.2. The examples for $b \equiv 0 \pmod 4$

$X_{12} = (17,20,25,31,40,57,71,76,98,105,121,124)$
$X_{16,1} = (2,24,36,37,42,51,61,66,74,78,85,99,103,104,116,126)$
$X_{16,2} = (1,20,25,28,43,48,64,68,73,75,77,88,96,104,111,121)$
$X_{18} = (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{22} = (6,10,16,19,27,29,39,43,45,47,58,59,65,74,82,90,93,97,108,111,114,125)$
$X_{26,1} = (2,7,8,19,21,23,24,29,35,43,47,52,60,65,68,74,80,82,88,92,99,106,108,116,120,124)$
$X_{26,2} = (3,10,12,20,21,22,25,28,30,37,45,53,57,59,67,70,74,75,82,98,105,110,118,119,124,125)$
$X_{26,3} = (4,5,7,18,26,28,37,46,47,53,58,63,67,74,76,80,84,87,92,94,100,104,110,118,125,126)$
$X_{26,4} = (4,10,20,23,27,30,40,44,47,55,58,61,64,72,82,85,90,93,94,108,109,111,116,118,119,124)$
$X_{30} = X_{12} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{34,1} = X_{16,1} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{34,2} = X_{16,2} \cup (2,10,18,31,34,37,45,52,61,63,79,83,89,95,97,110,112,125)$
$X_{36} + X_{18} \cup (6,10,16,27,29,38,43,56,59,65,74,82,90,97,100,108,114,125)$
$X_{40} = X_{22} \cup (2,8,21,31,35,40,44,48,60,63,76,84,91,94,98,110,116,122)$
$X_{44,1} = X_{26,1} \cup (3,10,15,28,34,37,45,55,61,66,79,83,86,94,98,107,112,126$

$X_{44,2} = X_{26,2} \cup (1,15,19,31,33,38,46,48,58,64,80,84,88,94,106,111,112,120)$
$X_{44,3} = X_{26,3} \cup (1,13,17,30,33,39,41,56,61,69,72,86,90,99,102,103,117,119)$
$X_{44,4} = X_{26,4} \cup (1,15,17,28,34,37,46,54,59,68,74,86,88,98,103,107,112,121)$
$X_{48} = X_{30} \cup (6,10,16,27,29,38,43,56,59,65,74,82,90,97,100,108,114,125)$
$X_{52,1} = X_{34,1} \cup (5,8,20,22,28,46,49,53,64,68,72,79,86,96,100,110,117,122)$
$X_{52,2} = X_{34,2} \cup (4,8,14,30,33,38,46,53,60,70,78,82,87,92,99,103,116,126)$
$X_{54} = X_{36} \cup (5,13,18,24,26,37,52,53,60,62,73,78,91,103,106,109,117,118)$
$X_{58} = X_{40} \cup (5,7,20,28,33,41,42,52,61,67,72,85,89,95,99,102,121,124)$
$X_{62,1} = X_{44,1} \cup (1,14,18,31,36,38,42,51,59,62,81,85,89,95,103,111,114,118)$
$X_{62,2} = X_{44,2} \cup (5,13,18,27,35,40,42,44,60,66,73,78,87,92,100,107,122,126)$
$X_{62,3} = X_{44,3} \cup (2,8,19,31,36,40,45,48,60,65,78,82,91,93,97,109,115,124)$
$X_{62,4} = X_{44,4} \cup (5,9,12,26,33,39,51,53,63,71,77,80,84,92,96,105,117,126)$

6.3. The examples for $b \equiv 3 \pmod 4$

$X_{15} = (4,11,12,34,46,48,71,77,85,89,94,96,104,116,126)$
$X_{21} = (2,8,17,21,23,28,35,40,44,49,61,64,71,73,82,89,94,98,108,121,124)$
$X_{25} = (4,11,14,18,23,28,30,41,46,52,53,57,68,69,73,77,83,91,92,99,101,103,109,116,123)$
$X_{29} = (2,9,14,17,18,22,26,27,34,38,42,54,56,60,66,69,71,72,73,78,86,96,98,103,106,117,118,122,124)$
$X_{33} = X_{15} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119).$
$X_{39} = X_{21} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{43} = X_{25} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{47} = X_{29} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{51} = X_{33} \cup (6,10,16,27,29,38,43,56,59,65,74,82,90,97,100,108,114,125)$
$X_{57} = X_{39} \cup (5,12,20,22,24,43,52,53,60,68,72,80,85,102,106,110,117,118)$
$X_{61} = X_{43} \cup (6,10,16,27,29,38,43,56,59,65,74,82,90,97,100,108,114,125)$

6.4. The examples for $b \equiv 1 \pmod 8$

$X_{17} = (11,12,23,30,31,44,50,57,69,70,76,83,94,110,116,120,123)$
$X_{19} = (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119,126)$
$X_{27} = (2,5,8,11,18,24,30,34,41,48,50,55,60,62,66,75,79,83,86,91,92,101,106,109,110,112,117)$
$X_{35} = X_{17} \cup (11,12,23,30,31,44,50,57,69,70,76,83,94,110,116,120,123)$
$X_{37} = X_{19} \cup (2,8,20,25,36,38,49,53,64,66,75,77,91,98,100,102,115,124)$
$X_{45} = X_{27} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$
$X_{53} = X_{35} \cup (6,10,16,27,29,38,43,56,59,65,74,82,90,97,100,108,114,125)$
$X_{55} = X_{37} \cup (6,10,16,22,28,43,48,56,65,67,74,80,82,96,99,110,114,125)$
$X_{63} = X_{45} \cup (1,15,19,32,33,39,45,47,58,63,81,84,88,93,107,111,113,119)$

6.5. The examples for $b \equiv 5 \pmod 8$

$X_{13,1} = (16,21,22,48,51,65,72,85,99,102,110,117,119)$
$X_{13,2} = (6,16,29,42,45,58,74,91,99,100,102,110,114)$
$X_{13,3} = (6,10,20,32,41,49,50,66,83,93,101,114,126)$
$X_{13,4} = (2,36,37,44,54,59,75,88,90,94,98,102,125)$
$X_{23,1} = (1,2,10,27,35,41,46,48,51,68,69,72,73,75,85,89,90,95,96,97,105,107,121)$
$X_{23,2} = (7,16,23,29,30,31,39,43,56,58,61,69,71,73,83,84,93,103,106,118,120,121,123)$
$X_{23,3} = (1,7,17,19,27,33,34,40,45,57,65,66,70,76,87,90,97,101,105,113,115,119,123)$
$X_{23,4} = (2,10,11,21,23,26,31,47,50,59,62,68,73,77,86,88,94,99,107,111,114,119,124)$
$X_{31,1} = X_{13,1} \cup (1,14,20,32,33,40,44,47,58,63,81,83,89,93,107,111,114,118)$

$X_{31,2} = X_{31,2} \cup (1,13,18,34,36,40,41,48,60,62,80,85,90,92,106,109,117,118)$
$X_{31,3} = X_{13,3} \cup (1,15,19,31,33,38,46,48,58,64,80,84,88,94,106,111,112,120)$
$X_{31,4} = X_{13,4} \cup 1,14,20,31,32,38,46,49,58,65,79,83,89,95,105,111,112,120)$
$X_{41,1} = X_{23,1} \cup (3,7,20,25,34,43,47,52,65,67,74,76,91,93,100,104,120,122)$
$X_{41,2} = X_{23,1} \cup (2,9,17,33,35,37,46,50,60,65,80,82,90,94,96,108,114,125)$
$X_{41,3} = X_{23,3} \cup (2,10,20,31,32,38,43,52,61,62,77,85,89,95,99,111,112,124)$
$X_{41,4} = X_{23,4} \cup (1,13,18,32,34,37,45,52,60,65,76,85,90,95,102,109,113,121)$
$X_{49,1} = X_{31,1} \cup (3,10,15,24,35,37,50,55,64,66,78,79,86,95,101,103,112,126)$
$X_{49,2} = X_{31,2} \cup (3,10,15,24,35,37,50,55,64,66,78,79,86,95,101,103,112,126)$
$X_{49,3} = X_{31,3} \cup (4,8,21,27,30,39,45,53,60,63,72,87,89,98,99,110,116,122)$
$X_{49,4} = X_{31,4} \cup (5,13,18,22,26,41,48,56,60,66,73,78,87,104,106,108,113,121)$
$X_{59,1} = X_{41,1} \cup (5,8,13,30,33,39,45,53,59,71,78,83,86,92,99,102,117,126)$
$X_{59,2} = X_{41,2} \cup (3,10,15,26,34,38,47,55,64,66,78,79,86,92,100,107,113,126)$
$X_{59,3} = X_{41,3} \cup (4,11,12,25,30,42,50,54,68,69,73,81,83,92,96,107,116,126)$
$X_{59,4} = X_{41,4} \cup (8,14,20,22,24,36,49,53,58,64,70,81,82,104,108,115,116,120)$

7. Discussion

This paper studies the non-isomorphic $E(s^2)$-optimal supersaturated designs in $\text{ssd}(m,N)$. In particular, for $N = 10$ runs, we give all the possible minimal row Gram structures. As we have seen, for $N = 10$ all minimal row Gram structures are realizable by some supersaturated design. However, there is no clear pattern as to how many non-isomorphic $E(s^2)$-optimal supersaturated designs exists for a given number of factors m. Nevertheless, it is interesting to observe that for $b \equiv 1 \pmod 8$ and $b \equiv 3 \pmod 8$, we found a unique $E(s^2)$-optimal supersaturated design. For the remaining cases, the number of non-isomorphic $E(s^2)$-optimal supersaturated designs range from 1 to 4.

This leaves us with some questions for further inquiry:

1. Are additional, statistically meaningful criteria that differentiate when more than one non-isomorphic $E(s^2)$-optimal supersaturated design exists?

2. Are all possible minimal row Gram structures realizable for $N = 14$? For general $N \equiv 2 \bmod 4$?

3. What about the case $N \equiv 0 \bmod 4$?

4. In many cases, Section 3 describes the minimal row Gram structures via graphs. Is there a connection between the properties of those graphs and the properties of the $E(s^2)$-optimal designs.

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