D-optimal $2 \times 2 \times s_3 \times s_4$ saturated factorial designs

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Abstract: In this paper, Resolution III saturated $s_1 \times s_2 \times s_3 \times s_4$, $s_4 \geq s_3 \geq s_2 \geq s_1 \geq 2$ factorial designs and specially the cases $2^2 \times (s - k) \times s$, $s - k \geq 2$, $k = 0, 1$ are studied, in order to obtain D-optimal plans.

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1. Introduction

Saturated factorial plans is a very interesting issue in theory of experimental designs, since the reduced number of observations is very useful in practice especially in screening experiments, where are used to determine which of many factors affects the measure of pertinent quality characteristics. In saturated designs the number of observation is equal to the number of parameters, so all degrees of freedom are consumed by the estimation of parameters, leaving no degrees of freedom for error variance estimation. The purpose of this paper is to give saturated resolution III designs, minimizing the generalized variance of the main effects and the general mean, that is, D-optimal designs. In recent years, there has been a considerable interest in optimal saturated main effect designs with two or three factors. Mukerjee et al. (1986) and Kraft (1990) showed all two-factor designs are equivalent with respect to D-optimality criterion. Later Mukerjee and Sinha (1990) studied the problem of finding optimal designs under different types of criteria preoccupies many researchers the last decades. Most of the work on constructing optimal designs for the estimation of parameters in fractional factorials is concentrated on factors at two levels. Chatzopoulos, Kolyva-Machera, and Chatterjee (2009), studied the optimality of designs which are obtained by adding p runs to an orthogonal array for experiments involving m factors each at s levels. Chatterjee, Kolyva-Machera, and Chatzopoulos (2011), considered the issue of optimality of fractional factorial experiments involving m factors each at 2 levels. Pericleous, Chatzopoulos, Kolyva-Machera and Kounias, study the problem of estimating the standardized linear and quadratic contrasts in fractional factorials with k factors, each at 3 levels, when the number of runs or assemblies is $N = 3$ and introduced a different notion of Balanced Arrays. Chatzopoulos and Kolyva-Machera (2005), studied the saturated $m_1 \times m_2 \times m_3 \times m_4$ designs and Chatzopoulos & Kolyva-Machera (2008), considered the problem of finding D-optimal saturated $4 \times m_2 \times m_3$ designs.
considered, for the two-factor case, the optimality results on almost saturated main effect designs. Pesotan and Raktoe (1988) worked also in the special case for $s^2$ factorials and a subclass of $s^3$ factorials.

Chatzopoulos and Mukerjee (1993) were the first who attempted to extend the two factor results to three factors. They consider $2 \times s_2 \times s_y$, $s_2 \geq 2$, $s_3 \geq s_2$ to derive D-optimal saturated main effect designs. Later Chatzopoulos and Narasimhan (2002), using techniques from Graph Theory and Combinatorics, claimed about the upper bound of the determinant of the saturated $3 \times s \times s_y$, $s_2 \geq 3$, $s_3 \geq s_2$ factorials when $s_i$ is odd. Chatzopoulos and Kolyva-Machera (2006) extend the results concerning D-optimal saturated main effect designs for $2 \times s_2 \times s_3$ to $3 \times s_2 \times s_3$ factorials, when $3 \leq s_2 \leq 6$ and $s_3 \geq s_2$. Karagiannis and Molyssiotis (2005) and Karagiannis and Molyssiotis (2008) extend the Graph theoretic approach of Chatzopoulos and Narasimhan (2002) and the results of Chatzopoulos and Kolyva-Machera (2006), and give the D-optimal saturated $3 \times s_2 \times s_3 \geq 3$, $s_3 \geq s_2$ designs. In this paper, we study the D-optimality for saturated $s_1 \times s_2 \times s_3 \times s_4$ factorials. Moreover, we give the upper bound of the determinant for the $2^2 \times (s - k) \times s$, $s - k \geq 2$, $k = 0, 1$, saturated designs and the corresponding design, which attains this bound. The paper is organized as follows. Some notations and preliminaries are first presented in Section 2. Section 3 deals with the main results of this paper.

2. Notations and preliminaries

In this paper, we follow the same notations as in Chatzopoulos and Kolyva-Machera (2006) adapted for four factors. Let us consider the setup of an $s_1 \times s_2 \times s_3 \times s_4$ factorial experiment, involving four factors $F_1 \times F_2 \times F_3$ and $F_4$, appearing at $s_1$, $s_2$, $s_3$, and $s_4$ levels, respectively, with $N = s_1 + s_2 + s_3 + s_4 - 3$ runs. For $1 \leq i \leq 4$ let the levels of $F_i$ be denoted by $r_i$ and coded as $0, 1, \ldots, s_i - 1$. Our interest is to find D-optimal resolution III designs. There are altogether $s_1^2 s_2^2 s_3^2$ treatment combinations denoted by $\tau_1 \tau_2 \tau_3 \tau_4$, that will hereafter be assumed to be lexicographically ordered.

Let, for $1 \leq i \leq 4$, $\mathbf{1}$ be the $s_i \times 1$ vector with each element unity, $I_i$ the identity matrix of order $s_i$, $\otimes$ denotes the Kronecker product of matrices and $P_i$ be an $(s_i - 1) \times s_i$ matrix such that $(s_i^{-1/2} \mathbf{1}, P_i')$ is orthogonal ($A'$ denotes the transpose of matrix $A$). The usual fixed effect model under the absence of interactions is $Y = W \beta + \epsilon$, where $Y$ is the response vector of the experiment, $\epsilon$ is the vector of uncorrelated random errors with zero mean and the same variance $\sigma^2$ and $\beta$ is the vector of unknown parameters, is considered. In our case $\beta = (\mu, \beta_1, \beta_2, \beta_3, \beta_4)'$, where $\mu$ is the unknown general mean and the elements of the $(s_i - 1) \times 1$ vectors $\beta_i$ are unknown contrasts representing a full set of mutually orthogonal contrasts belonging to the main effects $F_i$ and $W = [1_1 \otimes 1_2 \otimes 1_3 \otimes 1_4, W_1, W_2, W_3, W_4]$ where $W_1 = P_1' \otimes 1_2 \otimes 1_3 \otimes 1_4'$, $W_2 = 1_1 \otimes P_2' \otimes 1_3 \otimes 1_4'$, $W_3 = 1_1 \otimes 1_2 \otimes P_3' \otimes 1_4'$ and $W_4 = 1_1 \otimes 1_2 \otimes 1_3 \otimes P_4'$. It is easy to see that the D-optimal design does not depend on the choice of $P_i$, $1 \leq i \leq 4$.

Following Mukerjee and Sinha (1990) let $X_0 = [1_1 \otimes 1_2 \otimes 1_3 \otimes 1_4, X_1, X_2, X_3, X_4]$ where $X_1 = I_1 \otimes 1_2 \otimes 1_3 \otimes 1_4$, $X_2 = 1_1 \otimes I_2 \otimes 1_3 \otimes 1_4$, $X_3 = 1_1 \otimes 1_2 \otimes I_3 \otimes 1_4$, $X_4 = 1_1 \otimes 1_2 \otimes 1_3 \otimes I_4$. We denote $X_i^{(i)}$, $i = 1, 2, 3$ the matrices obtained by deleting the first column of $X_i$, $i = 1, 2, 3$. Consider the $u \times (s_1 + s_2 + s_3 + s_4 - 3)$ matrix $U$, which is a submatrix of $X_0$ given by $U = [X_1^{(1)}, X_2^{(1)}, X_3^{(1)}, X_4^{(1)}]$ which has full column rank. The $u$ rows of matrix $U$ like those of $W$, correspond to the lexicographically ordered treatment combinations. Moreover the columns of $U$ span those of $X_0$ and hence those of $W$, which also has full column rank.

Hence, one may obtain $W = UH$, where matrix $H$ is a nonsingular matrix of order $s_1 + s_2 + s_3 + s_4 - 3$. For any design $d$ in the class $D$ of the saturated resolution III designs with $N = s_1 + s_2 + s_3 + s_4 - 3$ runs, the design matrix is $W_d = U_dH$, where $U_d$ is a square matrix of order $s_1 + s_2 + s_3 + s_4 - 3$ such that for $1 \leq j \leq s_1 + s_2 + s_3 + s_4 - 3$ if the $j$-th run in $d$ is given by the treatment combination $\tau_1 \tau_2 \tau_3 \tau_4$ then the $j$-th row of $U_d$ is the row of $U$ corresponding to the treatment combination $\tau_1 \tau_2 \tau_3 \tau_4$. A design $d$ is said to be D-optimal in the class $D$, if it maximizes the
quantity $|\text{det}(W_d'W_d)|$. Since matrix $H$ is nonsingular a design is D-optimal if it maximizes the quantity $|\text{det}(U_d)|$, where:

$$U_d = [Z_1^{(1)}, Z_2^{(1)}, Z_3^{(1)}, Z_4].$$

The matrices $Z_i^{(1)}, 1 \leq i \leq 3$ and $Z_4$ are obtained from the matrices $X_1^{(1)}$ and $X_2$ in a similar way, as $U_d$ is obtained from $U$.

**Definition 2.1** For $1 \leq i \leq 3$, if the $i$-th factor enters the experiment at level 0 then the corresponding row of the matrix $Z_i^{(1)}$ is a row vector with $s_i - 1$ elements zero. On the other hand if the $i$-th factor enters the experiment at level $p, 1 \leq p \leq (s_i - 1)$, then the corresponding row of the matrix $Z_i^{(1)}$ equals the $p$-th row of the identity matrix of order $(s_i - 1)$. Similarly, if the fourth factor enters the experiment at level $p, 0 \leq p \leq s_4 - 1$, then the corresponding row of the matrix $Z_4$ equals to the $(p + 1)$-th row of the identity matrix $I_{s_4}$. Let $n_i^p, 0 \leq p \leq (s_i - 1)$, denote the number of these rows. It holds that

$$N = \sum_{p=0}^{(s_3-1)} n_i^p, \ i = 1, 2, 3, 4.$$

**Definition 2.2** For $1 \leq i \neq j \leq 4$ and $0 \leq p \leq (s_i - 1), 0 \leq q \leq (s_j - 1)$, let $n_{ij}^{pq}$ denote the number of runs where the $i$-th factor appears at level $p$ and the $j$-th factor appears at level $q$. It holds that

$$n_{ij}^p = \sum_{q=0}^{(s_j-1)} n_{ij}^{pq}, \ \text{for} \ j = 1, 2, 3, 4, \ j \neq i,$$

$$n_j^p = \sum_{p=0}^{(s_j-1)} n_{ij}^{pq}, \ \text{for} \ i = 1, 2, 3, 4, \ i \neq j,$$

$$N = \sum_{p=0}^{(s_3-1)} \sum_{q=0}^{(s_4-1)} n_{ij}^{pq}, \ \text{for} \ 1 \leq i \neq j \leq 4.$$

**Definition 2.3** For $1 \leq i \neq j \neq k \leq 4$ and $0 \leq p \leq (s_i - 1), 0 \leq q \leq (s_j - 1), 0 \leq r \leq (s_k - 1)$ let $n_{ijk}^{pqr}$ denote the number of runs where the $i$-th factor appears at level $p$, the $j$-th factor appears at level $q$ and the $k$-th factor appears at level $r$. It holds that

$$n_{ijk}^{pqr} = \sum_{r=0}^{(s_k-1)} n_{ijk}^{pqr}, \ \text{for} \ k = 1, 2, 3, 4, \ i \neq k \neq j \neq i,$$

$$n_{i}^{pqr} = \sum_{q=0}^{(s_j-1)} n_{ijk}^{pqr}, \ \text{for} \ j = 1, 2, 3, 4, \ k \neq j \neq i \neq k,$$

$$n_{i}^{pqr} = \sum_{p=0}^{(s_i-1)} n_{ijk}^{pqr}, \ \text{for} \ i = 1, 2, 3, 4, \ j \neq i \neq k \neq j,$$

$$N = \sum_{p=0}^{(s_3-1)} \sum_{q=0}^{(s_4-1)} \sum_{r=0}^{(s_4-1)} n_{ijk}^{pqr}, \ \text{for} \ 1 \leq i \neq j \neq k \neq i \leq 4.$$

**Remark 2.1** It holds that $n_i^p \geq 1, 1 \leq i \leq 4, 0 \leq p \leq (s_i - 1)$, since the design matrix of a saturated design has full column rank.

**Remark 2.2** By the choice of the labels for the levels one can always assume, without loss of generality (w.l.o.g.), that $n_i^p = \max(n_i^p, 0 \leq p \leq s_i - 1, 1 \leq i \leq 4)$.

The following lemmas are crucial for the main results of our paper and can be found in Chatterjee and Mukerjee (1993) and Chatzopoulos and Kolyva-Machera (2006).
Consider the saturated \( s_1 \times s_2 \) design \( e \), \( s_2 \geq s_1 \geq 2 \), with \( N = s_1 + s_2 - 1 \) runs and corresponding matrix \( X_e \). It holds that

\[
|\det(X_e)| = 1.
\]  

(2)

**Proof**  See Chatterjee and Mukerjee (1993).

\[
\begin{align*}
\text{Lemma 2.2} & \quad \text{Consider the saturated } 2 \times s_2 \times s_3 \text{ designs } d^{(2)}, \; s_3 \geq s_2 \geq 2, \; \text{with } N = s_2 + s_3 \text{ runs and corresponding matrix } U_{d^{(2)}}^2. \; \text{It holds that} \\
|\det(U_{d^{(2)}}^2)| & \leq s_2. \\
\end{align*}
\]  

(3)

**Proof**  See Chatterjee and Mukerjee (1993).

\[
\begin{align*}
\text{Lemma 2.3} & \quad \text{Consider the saturated } s_1 \times \ldots \times s_i \times \ldots \times s_k \text{ design } d. \; \text{If } s_i \geq 2 \; \text{and } n_i^p = 1 \; \text{for some } 0 \leq p \leq s_i - 1 \; \text{then } |\det(U_d)| = |\det(U_{d^p})|, \; \text{where } d^p \; \text{is a saturated } s_1 \times \ldots \times (s_i - 1) \times \ldots \times s_k \text{ design.} \\
\end{align*}
\]


\[
\begin{align*}
\text{Corollary 2.1} & \quad \text{Consider the saturated } s_1 \times s_2 \times s_3 \times s_4 \times s_5 \left( s_1 \geq s_2 \geq s_3 \geq s_4 \geq s_5 \geq 2 \right) \text{ design } d \; \text{with } N = s_1 + s_2 + s_3 + s_4 + s_5 - 3 \text{ runs. If } w = s_k - (s_1 + s_2 + s_3 - 3) \neq 0, \; \text{then using the pigeonhole principle we can easily verify that } n_k^w = 1, \; \text{for some } 0 \leq p \leq s_k - 1 \; \text{at least } w \text{ times}. \; \text{Applying, } w \times \text{times, } \text{Lemma 2.3, we get } |\det(U_d)| = |\det(U_{d^p})|, \; \text{where } d^p \; \text{is a saturated } s_1 \times s_2 \times s_3 \times (s_1 + s_2 + s_3 - 3) \text{ design.} \\
\end{align*}
\]

**Remark**  For \( s_1 = s_2 = 2 \) we have to study only the cases where \( 0 \leq s_k - s_i \leq 1 \), that is the cases \( 2^1 \times 2^1, 2 \geq 2 \) and \( 2^2 \times (s - 1) \times s, s \geq 3 \).

\[
\begin{align*}
\text{Lemma 2.4} & \quad \text{Let } d \; \text{be a saturated } s_1 \times s_2 \times s_3 \times s_4 \left( s_1 \geq s_2 \geq s_3 \geq s_4 \geq 2 \right) \text{ design. If } |\det(U_d)| = \prod_{i=1}^{k-1} n_i^p \; \text{and } n_i^0 \geq n_i^1 \geq \ldots \geq n_i^{(s_i-1)} \geq n_i^0 - 1, \; i = 1, 2, 3, \; \text{then } d \; \text{is } D\text{-optimal.} \\
\end{align*}
\]


3. Main results

**Lemma 3.1**  The determinant of the matrix \( U_d = \{Z_1, Z_2, Z_3\} \) given in (1), which corresponds to a \( s_1 \times s_2 \times s_3 \times s_4 \left( s_1 \geq s_2 \geq s_3 \geq s_4 \geq 2 \right) \) saturated factorial design \( d \) is left invariant by interchanging the levels of the factors.

**Proof**  For the fourth factor, we can interchange the columns which correspond to two levels and the proof is obvious. Similarly, for the nonzero levels of the first, second and the third factor, interchanging the columns \( p \) and \( q \), the levels \( (p-1) \) and \( (q-1) \) are interchanged. Moreover, for the first (or second or third) factor, adding all the columns of matrix \( Z_1^p \) (or \( Z_2^p \) or \( Z_3^p \)) to the column which corresponds to level \( p \), subtracting the sum of all columns of matrix \( Z_4 \) and multiplying the resulting column by \(-1\) the levels 0 and \( p \) are interchanged.

**Lemma 3.2**  Let \( d \) be a \( s_1 \times s_2 \times s_3 \times s_4 \left( s_1 \geq s_2 \geq s_3 \geq s_4 \geq 2 \right) \) saturated factorial design with corresponding matrix \( U_d = \{Z_1, Z_2, Z_3, Z_4\} \) as given in (1). Let \( n_i^{\text{max}} = w > 1 \) for some \( 0 \leq i, j, k \leq 4 \) and some \( 0 \leq p \leq s_i - 1, 0 \leq q \leq s_j - 1, 0 \leq r \leq s_k - 1 \). Then

\[
|\det(U_d)| = \begin{cases} 
|\det(U_{d^{(1)})})| & \text{for } (i, j, k) = (1, 2, 3), \\
|\det(U_{d^{(2)})})| & \text{for } (i, j, k) = (1, 2, 4), \\
|\det(U_{d^{(3)})})| & \text{for } (i, j, k) = (1, 3, 4), \\
|\det(U_{d^{(4)})})| & \text{for } (i, j, k) = (2, 3, 4), 
\end{cases}
\]
where \( d^{123}_{1}, d^{124}_{1}, d^{134}_{2} \) and \( d^{234}_{3} \) is \( s_1 \times s_2 \times s_3 \times (s_1 - w + 1) \times s_1 \times s_2 \times (s_1 - w + 1) \times s_1 \times s_2 \times s_3 \times s_w \) saturated factorial design, respectively.

**Proof** Let us assume that \( n_{123}^{\text{opt}} = w > 1, 0 \leq p \leq s_1 - 1, 0 \leq q \leq s_2 - 1, 0 \leq r \leq s_3 - 1 \), which means that the saturated design \( s_1 \times s_2 \times s_3 \times s_4 \) contains the runs \( pqr, pqr, \ldots, pqr \). By subtracting the row corresponding to \( pqr \) from the other rows which correspond to \( pqr \), adding the columns corresponding to levels \( x_1 \), \( \ldots, x_w \) to the column corresponding to level \( x_i \), and expanding \( \det(U_d) \) along the \( (w - 1) \) rows which contain levels \( x_1 \), \( \ldots, x_w \), we get \( |\det(U_d)| = |\det(U_d^{(n_{123})})| \), where \( d^{123}_{1} = s_1 \times s_2 \times s_3 \times (s_4 - w + 1) \) saturated design. The proof is similar for \( n_{124}^{\text{opt}} = w, n_{134}^{\text{opt}} = w \) and \( n_{234}^{\text{opt}} = w \). □

### 3.1. D-optimality of \( 2^s \times (s - 1) \times s \) saturated designs

**Lemma 3.3** Consider the saturated \( 2^s \times (s - 1) \times s \) design with \( N = 2s \) runs and corresponding matrix \( U_d \) as given in (1). For the D-optimal design it holds that:

\[
\begin{align*}
    n_{i}^{0} & = s, \quad i = 1, 2, \quad p = 0, 1. \\
    n_{i}^{1} & = n_{i}^{3} = 3, \quad n_{i}^{2} = 2, \quad 2 \leq p \leq (s - 2). \\
    n_{i}^{2} & = 2, \quad 0 \leq p \leq (s - 1).
\end{align*}
\]

**Proof** Expanding \( \det(U_d) \) along its first column, we have that \( |\det(U_d)| = \sum_{i=1}^{n_{i}^{0}} |\det(U_{d2}^{i})| \), where \( d^{i2}_{i} \), \( i = 1, 2, \ldots, n_{i}^{1} \) are \( 2 \times (s - 1) \times s \) saturated designs with corresponding matrices \( U_{d2}^{i} \). Let \( |\det(U_{d2}^{i})| = \max \{|\det(U_{d2}^{i})|, i = 1, 2, \ldots, n_{i}^{1}\} \). Then

\[
|\det(U_d)| \leq n_{i}^{0}|\det(U_{d2}^{i})|. \tag{4}
\]

From lemma 3.1, by interchanging the levels 0 and 1 of the first factor, it also holds

\[
|\det(U_d)| \leq n_{i}^{1}|\det(U_{d2}^{i})|. \tag{5}
\]

From (4)-(5), we get \( |\det(U_d)| \leq \frac{n_{i}^{0}n_{i}^{1}}{2} |\det(U_{d2}^{i})| = s|\det(U_{d2}^{i})| \). According to lemma 2.4, in order to find the D-optimal design \( d' \), it must hold that \( n_{i}^{0} \geq n_{i}^{1} \geq n_{i}^{3} \geq n_{i}^{2} - 1, \quad i = 2, 3, 4 \), which implies \( n_{i}^{0} = n_{i}^{1} = s, \quad n_{i}^{2} = 2, \quad 2 \leq p \leq (s - 2), \quad n_{i}^{2} = 2, \quad 0 \leq p \leq (s - 1) \). Expanding \( \det(U_d) \) along its second column, and following the same procedure we get \( n_{i}^{0} = n_{i}^{1} = s \). □

**Lemma 3.4** Consider the saturated \( 2^s \times (s - 1) \times s \) design with \( N = 2s \) runs and corresponding matrix \( U_d \) as given in (1). For the D-optimal design it holds that:

\[
    n_{i}^{0} = n_{i}^{1} = 1, \quad i = 1, 2, \quad 0 \leq q \leq (s - 1).
\]

**Proof** Suppose, w.l.o.g., that \( n_{i}^{0} = 2 \) for some \( 0 \leq p \leq (s - 1) \). Then from the pigeonhole principle, we get \( n_{i}^{0} = 2 \) for some \( q, 0 \leq p \neq q \leq (s - 1) \). From lemmas 3.1 and 3.2, we may assume that in a design \( d \) the following treatment combinations exist: \( 000^{i}, 011^{i}, 101^{i}, 110^{i}, 100^{i}, 010^{i} \). Consider now matrix \( U_d \), which corresponds to the design \( d \), as given in (1). Subtract the row corresponding to the treatment combination \( 000^{i} \) from the row corresponding to the treatment combination \( 011^{i} \). The row corresponding to the treatment combination \( 011^{i} \) is now \( r = (0, 0, 0, \ldots, 0, 0, 0, \ldots, 0, 0, \ldots, 0) \), where the second ace is at the \( (j + 2) \)-th column of \( r \), that is at the \( j \)-th column of \( Z_{1}^{j} \). Then, subtract the row \( r \) from the row corresponding to the treatment combination \( 111^{i} \). Continue by adding the column of \( Z_{1}^{j} \), which corresponds to \( r \), to the column of \( Z_{2}^{j} \) which corresponds to \( r \). Consequently, treatment combination \( 101^{i} \) is now in the position of treatment combination \( 101^{i} \). Add the row corresponding to the treatment combination \( 000^{i} \) to row \( r \). The resulting row \( r \) corresponds to the treatment combination \( 011^{i} \). Hence, the design \( d \) contains the treatment combinations \( 000^{i}, 011^{i}, 101^{i}, 110^{i}, 100^{i}, 010^{i} \), which implies \( n_{i}^{0} = 2 \). Then, proceeding as in lemma 3.2, we have that \( |\det(U_d)| = |\det(U_{d2}^{i})| \).
where \(d_2\) is \(2 \times 2 \times (s - 2) \times (s - 1)\) saturated design.

\[ \text{COROLLARY 3.1 } \text{For the D-optimal saturated } 2^2 \times (s - 1) \times s \text{ design } d \text{ with } N = 2s \text{ runs, if there exists the treatment combination } 00r_3r_4 (01r_3r_4) \text{ then there exists the treatment combination } 11r_3r_4 (10r_3r_4). \]

\[ \text{LEMMA 3.5 } \text{Consider the saturated } 2^2 \times (s - 1) \times s \text{ design } d \text{ with } N = 2s \text{ runs and corresponding matrix } U_d \text{ as given in (1). For the D-optimal design it holds that:} \]

\[
n_{oq}^{i,3} = 1, \quad i = 1, 2, \quad 0 \leq p \leq 1, \quad 2 \leq q \leq (s - 2).
\]

\[ \text{Proof } \text{The proof is similar as in lemma 3.4.} \]

\[ \text{COROLLARY 3.2 } \text{Let us now consider the saturated } 2^2 \times (s - 1) \times s \text{ design } d \text{ with } N = 2s \text{ runs. Then, from lemma 3.4 and using the pigeonhole principle, we get:} \]

\[
n_{oq}^{i,4} \leq 1, \quad 0 \leq p, q \leq (s - 1),
\]

\[
n_{oq}^{i,6} = 2, \quad 1 \leq i \leq 2, \quad 0 \leq p \leq 1, \quad 0 \leq q \leq 1.
\]

\[ \text{COROLLARY 3.3 } \text{For the D-optimal saturated } 2^2 \times (s - 1) \times s \text{ design } d \text{ with } N = 2s \text{ runs it holds that:} \]

\[
n_{oq}^{i,12} = \frac{s}{2} \text{ if } s \equiv 0 \text{ mod 2, } \quad 0 \leq p, q \leq 1,
\]

\[
n_{00}^{i,12} = n_{o1}^{i,12} = \frac{i + 1}{2} \quad \text{and} \quad n_{o1}^{i,12} = n_{10}^{i,12} = \frac{i - 1}{2} \quad \text{or} \quad \left\{ \begin{array}{c}
\text{if } s \equiv 1 \text{ mod 2.}
\end{array} \right.\]

\[ \text{LEMMA 3.6 } \text{Consider the saturated } 2^2 \times (s - 1) \times s \text{ design } d \text{ with } N = 2s \text{ runs and corresponding matrix } U_d \text{ as given in (1). For the D-optimal design it holds that:} \]

\[
n_{o0}^{i,22} = n_{o1}^{i,22} = n_{10}^{i,22} = n_{11}^{i,22} = n_{12}^{i,22} = n_{13}^{i,22} = 1. \quad (6)
\]

\[ \text{Proof } \text{From lemma 3.3, we have } n_{o0}^{i} = 3, p = 0, 1 \text{ and from lemma 3.2 and corollary 3.2 the D-optimal design includes one of the following sets of treatment combinations: } (00pr_2, 01pr_2, 11pr_2) \text{ or } (00pr_3, 01pr_3, 10pr_3) \text{ or } (11pr_3, 01pr_3, 10pr_3). \text{ Applying lemma 3.1, we can always choose, w.l.o.g. the treatment combination } 000r_4, 010r_4, 110r_4. \text{ This choice, using pigeonhole principle, implies the existence of the treatment combinations } 001r_4, 111r_4, 101r_4 \text{ and the proof of (6) is obvious.} \]

\[ \text{THEOREM 3.1 } \text{Consider the saturated } 2^2 \times (s - 1) \times s \text{ design } d \text{ with } N = 2s \text{ runs and corresponding matrix } U_d \text{ as given in (1). It holds that:} \]

\[
|\text{det}(U_d)| \leq \begin{cases} 
\frac{s^2}{2} & \text{if } s \equiv 0 \text{ mod 2,} \\
\frac{s^2}{2} & \text{if } s \equiv 1 \text{ mod 2.}
\end{cases} \quad (7)
\]

\[ \text{Proof } \text{Let } u = n_{o0}^{i,12} = n_{10}^{i,12}. \text{ So, from corollary 3.3, we have } u = s/2 \text{ if } s \equiv 0 \text{ mod 2 or } u = (s + 1)/2 \text{ if } s \equiv 1 \text{ mod 2. Moreover, from lemmas 3.1-3.6 and corollaries 3.1-3.2, w.l.o.g., the D-optimal saturated design } 2^2 \times (s - 1) \times s \text{ can be written as:} \]
Let $\theta_{2k}$ be a $1 \times k$ vector with all elements equal to zero, $I_k$ be the identify matrix of order $k$. For $m < k$, it can be easily seen that:

\[
I_k = \begin{pmatrix}
e_1k & e_2k & \cdots & e_kk \\
e_1m & 0 & \cdots & 0 \\
e_mm & 0 & \cdots & 0 \\
es_km & 0 & \cdots & 0
\end{pmatrix} = \begin{pmatrix}
e_1m & 0 & \cdots & 0 \\
e_mm & 0 & \cdots & 0 \\
e_{k-m}m & 0 & \cdots & 0 \\
e_{k-m}k & 0 & \cdots & 0
\end{pmatrix}.
\]

Matrix $U_d$ as given in (1), can be written as:

\[
U_d = \begin{pmatrix}
0 & 0 & 0 & e_{1s} \\
0 & 0 & e_{1(s-2)} & e_{2s} \\
0 & e_{(u-1)(s-2)} & e_{us} & e_{1s} \\
1 & 0 & e_{1(s-2)} & e_{2s} \\
1 & 0 & e_{1(s-2)} & e_{us} \\
1 & 0 & e_{(u-1)(s-2)} & e_{1s} \\
0 & 0 & e_{u(s-2)} & e_{(u+1)s} \\
0 & 0 & e_{u(s-2)} & e_{us} \\
0 & 0 & e_{u(s-2)} & e_{(u+2)s} \\
0 & 0 & e_{u(s-2)} & e_{us} \\
0 & e_{(s-2)(s-2)} & e_{ss} & e_{1s} \\
1 & 0 & e_{1(s-2)} & e_{(u+2)s} \\
1 & 0 & e_{1(s-2)} & e_{ss} \\
1 & 0 & e_{1(s-2)} & e_{(u+1)s} \\
1 & 0 & e_{1(s-2)} & e_{ss}
\end{pmatrix}.
\]
Using relation (8), and after permutation of columns matrix $U_d$ can be written as:

$$
U_d = \begin{pmatrix}
0_{1 \times (u-1)} & e_{1u} & 0 & 0 & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{1(u-1)} & e_{2u} & 0 & 0 & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
e_{(u-1)(u-1)} & e_{uu} & 0 & 0 & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
0_{1 \times (u-1)} & e_{1u} & 1 & 1 & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{1(u-1)} & 0_{1 \times u} & 0 & 1 & 0_{1 \times (s-u-1)} & e_{1(s-u)} \\
0_{1 \times (u-1)} & 0_{1 \times u} & 0 & 1 & e_{1(s-u-1)} & e_{2(s-u)} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0_{1 \times (u-1)} & 0_{1 \times u} & 0 & 1 & e_{(s-u-1)(s-u)} & e_{(s-u)(s-u)} \\
e_{1(u-1)} & 0_{1 \times u} & 1 & 0 & 0_{1 \times (s-u-1)} & e_{2(s-u)} \\
0_{1 \times (u-1)} & 0_{1 \times u} & 1 & 0 & e_{1(s-u-1)} & \vdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0_{1 \times (u-1)} & 0_{1 \times u} & 1 & 0 & e_{(s-u-1)(s-u)} & e_{1(s-u)} 
\end{pmatrix}
$$

(9)

Now subtract the $(2u)$-th column from the $(2u+1)$-th column and add the last $s-u$ columns to the $(2u+1)$-th column. Matrix $U_d$, as given in (9), can be written as:

$$
U_d = \begin{pmatrix}
U_{d1} & 0_{2u \times (s-u)} \\
A & U_2
\end{pmatrix}
$$

Matrix $U_{d1}$ is the design matrix of the saturated $u \times u \times 2$ design $d_1$ with $N_1 = 2u$ runs. Matrix $U_2$ is not design matrix as its first column is $(2,\ldots,2,0,\ldots,0)'$, but $|\det(U_2)| = 2|\det(U_{d1})|$, where matrix $U_{d1}$ is the design matrix of the saturated $2 \times (s-u) \times (s-u)$ design $d_1$, with $N_2 = 2(s-u)$ runs. Hence, $|\det(U_d)| = 2|\det(U_{d1})| |\det(U_{d1})|$. From (3), we get $|\det(U_d)| \leq 2 \cdot u \cdot (s-u)$. Recalling that $u = s/2$ if $s \equiv 0 \bmod 2$, or $u = (s+1)/2$ if $s \equiv 1 \bmod 2$, we get that (7) holds.

Theorem 3.2  Let $u = (s_1 + 1)/2$ if $s \equiv 1 \bmod 2$, or $u = s_1/2 + 1$ if $s \equiv 0 \bmod 2$. The saturated $2^2 \times s_1 \times s_u$ design $d'$ with the following $N = s_1 + s_u + 1$ treatment combinations $00i (0 \leq i \leq u-1)$, $110(u-1)$, $1i(i+1)i (0 \leq i \leq u-2)$, $100u$, $10i(i+1)i (u \leq i \leq s_1 - 1)$, $010s_{s_1}$, $01ii (u \leq i \leq s_1 - 1)$, $01(s_1 - 1)i (s_1 + 1 \leq i \leq s_u - 1)$ is a $D$-optimal design in the class of all $2^2 \times s_1 \times s_u$ designs.

Proof The proof is obvious from lemma 2.3, lemmas 3.1-3.6 and theorem 3.1.

3.2. $D$-optimality of $2^2 \times s^2$ saturated designs

Lemma 3.7 Consider the saturated $2^2 \times s^2$ design $d$ with $N = 2s + 1$ runs and corresponding matrix $U_d$ as given in (1). For the $D$-optimal design, it holds that:

$n_0^0 = s + 1$ and $n_1^i = s$, or $n_0^i = s$ and $n_1^i = s + 1$, $i = 1, 2$.

$n_0^3 = 3$, $n_0^p = 2$, $i = 3, 4$, $1 \leq p \leq s - 1$.

Proof The proof is similar as lemma 3.3.
Corollary 3.4 For the saturated $2^2 \times s^2$ design $d$ with $N = 2s + 1$ runs, from lemma 3.2 and using the pigeonhole principle we get:

\[
\begin{align*}
n_{ij}^{pq} &\leq s + 1, \quad 0 \leq p, q \leq 1, \\
n_{ij}^{pq} &\leq 2, \quad 0 \leq p, q \leq s - 1, \\
n_{ij}^{pq} &\leq 2, \quad 1 \leq i \leq 2, \quad 0 \leq p \leq 1, \quad 3 \leq j \leq 4, \quad 0 \leq q \leq s - 1.
\end{align*}
\]

Lemma 3.8 Consider the saturated $2^2 \times s^2$ design $d$ with $N = 2s + 1$ runs and corresponding matrix $U_d$ as given in (1). For the D-optimal design, it holds that:

\[
\begin{align*}
n_{ij}^{1q} &\equiv 1, \quad i = 1, 2, \quad 1 \leq q \leq (s - 1). \quad (10) \\
n_{ij}^{00} &\equiv 2, \quad \text{or} \quad n_{ij}^{10} \equiv 2, \quad i = 1, 2, \quad 3 \leq j \leq 4. \quad (11)
\end{align*}
\]

Proof For the proof of relation (10) see lemma 3.4. The proof of relation (11) is obvious, since $n_{ij}^{0} = s + 1$ or $n_{ij}^{0} = s + 1$. □

Corollary 3.5 For the D-optimal saturated $2^2 \times s^2$ design $d$ with $N = 2s + 1$ runs it holds that:

\[
\begin{align*}
n_{ij}^{1q} &\equiv 1, \quad i = 1, 2, \quad 1 \leq q \leq (s - 1). \quad (10) \\
n_{ij}^{00} &\equiv 2, \quad \text{or} \quad n_{ij}^{10} \equiv 2, \quad i = 1, 2, \quad 3 \leq j \leq 4. \quad (11)
\end{align*}
\]

Proof For the proof of relation (10) see lemma 3.4. The proof of relation (11) is obvious, since $n_{ij}^{0} = s + 1$ or $n_{ij}^{0} = s + 1$. □

Theorem 3.3 Consider the saturated $2^2 \times s^2$ design $d$ with $N = 2s + 1$ runs and corresponding matrix $U_d$ as given in (1). It holds that:

\[
|\text{det}(U_d)| \leq \frac{ss + 1}{2}. \quad (12)
\]

Proof If $s \equiv 0$ mod 2, then $u = s/2 = n_{12}^{00} = n_{12}^{01} = n_{12}^{11}$ and $n_{12}^{10} = u + 1$, while if $s \equiv 1$ mod 2, then $u = (s - 1)/2 = n_{12}^{01}$ and $n_{12}^{00} = n_{12}^{10} = n_{12}^{11} = u + 1$. From lemmas 3.7-3.8 and corollaries 3.4-3.5, the D-optimal saturated $2^2 \times s^2$ design, w.l.o.g., can be written as:
By interchanging the levels 0 and \((s - 1)\) of the 4-th factor, according to lemma 3.1, the determinant of the matrix \(U_d\) is left invariant. Hence the D-optimal saturated \(2^2 \times s^2\) design, w.l.g., can be written as:

\[
\begin{pmatrix}
1 & 0 & 0 & u - 1 \\
1 & 0 & 1 & s - 1 \\
1 & 0 & 2 & 1 \\
\vdots & \vdots & \vdots & \vdots \\
1 & 0 & u - 1 & u - 2 \\
1 & 0 & u & 0 \\
0 & 1 & 1 & 1 \\
\vdots & \vdots & \vdots & \vdots \\
0 & 1 & u - 1 & u - 1 \\
0 & 1 & u & s - 1 \\
1 & 1 & 0 & u \\
1 & 1 & u + 1 & u + 1 \\
\vdots & \vdots & \vdots & \vdots \\
1 & 1 & s - 2 & s - 2 \\
1 & 1 & s - 1 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & u + 1 & u \\
\vdots & \vdots & \vdots & \vdots \\
0 & 0 & s - 1 & s - 2 \\
\end{pmatrix}
\]

Matrix \(U_d\) as given in (1), can be written as:

\[
\begin{pmatrix}
1 & 0 & 0 & u - 1 \\
1 & 0 & 1 & 0 \\
\vdots & \vdots & \vdots & \vdots \\
1 & 0 & u - 1 & u - 2 \\
1 & 0 & u & s - 1 \\
0 & 1 & 1 & 1 \\
\vdots & \vdots & \vdots & \vdots \\
0 & 1 & u - 1 & u - 1 \\
0 & 1 & u & s - 1 \\
1 & 1 & 0 & u \\
1 & 1 & u + 1 & u + 1 \\
\vdots & \vdots & \vdots & \vdots \\
1 & 1 & s - 1 & s - 1 \\
0 & 0 & 0 & s - 1 \\
0 & 0 & u + 1 & u \\
\vdots & \vdots & \vdots & \vdots \\
0 & 0 & s - 1 & s - 2 \\
\end{pmatrix}
\]
Using relation (8), and after a suitable permutation of columns of the matrix $U_d$, in order to make the left bottom block of the matrix $U_d$ a zero matrix, matrix $U_d$ can be written as:

$$
U_d = \begin{pmatrix}
1 & 0 & 0_{1 \times (s-1)} & e_{us} \\
1 & 0 & e_{1(s-1)} & e_{1s} \\
\vdots & \vdots & \vdots & \vdots \\
1 & 0 & e_{(u-1)(s-1)} & e_{(u-1)s} \\
1 & 0 & e_{u(s-1)} & e_{ss} \\
0 & 1 & e_{1(s-1)} & e_{2s} \\
\vdots & \vdots & \vdots & \vdots \\
0 & 1 & e_{(u-1)(s-1)} & e_{us} \\
0 & 1 & e_{u(s-1)} & e_{1s} \\
1 & 1 & 0_{1 \times (s-1)} & e_{(u+1)s} \\
1 & 1 & e_{(u+1)(s-1)} & e_{(u+2)s} \\
\vdots & \vdots & \vdots & \vdots \\
1 & 1 & e_{(s-1)(s-1)} & e_{ss} \\
0 & 0 & 0_{1 \times (s-1)} & e_{ss} \\
0 & 0 & e_{(u+1)(s-1)} & e_{(u+1)s} \\
\vdots & \vdots & \vdots & \vdots \\
0 & 0 & e_{(s-1)(s-1)} & e_{(s-1)s}
\end{pmatrix}.
$$

Analytically, the permutation is: the first $u$ columns of matrix $U_d$ are the first $u$ columns of matrix $Z_1^{(u)}$, columns $(u + 1) - 2u$ of matrix $U_d$ are the first $u$ columns of matrix $Z_u$ $(2u + 1)$-th column of matrix $U_d$ is matrix $Z_1^{(u)}$, $(2u + 2)$-th column of matrix $U_d$ is matrix $Z_2^{(u)}$, while the remaining $(2s + 1) - (2u + 2)$ columns of matrix $U_d$ are the rest columns of matrices $Z_3^{(u)}$ and $Z_u$. 

$$
U_d = \begin{pmatrix}
0_{1 \times u} & e_{(u-1)u} & e_{uu} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{1u} & e_{(s-1)u} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{2u} & e_{1u} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
\vdots & \vdots & \vdots & \vdots \\
e_{(u-1)u} & e_{(u-2)u} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{uu} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u-1)} & e_{1x}
\end{pmatrix}.
$$

$$
U_d = \begin{pmatrix}
0_{1 \times u} & e_{uu} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{1u} & e_{1u} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
\vdots & \vdots & \vdots & \vdots \\
e_{(u-1)u} & e_{(u-1)u} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
e_{uu} & e_{uu} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
0_{1 \times u} & e_{uu} & 0_{1 \times (s-u-1)} & 0_{1 \times (s-u)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{uu} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(u+1)(s-u-1)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-2)(s-u-1)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-1)(s-u-1)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-1)(s-u-1)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-2)(s-u)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-1)(s-u)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-1)(s-u)} \\
0_{1 \times u} & 0_{1 \times u} & 0_{1 \times (s-u-1)} & e_{(s-2)(s-u)]}
\end{pmatrix}.
$$
Now subtract the $(2u + 2)$th column from the $(2u + 1)$th column. Then, matrix $U_d$ is a block triangular matrix. It holds that $\det(U_d) = \det(U_{d1})\det(U_{d2})$, where matrix $U_{d1}$ is a $(2u + 1) \times (2u + 1)$ matrix, which does not correspond to any design and matrix $U_{d2}$ is the design matrix of the saturated $2 \times (s - u) \times (s - u)$ design $d_2$ with $N_2 = 2(s - u)$ runs. From (3), we get $|\det(U_{d2})| \leq (s - u)$. Moreover, expanding $\det(U_{d1})$ along its last column we get that $|\det(U_{d1})| \leq \sum_{i=1}^{2u} |\det(X_i)|$, where, after some manipulations, $X_i$ correspond to two factor saturated designs $e_i$, with, according to lemma 2.1, $|\det(X_i)| = 1$. Hence, $|\det(U_d)| \leq (2u + 1)(s - u)$. Recalling that $u = s/2$ if $s \equiv 0 \mod 2$, or $u = (s - 1)/2$ if $s \equiv 1 \mod 2$, we get that (11) holds.

**Theorem 3.4** Let $u = s/2$ if $s \equiv 0 \mod 2$, or $u = (s - 1)/2$ if $s \equiv 1 \mod 2$. The saturated $2^2 \times s^2$, $s \geq 2$ design $d^*$ with the following $N = 2s + 1$ runs $100(u - 1)$, $101(s - 1)$, $10(i + 1)ii (1 \leq i \leq u - 2)$, $10u0$, $01ii (1 \leq i \leq u - 1)$, $01u(s - 1)$, $110u$, $11ii (u + 1 \leq i \leq s - 2)$, $11(s - 1)0$, $0000$, $00(i + 1)ii (u \leq i \leq s - 2)$, is a D-optimal design in the class of all $2^2 \times s^2$, $s \geq 2$ saturated designs.

**Proof** From lemma 2.3, lemmas 3.1, 3.2, 3.7, 3.8 and theorem 3.3, the proof is obvious.

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**References**


