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BALANCED OPTIMAL SATURATED MAIN EFFECT PLANS OF THE 2^n FACTORIAL AND THEIR RELATION TO (v, k, λ) CONFIGURATIONS[1]

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This paper characterizes balanced saturated main effect plans of the 2^n factorial in terms of $D'D$ rather than $X'X$, where D is the $(n+1) \times n$ treatment combination matrix and X is the $(n+1) \times (n+1)$ design matrix. Besides this result, balanced optimal (in the sense of maximum determinant of $X'X$) saturated main effect plans of the 2^{4m-1} factorial are discussed for various classes of designs, each class consisting of designs having $(0, 0, \cdots 0)$ and n treatment combinations with exactly t 1's among them. The optimality results are achieved by applying theorems associated with incidence matrices of (v, k, λ) configurations. In addition results are given for designs associated with the permuted (v, k, λ) configurations. Finally, the approach taken in the paper can be applied to 2^n factorials with $n \neq 4m - 1$.

1. Summary. This paper presents a characterization of balanced saturated main effect plans in terms of $D'D$ rather than $X'X$, where D is the $(n+1) \times 1$ treatment combination matrix consisting of 0's and 1's and X is the $(-1, 1)$ design matrix of order $(n+1) \times 1$. Balanced optimal saturated main effect plans are discussed for various classes of the 2^{4m-1} factorial, each class consisting of designs having $(0, 0, \cdots, 0)$ and n treatment combinations with t 1's among them. The results rely heavily on an optimality theorem concerning (v, k, λ) configurations, where the number of 1's in the incidence matrix is equal to t. Also, complementary results are obtained by using a permutation of the levels. Finally, the results can be extended to 2^n factorials with $n \neq 4m - 1$.

2. Introduction. Fractional factorials present some challenging problems in treatment designs. Even when dealing with the simplest situation, such as main effect plans of the 2^n factorial, one is confronted with problems of a highly complex combinatorial nature. Some of these problems have been pointed out and investigated by Federer, Paik, Raktoe, and Werner (1972), Paik and Federer (1970), (1972), and Raktoe and Federer (1970b), (1971). Problems for other types of plans from the 2^n factorial and other factorials are currently being studied intensively by Srivastava and Chopra (1971), Srivastava and Anderson (1970), Banerjee (1970), Srivastava, Raktoe, and Pesotan (1971), and Pesotan, Raktoe

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and Federer (1972). These and other authors have demonstrated the mathematical and statistical richness of factorial experiments.

To make this paper relatively self-contained we introduce the following notations and definitions:

(i) In a 2^n factorial experiment with n factors at two levels each, a treatment combination is an n-tuple $(x_1, x_2, \cdots, x_n)$, with $x_i \in \{0, 1\}$.

(ii) A set of $(n + 1)$ treatment combinations arranged in arbitrary order in an $(n + 1) \times n$ matrix D (a row being a treatment combination) with the aim of estimating the vector β, consisting of the mean and the main effects (when the assumption that all other effects are negligible is justified) is called a saturated main effect plan.

(iii) The $(n + 1) \times (n + 1)$, $(-1, 1)$-matrix X_D corresponding to D and the parameters in (ii) is called the design matrix of D; $X_D'X_D$ is called the information matrix of the design D.

(iv) I will be a square identity matrix, J a rectangular matrix consisting of $+1$'s and $\mathbf{1}$ will be a column vector of $+1$'s; 0 is either a matrix or a vector of zeros.

(v) A balanced saturated main effect plan of the 2^n factorial is a design D such that: (a) each element of β is estimated with the same variance, (b) the covariance between the estimates of the mean μ and a main effect is a constant, and (c) the covariance between estimates of two main effects is another constant.

(vi) Optimality of a saturated main effect plan may be defined in many ways. We will be using maximum determinant of $X_D'X_D$ as our criterion for denoting a design optimal.

3. Balanced saturated main effect plans. Let $\mathscr{D}$ be the class of all possible designs which can be formed by selecting $n + 1$ treatment combinations from among 2^n treatment combinations. Obviously the cardinality of $\mathscr{D}$ is equal to $(2^n!)/(n + 1)!\,(2^n - n - 1)!$. If D is any arbitrary design in $\mathscr{D}$, then the relation

$$X_D = [\mathbf{1}_{(n+1)\times 1} \vdots 2D_{(n+1)\times n} - J_{(n+1)\times n}] \tag{3.1}$$

leads at once to the following result (which has already been established through a different approach in a paper by Raktoe and Federer (1970a).

$$X_D'X_D = \left[\begin{array}{c|c} n+1 & z' \\ \hline z & Z \end{array}\right], \tag{3.2}$$

where

$$z_{n\times 1} = -(n + 1)\mathbf{1}_{n\times 1} + 2D'_{n\times(n+1)}\mathbf{1}_{(n+1)\times 1}\,, \quad \text{and}$$

$$Z_{n\times n} = (n + 1)J_{n\times n} - 2D'_{n\times(n+1)}J_{(n+1)\times n} - 2J'_{n\times(n+1)}D_{(n+1)\times n} + 4D'_{n\times(n+1)}D_{(n+1)\times n}\,.$$

Utilizing (3.2) we see that a design D will be balanced if and only if

$$D'D = \tfrac{1}{4}(n + 1 - b)I_{n\times n} + \tfrac{1}{4}(n + 1 + 2a + b)J_{n\times n} \tag{3.3}$$

where a and b are integers such that $\frac{1}{2}(n+1+a)$ and $\frac{1}{4}(n+1+2a+b)$ are integers between 0 and $n+1$.

The proof of this proposition is as follows. From the definition in (v) of Section 2 we know that a design D is balanced if and only if the information matrix is of the form

$$X_D'X_D = \left[\begin{array}{c|c} n+1 & a\mathbf{1}'_{1\times n} \\ \hline a\mathbf{1}_{n\times 1} & (n+1-b)I_{n\times n} + bJ_{n\times n} \end{array}\right]. \tag{3.4}$$

Hence, from (3.2) we have $a\mathbf{1}' = -(n+1)\mathbf{1} + 2\mathbf{1}'D$ and $(n+1)J - 2D'J - 2J'D + 4D'D = (n+1-b)I + bJ$, so that $(n+1)J - (a+n+1)J - (a+n+1)J + 4D'D = (n+1-b)I + bJ$. Hence:

$$D'D = \tfrac{1}{4}(n+1-b)I + \tfrac{1}{4}(n+1+2a+b)J. \tag{3.5}$$

Since a diagonal element of $D'D$ is the squared length of a (0, 1)-vector, it follows immediately that $\frac{1}{4}(n+1-b) + \frac{1}{4}(n+1+2a+b) = \frac{1}{2}(n+1+a)$ is an integer between 0 and $n+1$. The innerproduct of two (0, 1)-vectors is quite clearly an integer between 0 and $n+1$ and hence $\frac{1}{4}(n+1+2a+b)$ is such a number. This completes the proof of the proposition.

REMARK 3.1. One of the referees has pointed out that result (3.3) may also be proved by noting the following:

(i) Each column of D must have the same number of 1's, say r, since $a =$ (number of 1's) $-$ (number of 0's) for each column. Since the (number of 1's) $+$ (number of 0's) $= n+1$ it follows that $0 < r = \frac{1}{2}(n+1+a) < n+1$.

(ii) It is easy to show that for any two columns of D the number of (1, 1) matches must be constant, say λ, since for any pair of columns $b =$ (number of (1, 1) matches) $-$ (number of (1, 0) matches) $-$ (number of (0, 1) matches) $+$ (number of (0, 0) matches). Hence $b = \lambda - (r-\lambda) - (r-\lambda) + [(n+1) - \lambda - 2(r-\lambda)]$.

(iii) Therefore $\lambda = \frac{1}{4}[b + 4r - (n+1)] = \frac{1}{4}(n+1+2a+b)$, so that $D'D = rI + \lambda(J-1) = (r-\lambda)I + \lambda J$. This proof does not depend on result (3.2).

REMARK 3.2. From (3.4) one can show in a straightforward manner that the characteristic roots of the information matrix $X_D'X_D$ for a balanced design $D \in \mathscr{D}$ are:

$$\begin{aligned} \lambda_1 &= (n+1-b) \quad \text{with multiplicity} \quad n-1, \\ \lambda_2 &= \tfrac{1}{2}[2(n+1) + (n-1)b] + \tfrac{1}{2}[(n-1)^2b^2 + 4na^2]^{\frac{1}{2}}, \\ \lambda_3 &= \tfrac{1}{2}[2(n+1) + (n-1)b] - \tfrac{1}{2}[(n-1)^2b^2 + 4na^2]^{\frac{1}{2}}. \end{aligned} \tag{3.6}$$

Using (3.6) it follows that a balanced design will be singular (i.e. det $X_D'X_D = 0$) if and only if $a = \{(n+1)/n[(n+1)+(n-1)b]\}^{\frac{1}{2}}$ or $b = n+1$. Hence a singular balanced design $D \in \mathscr{D}$ is characterized by

$$\begin{aligned} &D'D = \tfrac{1}{2}(n+1+a)J \qquad \text{or} \\ &D'D = \tfrac{1}{4}(n+1-b)I \\ &\qquad + \tfrac{1}{4}([n+1] + 2\{(n+1)/n[(n+1)+(n-1)b]\}^{\frac{1}{2}} + b)J. \end{aligned} \tag{3.7}$$

How useful the singularity test (3.7) is depends in practice on whether calculation of the rank of $[\mathbf{1} \vdots D]$ or the determinant of $[\mathbf{1} \vdots D]$ requires more time than the calculation of $D'D$ and seeing if it is of the form. Aside from the practicality of (3.7) this characterization could become a tool in enumeration problems.

REMARK 3.3. Using (3.6) the maximization of det $X_D'X_D$ results in the solution $a = 0$ and $b = 0$. This then provides us with a characterization of optimal balanced designs, or Hadamard designs. In this case $D'D = \frac{1}{4}(n+1)I + \frac{1}{4}(n+1)J$. Denoting the class of balanced designs in $\mathscr{D}$ by $\mathscr{D}^+$ we should observe that the Hadamard designs are not only det-optimal in $\mathscr{D}^+$ but also in $\mathscr{D}$. Of course this fact was observed by Plackett and Burman (1946) and also by the authors (1970a). Since a necessary condition for the existence of these plans is that $(n+1)$ is divisible by 4 we may write $n + 1 = 4m$ so that the characterization becomes $D'D = mI + mJ$.

4. The weight of a design, (v, k, λ) configurations and optimality. Let $w(D) = \mathbf{1}'D\mathbf{1}$ (= the number of 1's) be the weight function for a design $D \in \mathscr{D}$. The weight function can be given the following interpretation. If the low level 0 of any factor costs 0 and the high level 1 costs 1 unit then $w(D)$ is the total cost of design D. Define two designs D_1 and D_2 in $\mathscr{D}$ to be weight equivalent, in symbols $D_1 = wD_2$, if and only if $w(D_1) = w(D_2)$. The equivalence relation $= w$ leads to a partitioning of $\mathscr{D}$ into the set of equivalence classes $\mathscr{D}/_{=w}$. This means that if $\mathscr{H}$ is an equivalence class in $\mathscr{D}/_{=w}$, all designs in $\mathscr{H}$ have the same weight. Werner (1971) in her masters thesis has given a counting formula for the cardinality of $\mathscr{D}/_{=w}$ and also for any equivalence class $\mathscr{H} \in \mathscr{D}/_{=w}$. These results are reported in the paper by Federer, Paik, Raktoe, and Werner (1972).

Consider the class $\mathscr{D}^0 \subset \mathscr{D}$ consisting of all designs such that each one has $(0, 0, \cdots, 0)$ in it. Clearly the cardinality of $\mathscr{D}^0$ is equal to $(2^n - 1)!/(n!)(2^n - n - 1)!$ The cardinality of $\mathscr{D}^0/_{=w}$ and of any equivalence class in $\mathscr{D}^0/_{=w}$ was also developed by Werner and is given in the above mentioned paper. If a design $D^0 \in \mathscr{D}^0$ is selected, then from Raktoe and Federer (1970a) it follows that

$$|\det X_{D^0}| = 2^n \left|\det \mathbf{1} \begin{array}{c} \vdots\ 0' \\ \cdots \\ \vdots\ D^* \end{array}\right| = 2^n |\det D^*| \tag{4.1}$$

where D^* is an $n \times n$ (0, 1)-matrix without rows consisting entirely of zeros. From Williamson (1946) and Ryser (1956) we know that

$$|\det D^*| \leqq 2^{-n}(n+1)^{(n+1)/2} \tag{4.2}$$

with equality holding if and only if D^* is obtained from a Hadamard matrix, i.e. in the case of equality we have

$$|\det D^*| = 2^{-(4m-1)}(4m)^{2m} . \tag{4.3}$$

Let $\mathscr{D}^*$ be the class of designs such that a design $D^* \in \mathscr{D}^*$ consists of n

treatment combinations and such that $(0, 0, \cdots, 0)$ is not in D^*. Clearly the cardinality of $\mathscr{D}^*$ is equal to the cardinality of $\mathscr{D}^0$. Under the equivalence relation $= w$, similarly defined for two designs in $\mathscr{D}^*$, the set of equivalence classes is $\mathscr{D}^*/_{=w}$. Let $\mathscr{H}^*(t)$ denote the equivalence class in $\mathscr{D}^*/_{=w}$ such that each $D^* \in \mathscr{H}^*(t)$ has $w(D^*) = t$. It can be easily verified that for the 2^n factorial the range of t is given by

$$n \leqq t \leqq n^2 - n + 1 . \tag{4.4}$$

Following Ryser (1963) we define a v, k, λ configuration (or v, k, λ design) to be an arrangement of v elements into v sets such that each set contains exactly k distinct elements and such that each pair of sets has exactly λ elements in common, where $0 \leqq \lambda < k < v$. (Note that we are allowing λ to be equal to 0.) In design terminology a v, k, λ configuration is a balanced incomplete block design with parameters v, $b = v$, k, $r = k$, and λ. The $v \times v$ (0, 1)-incidence matrix of a v, k, λ configuration satisfies the properties:

$$A'A = AA' = (k - \lambda)I + \lambda J \tag{4.5}$$

$$|\det A| = k(k - \lambda)^{(v-1)/2} . \tag{4.6}$$

Let Q be a (0, 1)-matrix of order v, containing exactly t 1's, i.e. $w(Q) = \mathbf{1}'Q\mathbf{1} = t$. Let $k = t/v$ and set $\lambda = k(k - 1)/(v - 1)$, with $0 \leqq \lambda < k < v$, then it follows from Ryser's (1956) results that:

$$|\det Q| \leqq k(k - \lambda)^{(v-1)/2} \tag{4.7}$$

with equality holding if and only if Q is the incidence matrix of a v, k, λ configuration.

Taking (4.4) into account, we note that for a $v = n$, $k = t/n$, $\lambda = (t/n)(t/n - 1)/(n - 1) = t(t - n)/n^2(n - 1)$ configuration to make sense, we must consider the values $n, 2n, 3n, \cdots, (n - 1)(n)$ for t. Setting $t = dn$, $d = 1, 2, \cdots, n - 1$, we see that $k = d$, $\lambda = d(d - 1)/(n - 1)$. Hence for a $v = n$, $k = d$, $\lambda = d(d - 1)/(n - 1)$ configuration to exist we must have that λ is a nonnegative integer, i.e., $d(d - 1)$ is divisible by $(n - 1)$. As an illustration, the following table shows values of v, k, λ for $v = n \leqq 7$:

(4.8)

v	2	3	4	5
(k, λ)	(1, 0)	(1, 0), (2, 1)	(1, 0), (3, 2)	(1, 0), (4, 3)
v	6	7	etc.	
(k, λ)	(1, 0), (5, 4)	(1, 0), (3, 1), (4, 2), (6, 5)	etc.	

Clearly, λ is a nonnegative integer *for all n* if $t = n$ or $t = (n - 1)n$. In these cases we have the $n, 1, 0$ and $n, n - 1, n - 2$ configurations respectively. Using the definition of $\mathscr{D}^*$ and denoting an equivalence class of fixed weight t in $\mathscr{D}^0/_{=w}$ by $\mathscr{H}^0(t)$, it follows immediately that the cardinality of $\mathscr{H}^0(n)$ and $\mathscr{H}^0(n(n - 1))$ is equal to 1. The unique optimal balanced design of weights n

and $n(n-1)$ are therefore:

$$(4.9)\qquad D_1^0 = \begin{bmatrix} 0 & 0 & 0 \cdots 0 & 0 \\ 1 & 0 & 0 \cdots 0 & 0 \\ 0 & 1 & 0 \cdots 0 & 0 \\ \cdot & \cdot & \cdot \quad \cdot \quad \cdot & \cdot \\ 0 & 0 & 0 \cdots 0 & 1 \end{bmatrix}, \qquad D_2^0 = \begin{bmatrix} 0 & 0 & 0 \cdots 0 & 0 \\ 0 & 1 & 1 \cdots 1 & 1 \\ 1 & 0 & 1 \cdots 1 & 1 \\ \cdot & \cdot & \cdot \quad \cdot \quad \cdot & \cdot \\ 1 & 1 & 1 \cdots 1 & 0 \end{bmatrix}.$$

These designs are such that $D_1^{0\prime} D_1^0 = I$ and $D_2^{0\prime} D_2^0 = I + (n-2)J$.

There are various classes of 2^n factorials one can study taking into account the weight function. There are four exhaustive cases, namely:

$$(4.10)\qquad \text{(i)}\ \ n = 4m, \qquad \text{(iii)}\ \ n = 4m - 2$$
$$\text{(ii)}\ \ n = 4m - 1, \qquad \text{(iv)}\ \ n = 4m - 3.$$

Let us limit ourselves in this paper to case (ii). The same approach however can be used to resolve the other cases. If $n = 4m - 1$, then the range of $w(D^*)$ for any design $D^* \in \mathscr{D}^*$ is:

$$(4.11)\qquad 4m - 1 \leqq t = w(D^*) \leqq (4m-1)(4m-2) + 1.$$

For the $v = 4m - 1$, $k = t/(4m-1)$, $\lambda = t(t - 4m + 1)/(4m-1)^2(4m-2)$ configuration to make sense, we must have $t \in \{4m-1, 2(4m-1), \cdots, (4m-2)(4m-1)\}$. Let $t = q(4m-1)$, with $q \in \{1, 2, \cdots, (4m-2)\}$, then $k = q$, $\lambda = q(q-1)/(4m-2)$. Now, λ must be a nonnegative integer, i.e. $q(q-1)$ must be divisible by $4m-2$. The only choices of q which satisfy this condition are $q_1 = 1$, $q_2 = 2m$, $q_3 = 2m-1$, and $q_4 = 4m-2$. The first and last solutions lead to the configurations corresponding to the unique designs in (4.9). The solutions q_2 and q_3 along with (4.7) lead us to the following result:

THEOREM 4.1. *The balanced saturated main effect plans corresponding to the* $v = 4m-1$, $k = 2m$ *and* $\lambda = m$ *configuration is* det-*optimal in the equivalence class* $\mathscr{H}^0(2m(4m-1))$ *and the balanced saturated main effect plan corresponding to the* $v = 4m-1$, $k = 2m-1$, $\lambda = m-1$ *configuration is* det-*optimal in the equivalence class* $\mathscr{H}^0((2m-1)(4m-1))$.

REMARK 4.1. The balanced saturated main effect plan in the first part of Theorem 4.1 is the incidence matrix of the Hadamard (v, k, λ) configuration augmented with $(0, 0, \cdots, 0)$. It is well known that when t *is not fixed*, then the plan is optimal in $\mathscr{D}^0$ and in $\mathscr{D}$. But clearly we are not interested in these classes but rather in classes consisting of designs with fixed weights. Note that the balanced optimal plans of Theorem 4.1 satisfy the following equations respectively:

$$(4.10)\qquad D^{0\prime} D^0 = mI + mJ$$
$$D^{0\prime} D^0 = mI + (m-1)J.$$

5. Permuted optimal plans and permuted v, k, λ configurations. Again restricting ourselves to the 2^{4m-1} factorial and looking at the four configurations of the previous section, i.e. (i) $v = 4m - 1$, $k = 1$, $\lambda = 0$ (ii) $v = 4m - 1$, $k = 2m$, $\lambda = m$, (iii) $v = 4m - 1$, $k = 2m - 1$, $\lambda = m - 1$, and (iv) $v = 4m - 1$, $k = 4m - 2$, $\lambda = 4m - 3$, then if we permute 0's to 1's and 1's to 0's in the incidence matrices of these configurations we obtain the *permuted configurations* ($\bar{\text{i}}$) $v = 4m - 1$, $k = 4m - 2$, $\lambda = 4m - 3$, ($\overline{\text{ii}}$) $v = 4m - 1$, $k = 2m - 1$, $\lambda = m - 1$, ($\overline{\text{iii}}$) $v = 4m - 1$, $k = 2m$, $\lambda = m$, and ($\overline{\text{iv}}$) $v = 4m - 1$, $k = 1$, $\lambda = 0$. Clearly the configurations (i) to (iv) are closed under permutation of 1's to 0's and 0's to 1's.

Consider the *permuted* saturated main effect plans obtained from the configurations ($\bar{\text{i}}$) to ($\overline{\text{iv}}$) and augmentation of $\mathbf{1}' = (1, 1, \cdots, 1)$. Equivalently these designs are obtained by the permutation map:

$$\tau : \begin{bmatrix} 0' \\ \cdots \\ D^* \end{bmatrix} \rightarrow \begin{bmatrix} \mathbf{1}' \\ \cdots \\ \bar{D}^* \end{bmatrix} \tag{5.1}$$

where $\bar{D}^*$ is the matrix obtained from D^* by replacing 0's by 1's and 1's by 0's. In other words, if D^* is the incidence matrix of a v, k, λ configuration then $\bar{D}^*$ is the incidence matrix of the permuted v, k, λ configuration.

Paik and Federer (1970) and more recently Srivastava, Raktoe, and Pesotan (1971) (in a more general setting) have shown that if $D \in \mathscr{D}$ is a saturated main effect plan and $\bar{D} \in \mathscr{D}$ is obtained from D by permuting the levels 0 and 1 of the factors, then the corresponding information matrices have the same determinant.

By invoking this invariance result it follows immediately that the permuted designs corresponding to configurations ($\bar{\text{i}}$) and ($\overline{\text{iv}}$) are unique optimal designs with weights equal to $(4m - 1)^2$ and $2(4m - 1)$ respectively. A theorem similar to Theorem 4.1 can be stated which has as results that the permuted designs corresponding to configurations ($\overline{\text{ii}}$) and ($\overline{\text{iii}}$) are optimal in the equivalence classes $\mathscr{H}^1(2m(4m - 1))$ and $\mathscr{H}^1((2m + 1)(4m - 1))$ respectively, where $\mathscr{H}^1$ is an equivalence class in $\mathscr{D}^1/_{=w}$, $\mathscr{D}^1$ being the class of designs in $\mathscr{D}$ having always the treatment combination $(1, 1, \cdots, 1)$ in them. The four optimal designs are characterized by the following four equations:

$$\begin{aligned} D^{1\prime}D^1 &= I + (4m - 2)J \\ D^{1\prime}D^1 &= mI + mJ \\ D^{1\prime}D^1 &= mI + (m + 1)J \\ D^{1\prime}D^1 &= I + J\,. \end{aligned} \tag{5.2}$$

REMARK 5.1. From Srivastava, Raktoe, and Pesotan (1971) it follows that the information matrices of the optimal designs and the corresponding permuted ones are orthogonally similar. From the fractional replicate viewpoint and optimality criteria based on the spectrum of the information matrix, the optimal designs and the corresponding permuted ones are information wise equivalent. However, physically and economically these designs are quite different, so that choosing among them can be done on the bases of a physical property or as set out in this paper on the basis of the weights.

6. Discussion. In this paper we have explored the case $n = 4m - 1$, i.e. the number of two level factors is equal to $4m - 1$. The results may be extended to the other three cases mentioned in the paper. To our knowlege, this is the first paper which shows how the number of 1's are important in classifying and characterizing balanced optimal plans. Work on the distribution of 1's in saturated main effect plans and their relation to values det $X_D'X_D$ was started by Werner (1971). She attempted to tie up the value of the determinant of $X_D'X_D$ with the number of 1's in D. The results obtained herein apply to this problem in that for a given number of ones in D^* it is shown that when a v, k, λ configuration exists then the corresponding plan D^0 is optimal in the sense that the determinant of $X'_{D^0}X_{D^0}$ is maximum. When a v, k, λ configuration does not exist then one may study $(v, k, \lambda_1, \lambda_2, \cdots, \lambda_s)$ configurations (i.e. partially balanced configurations) for the various values of weight function of D^*. Proceeding in this manner, one may be able to determine the various values for the determinant of $X'_{D^0}X_{D^0}$.

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