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Construction of D-optimal saturated designs for main effects and F_1 -second-order interactions in the presence of a free factor

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ABSTRACT

The allocation of resources in a 2^k -factorial experiment is crucial when the experimental resources are limited. In practice, when resources are limited, it is common for investigators to use all the information at their disposal to reduce the amount of resources needed for an experiment without trading the accuracy of the experiment. Suppose we have $k + 1$ factors and the investigator knows one of the factors (we call this factor an extra factor throughout the paper) does not interact with any of the remaining k factors. Furthermore, the investigator believes among the remaining k factors, one factor potentially interacts with the rest of the $k - 1$ factors. In this paper, we show how a D-optimal saturated design can be constructed for this problem with the minimum number of runs. In the process, we show the investigator can even forgo the presence of the extra factor in certain runs without compromising the D-optimality of the saturated design.

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1. Introduction

In a 2^k -factorial experiment, the allocation of resources is crucial when the experimental resources are limited. When that is the case, it is desirable for the investigator to conduct the screening experiment with a saturated design (SD). That is a design with the minimum number of runs that would ensure the unbiased estimation of the main effects and interactions of interest given the remaining parameters are negligible. Thus a saturated design is defined as a square non-singular matrix with entries from $\{-1, 1\}$ that is used as a design matrix to obtain the unbiased estimation of the parameters of interest that have been identified by the investigator. Note that once the SD is chosen the OLS can be used to estimate the parameters of interest. Concretely, the linear model for an SD is $Y = X\beta + \epsilon$, where Y is the response variable and ϵ is the usual error term. The matrix X is a saturated design matrix for the given vector parameter of interest β . Using the OLS, the parameter of interest β is estimated as $\hat{\beta} = (X^T X)^{-1} X^T Y = X^{-1} Y$. Since X is a square non-singular matrix, $\hat{\beta} = X^{-1} Y$. Note that when the investigator is choosing a saturated design it is desirable to choose a design that is optimal. However, a design can be optimal with respect to various criteria. In the 2^k -factorial experiment, the D -optimality criterion is one of the most popular criteria used in practice

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to choose an optimal design. This is because when a design X is D-optimal, the volume of the confidence ellipsoid of the vector parameter is minimized since the determinant of the Fisher information $X^T X$ is inversely proportional to the volume of the confidence ellipsoid of the vector parameter β . See Wald (1943) and Kiefer (1959). Thus maximizing the determinant of $X^T X$ is equivalent to minimizing the volume of the confidence ellipsoid for β . For SDs, since X is a square matrix, we maximize the determinant of $X^T X$ just by maximizing the determinant of the absolute value of X . Note that there is a vast literature about the construction of saturated and D-optimal saturated designs. See Hedayat and Pesotan (1992), Hedayat and Pesotan (2007), Hedayat and Zhu (2011), and Domagni et al. (2024).

In this paper, we consider a 2^k -factorial experiment with $k + 1$ factors $F_1, \dots, F_k, F^e$. The investigator believes that among the k factors, factor F_1 is the only one that potentially interacts with the rest of the $k - 1$ factors. Furthermore, the investigator knows the extra factor F^e doesn't interact with any of the k factors. The goal of the investigator is to conduct the experiment with a D-optimal saturated design for the unbiased estimation of the mean, the main effects, and the interactions in this problem. We solve the problem by coming up with an algorithm for the construction of D-optimal saturated design matrices for the problem. In the process, we show the problem is as hard as the Hadamard determinant problem. For simplicity, we use the following notations and definitions throughout the paper. We let F_0 be the factor underlying the mean, $F_1, \dots, F_k$ be the factors underlying the main effects of $F_1, \dots, F_k$, and F_e be the factor underlying the main effect of the extra factor. The second-order interactions of factor F_1 with each of the $k - 1$ factors namely $F_1 F_2, F_1 F_3, \dots, F_1 F_k$ will be called F_1 -second-order interactions and we write them as $F_{12}, \dots, F_{1k}$. We also define $\mathcal{D}(k, 1, e)$ as the set of all saturated designs that ensure the unbiased estimation of the mean, k main effects, the extra main effect F^e , and the F_1 -second-order interactions for a given k .

2. Construction of D-optimal saturated designs in $\mathcal{D}(k, 1, e)$

2.1. Motivation

The results in Table 1 are the results of a two-level factorial experiment where each factor has two levels coded as + and – that correspond to high level and low level, respectively. See Heyden et al. (1999). This experiment is conducted to understand the assay ridogrel and its related compound in ridogrel oral film-coated tablet simulation. The percentage recovery of the main compound is one of the response variables of interest. For scientific reasons, the experimenters considered only eight factors in assessing the importance of the factors on the response which is the percentage recovery of the main compound (MC). Note that the eight factors considered were pH of the buffer (A), column manufacturer (B), column temperature (D), percent of organic solvent in the mobile phase at the start of the gradient (E), percent of organic solvent in the mobile phase at the end of the gradient (F), the flow of the mobile phase (H), the detection wavelength (I), and the concentration of the buffer (J). The three other factors namely factors C, G, and K in Table 1 were omitted from the analysis because the experimenters knew beforehand that those factors did not affect the response variable which in this case is the percentage recovery of the main compound (MC). The experimenters ignored the interactions, fitted a main effects model to the observations and got

$$\hat{y} = 101.04 + 0.34A - 0.22B - 0.36D - 0.56E + 0.44F - 0.01H + 0.26I - 0.31J. \quad (1)$$

Table 1. Experiment reported in Heyden et al. (1999).

Run	A	B	C	D	E	F	G	H	I	J	K	MC
1	+	+	+	−	+	+	−	+	−	−	−	101.6
2	+	+	−	+	−	−	−	+	+	+	−	101.7
3	+	−	+	+	−	+	−	−	−	+	+	101.6
4	+	−	−	−	+	+	+	−	+	+	−	101.9
5	+	−	+	−	−	−	+	+	+	−	+	101.8
6	−	+	+	+	−	+	+	−	+	−	−	101.1
7	−	+	−	−	−	+	+	+	−	+	+	101.1
8	−	−	−	+	+	+	−	+	+	−	+	101.6
9	−	−	+	+	+	−	+	+	−	+	−	98.4
10	−	+	+	−	+	−	−	−	+	+	+	99.7
11	+	+	−	+	+	−	+	−	−	−	+	99.7
12	−	−	−	−	−	−	−	−	−	−	−	102.3

Note that for this model the experimenter concluded that none of the factors has a significant effect on the response variable (MC) because the most significant factors were E and F with p -values equal to 0.16 and 0.24, respectively. Furthermore, an $R^2 = 0.78$ and $\hat{\sigma} = 1.045$ were reported on 3 degrees of freedom. In Phoa et al. (2009), the experiment in Table 1 was reanalyzed taking into account interactions, and the following model was found

$$\hat{y} = 101.04 - 0.56E + 0.44F - 0.30H + 0.88EF. \quad (2)$$

This model has an $R^2 = 0.96$ which indicates a good fit. Furthermore, factor H is significant at the 5% level (p -value = 0.012) and E , F , and EF are significant at the 1% level.

It is important to point out that the design in Table 1 is the Plackett-Burman design where the column underlying the grand mean has been omitted. Thus the main effects are partially aliased with second-order interactions. Since some interaction(s) are not negligible, the main effects estimated in the main effect model in Equation (1) are biased. This is what misled the experimenters to draw the wrong conclusion that none of the main effects is significant. By introducing a model that takes into account the interaction Phoa et al. were able to identify the important effects and interactions that affect the response variable. The takeaway message here is that if for one reason or another, the experimenter can identify the potential main effects and interactions, he may cut down the number of runs needed to conduct the experiment without compromising the identification of the important effects and interactions. That is the main purpose of the remainder of this paper.

2.2. Preliminaries

As we have seen in the example above, in screening design it is common to encounter situations in which only one factor interacts with some of the other factors. In the rest of this paper, we consider a two-level factorial experiment with $k + 1$ factors $F_1, \dots, F_k$, and F^e (extra factor). We investigate the class of saturated design matrices for a vector parameter β that includes the mean, the $k + 1$ main effects, and the second-order interactions of factor F_1 with the factors $F_2, \dots, F_k$. More precisely, for such a problem there are $k + 1$ main effects $F_1, \dots, F_k$ and F^e , the mean F_0 and $k - 1$ second-order interactions $F_{12}, \dots, F_{1k}$. The total number of parameters to estimate is $2k + 1$. A saturated design would therefore require $2k + 1$ runs. The corresponding linear model is on the form

$$Y_i = \beta_0(F_0)_i + \beta_1(F_1)_i + \dots + \beta_k(F_k)_i + \beta^e(F^e)_i + \beta_{12}(F_{12})_i + \dots + \beta_{1k}(F_{1k})_i + \epsilon_i, \quad (3)$$

F_1	F_2	F_3	F^e	F_0		F_{12}	F_{13}		F_1	F_2	F_3	F^e	F_0	F_{12}	F_{13}
+	+	+	+	+	$\Rightarrow$	+	+	$\Rightarrow$	+	+	+	+	+	+	+
+	-	-	+	+		-	-		+	-	-	+	+	-	-
+	-	+	-	+		-	+		+	-	+	-	+	-	+
-	-	+	+	+		+	-		+	+	-	+	+	+	-
-	+	+	-	+		-	-		-	-	+	+	+	+	-
-	+	-	+	+		-	+		-	+	+	-	+	-	-
+	+	-	+	+		+	-		-	+	-	+	+	-	+

Figure 1. Example of a candidate saturated design in $\mathcal{D}(k, 1, e)$.

where $i \in \{1, \dots, 2k + 1\}$, ϵ_i , Y_i and $(F_{\cdot})_i$ are respectively the i th error term, the response variable and the corresponding runs. $\beta = [\beta_0, \beta_1, \dots, \beta_k, \beta^e, \beta_{12}, \dots, \beta_{1k}]^\top$ is the vector parameter of interest.

To solve the problem of constructing a D-optimal saturated design for the model in Equation (3), we first assume the extra factor F^e was not present in the model so that we obtain a new model given by

$$Y_i = \beta_0(F_0)_i + \beta_1(F_1)_i + \dots + \beta_k(F_k)_i + \beta_{12}(F_{12})_i + \dots + \beta_{1k}(F_{1k})_i + \epsilon_i, \quad (4)$$

where the vector parameter $\beta = [\beta_0, \beta_1, \dots, \beta_k, \beta_{12}, \dots, \beta_{1k}]^\top$. The difference between the model in Equation (3) and that in Equation (4) is the extra factor F^e present in (3) and not in (4). Throughout the paper, we define $\mathcal{D}(k, 1, e)$ as the set of all saturated design matrices that ensure the unbiased estimation of the vector parameter β for the model in Equation (3). Furthermore, we define $\mathcal{D}(k, 1)$ as the set of all saturated design matrices that ensure the unbiased estimation of the vector parameter β for the model in Equation (4). In Domagni et al. (2024), it has been shown how a D-optimal saturated design can be constructed for the model in Equation (4). We use the D-optimal design for the model in Equation (4) as a building block to construct a D-optimal saturated design for the model in Equation (3).

To gain more intuition about the problem, we give an example of the particular case of $k = 3$ as follows. For $k = 3$ the number of parameters to estimate is 7, namely, $F_0, F_1, F_2, F_3, F^e, F_{12}, F_{13}$. It follows that a saturated design would require 7 runs. Suppose we choose the candidate design with the runs $\{(++++) , (+-+-), (+-+-), (-++-), (-++-), (-+-+), (-+-+), (++)--\}$. Then the candidate saturated design matrix would be a square matrix of order 7 that is obtained by converting the runs into the underlying design matrix. As illustrated in Figure 1, the first matrix underlies the main effects plus mean F_1, F_2, F_3, F^e and F_0 . The second matrix underlies the second order interactions F_{12} and F_{13} and is obtained by taking the Schür product of F_1 with F_2 and F_3 respectively. The third matrix is the actual candidate saturated design matrix obtained by combining the first and second matrices. Note that this third matrix is the candidate saturated design matrix for the model in Equation (3). It is worth pointing out that for convenience we set the factors in the order F_1, F_2, F_3, F_0 so that the first and last entries of each run correspond to F_1 and F_0 respectively.

Suppose the extra factor F^e is omitted from the model in Equation (3). Then the model obtained after omission is just the model in Equation (4). For $k = 3$, we can build an example of a candidate-saturated design matrix for the model in Equation (4) by deleting the column underlying the extra factor F^e and the last row of the candidate-saturated design matrix for the model in Equation (3). In Figure 2, the first matrix underlying F_1, F_2, F_3 ,

$$\begin{array}{c}
 \begin{array}{cccc} F_1 & F_2 & F_3 & F_0 \end{array} \\
 \begin{bmatrix} + & + & + & + \\ + & - & - & + \\ + & - & + & + \\ - & - & + & + \\ - & + & + & + \\ - & + & - & + \end{bmatrix}
 \end{array}
 \Rightarrow
 \begin{array}{c}
 \begin{array}{cc} F_{12} & F_{13} \end{array} \\
 \begin{bmatrix} + & + \\ - & - \\ - & + \\ + & - \\ - & - \\ - & + \end{bmatrix}
 \end{array}
 \Rightarrow
 \begin{array}{c}
 \begin{array}{cccccc} F_1 & F_2 & F_3 & F_0 & F_{12} & F_{13} \end{array} \\
 \begin{bmatrix} + & + & + & + & + & + \\ + & - & - & + & - & - \\ + & - & + & + & - & + \\ - & - & + & + & + & - \\ - & + & + & + & - & - \\ - & + & - & + & - & + \end{bmatrix}
 \end{array}$$

Figure 2. Example of a candidate saturated design in $\mathcal{D}(k, 1)$.

and F_0 is the matrix obtained from the first matrix in Figure 1 by deleting the column of F^e and the last row. The second matrix in Figure 2 is the matrix underlying the interactions F_{12} and F_{13} . The third matrix in Figure 2 is the actual candidate saturated design matrix for the model in Equation (4). The corresponding runs for this example would be $\{(+ + +), (+ - -), (+ - +), (- - +), (- + +), (- + -)\}$ and the parameters of interest would be the effects and interactions of $F_0, F_1, F_2, F_3, F_{12}$, and F_{13} .

Note that for each run underlying F_1, F_2 and F_3 , one can construct the corresponding interactions F_{12} and F_{13} by taking the Schür product of F_1 with F_2 and F_3 respectively. Thus, for the run $(+ - +)$ underlying F_1, F_2 , and F_3 , the interactions are obtained as $F_{12} = (+) * (-) = -$ and $F_{13} = (+) * (+) = +$. Note that for that particular run, $F_1 = +, F_{12} = F_2 = -1$, and $F_{13} = F_3 = +$. Furthermore, since the mean F_0 is always equal to $+$ we can say $F_0 = F_1 * F_1 = (+) * (+) = +$. Thus for the run $(+ - +)$, it is easy to see that the row vector underlying $[F_1 \ F_2 \ F_3 \ F_{12} \ F_{13} \ F_0]$ is in the form $[+ \ - \ + \ | \ + \ - \ +] = [r^\top \ r^\top]$, where $r^\top = [+ \ - \ +]$. On the other hand, if we consider the run $(- - +)$, then $F_1 = -, F_{12} = (-) * (-) = +, F_{13} = (-) * (+) = -, \text{ and } F_0 = F_1 * F_1 = F_{11} = (-) * (-) = +$. The row vector underlying $[F_1 \ F_2 \ F_3 \ F_{12} \ F_{13} \ F_0]$ is in the form $[- \ - \ + \ | \ + \ + \ -] = [-r^\top \ r^\top]$, where $r^\top = [+ \ + \ -]$. Note that the Schür of F_1 with itself yields $F_{11} = F_1 * F_1 = F_0$. Since F_0 and F_{11} represent the same vector we shall use F_{11} and F_0 interchangeably. It shall be understood that the mean vector F_0 is also the interaction of F_1 with itself which is F_{11} .

In general, for any row vector of run $r = [r_1, \dots, r_k]$ underlying the row vector of factors $[F_1, \dots, F_k]$, the corresponding row in the design matrix underlying the factors $[F_1, \dots, F_k \ F_{11}, \dots, F_{1k}]$ may be in one of two forms depending on whether $F_1 = r_1$ is $+$ or $-$. If $F_1 = r_1 = +$, then the row underlying $[F_1, F_2, \dots, F_k \ F_{11}, F_{12}, \dots, F_{1k}] = [+ , F_2, \dots, F_k \ (+) * F_1, (+) * F_2, \dots, (+) * F_k] = [+ , r_2, \dots, r_k \ (+) * r_1, (+) * r_2, \dots, (+) * r_k] = [+ , r_2, \dots, r_k \ +, r_2, \dots, r_k] = [r^\top, r^\top]$ where $r^\top = [+ , r_2, \dots, r_k]$.

If on the other hand, $F_1 = r_1 = -$, then the row underlying $[F_1, F_2, \dots, F_k \ F_{11}, F_{12}, \dots, F_{1k}] = [- , F_2, \dots, F_k \ (-) * F_1, (-) * F_2, \dots, (-) * F_k] = [- , r_2, \dots, r_k \ (-) * r_1, (-) * r_2, \dots, (-) * r_k] = [- , r_2, \dots, r_k \ +, -r_2, \dots, -r_k] = [-r^\top, r^\top]$ where $r^\top = [+ , -r_2, \dots, -r_k]$.

Note that the forms of the rows underlying $[F_1, F_2, \dots, F_k \ F_{11}, F_{12}, \dots, F_{1k}]$ will play a key role in the proofs of the theorems coming up. We recapitulate the forms in the remark below as follows.

Remark 2.1: Suppose $r^\top = [r_1, r_2, \dots, r_k]$ is a choice of run underlying $[F_1, F_2, \dots, F_k]$.

- (1) If $F_1 = r_1 = +$, then the corresponding row in the design matrix underlying $[F_1, F_2, \dots, F_k \quad F_{11}, F_{12}, \dots, F_{1k}]$ is in the form $[r^\top, r^\top]$, where $r^\top = [+ , r_2, \dots, r_k]$.
- (2) If $F_1 = r_1 = -$, then the corresponding row in the design matrix underlying $[F_1, F_2, \dots, F_k \quad F_{11}, F_{12}, \dots, F_{1k}]$ is in the form $[-r^\top, r^\top]$, where $r^\top = [+ , -r_2, \dots, -r_k]$.

In Figure 2, $F_1 = r_1 = +$ for the first three runs and $F_1 = r_1 = -$ for the last three runs underlying $[F_1, F_2, F_3]$. Thus, using Remark 2.1, we observe the candidate-saturated design matrix is in the form

$$\begin{bmatrix} F_1 & F_2 & F_3 & F_{11} & F_{12} & F_{13} \\ + & + & + & + & + & + \\ + & - & - & + & - & - \\ + & - & + & + & - & + \\ - & - & + & + & + & - \\ - & + & + & + & - & - \\ - & + & - & + & - & + \end{bmatrix} = \begin{bmatrix} M & M \\ -N & N \end{bmatrix},$$

where

$$M = \begin{bmatrix} + & + & + \\ + & - & - \\ + & - & + \end{bmatrix}, \quad \text{and} \quad N = \begin{bmatrix} + & + & - \\ + & - & - \\ + & - & + \end{bmatrix}.$$

In Figure 1, we have an extra factor F^e that does not interact with any other factor. Note that for the underlying $[F_1, F_2, F_3]$, the factor $F_1 = +$ in the first four runs and $F_1 = -$ for the last three runs. Thus, using Remark 2.1, we observe that the candidate-saturated design matrix is in the form

$$\begin{bmatrix} F_1 & F_2 & F_3 & F^e & F_0 & F_{12} & F_{13} \\ + & + & + & + & + & + & + \\ + & - & - & + & + & - & - \\ + & - & + & - & + & - & + \\ + & + & - & + & + & + & - \\ - & - & + & + & + & + & - \\ - & + & + & - & + & - & - \\ - & + & - & + & + & - & + \end{bmatrix} = \begin{bmatrix} M & c & M \\ -N & d & N \end{bmatrix}$$

where

$$M = \begin{bmatrix} + & + & + \\ + & - & - \\ + & - & + \\ + & + & - \end{bmatrix}, \quad N = \begin{bmatrix} + & + & - \\ + & - & - \\ + & - & + \end{bmatrix}, \quad c = \begin{bmatrix} + \\ + \\ - \\ + \end{bmatrix}, \quad \text{and} \quad d = \begin{bmatrix} + \\ - \\ + \end{bmatrix}.$$

Remark 2.2: A few remarks can be made as follows.

- (1) $F_0 = F_1 * F_1 = F_{11}$. That is the mean F_0 can be written as the Schür product of F_1 by itself. This simple fact will be crucial in the theorems we develop in the upcoming section.

- (2) The choice of candidate saturated design matrix in $\mathcal{D}(k, 1, e)$ given in Figure 1 is in the form

$$\begin{bmatrix} M & c & M \\ -N & d & N \end{bmatrix}.$$

We will show this form is a necessary condition for any element in $\mathcal{D}(k, 1, e)$.

- (3) The candidate design matrix in Figure 1 is an element of $\mathcal{D}(k, 1, e)$ if and only if it is a non-singular matrix. We will give necessary and sufficient conditions on a candidate saturated design matrix to be an element of $\mathcal{D}(k, 1, e)$.

2.3. Construction of saturated and D-optimal saturated design matrices in $\mathcal{D}(k, 1, e)$

In the remainder of this section, we explore the construction of an element $\mathcal{D}(k, 1, e)$. We assume without loss of generality that the vector parameter of interest is of the form $\beta = [\beta_1, \dots, \beta_k, \beta^e, \beta_0, \beta_{12}, \dots, \beta_{1k}]^\top$ with parameters appearing in that order. For convenience, we give the following definitions.

Definition 2.1: We give the following definitions.

- (1) We define $\mathcal{M}_k\{-1, 1\}$ as the set of non-singular matrices of order k with entries from $\{-1, 1\}$ for which the first column is the vector 1_k .
- (2) We define Θ_k to be the maximal value of the absolute value of the determinant of matrices in $\mathcal{M}_k\{-1, 1\}$.

Note that for each element in $\mathcal{D}(k, 1, e)$, the factor F_1 interacts with all the $k-1$ factors $F_2, \dots, F_k$ except the extra factor F^e . Thus F_1 plays a key role in the construction of a saturated design that is an element in $\mathcal{D}(k, 1, e)$. We define the factor F_1 as the pivot factor. Since the entries of F_1 take values from $\{-1, 1\}$ we assume without loss of generality that F_1 is of the form $F_1 = \begin{bmatrix} \vec{1}_{f_+}^\top & -\vec{1}_{f_-}^\top \end{bmatrix}^\top$, where f_+ and f_- are respectively the frequencies of 1 and -1 entries in the vector F_1 with $f_+ + f_- = 2k + 1$. For convenience we write $F_2, \dots, F_k$ as block vectors $F_2 = \begin{bmatrix} m_2^\top & n_2^\top \end{bmatrix}^\top, \dots, F_k = \begin{bmatrix} m_k^\top & n_k^\top \end{bmatrix}^\top$, and the extra factor F^e as $F^e = \begin{bmatrix} c^\top & d^\top \end{bmatrix}^\top$, where $m_2, \dots, m_k$ and c are vectors of length f_+ and $n_2, \dots, n_k$ and d are vectors of length f_- with entries from $\{-1, 1\}$. With these observations, let D be an arbitrary element in $\mathcal{D}(k, 1, e)$. Then D can be written as

$$D = \begin{bmatrix} F_1 & F_2 & \dots & F_k & F^e & F_{11} & F_{12} & \dots & F_{1k} \\ + & m_{11} & \dots & m_{1k} & c_{11} & + & m_{11} & \dots & m_{1k} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ + & m_{1f_+} & \dots & m_{kf_+} & c_{1f_+} & + & m_{1f_+} & \dots & m_{kf_+} \\ - & n_{11} & \dots & n_{1k} & c_{21} & + & -n_{11} & \dots & -n_{1k} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ - & n_{1f_-} & \dots & n_{kf_-} & c_{2f_-} & + & -n_{1f_-} & \dots & -n_{kf_-} \end{bmatrix} = \begin{bmatrix} M & c_1 & M \\ -N & c_2 & N \end{bmatrix},$$

where

$$M = \begin{bmatrix} + & m_{11} & \dots & m_{1k} \\ \vdots & \vdots & \ddots & \vdots \\ + & m_{1f_+} & \dots & m_{kf_+} \end{bmatrix}$$

is an $f_+ \times k$ matrix,

$$N = \begin{bmatrix} + & -n_{11} & \dots & -n_{1k} \\ \vdots & \vdots & \ddots & \vdots \\ + & -n_{1f_-} & \dots & -n_{kf_-} \end{bmatrix}$$

is an $f_- \times k$ matrix, $c_1 = [c_{11}, \dots, c_{1f_+}]^\top$ is a vector of length f_+ , and $c_2 = [c_{21}, \dots, c_{2f_-}]^\top$ is a vector of length f_- .

In the following Lemma 2.1, we give a necessary condition on the frequencies f_+ and f_- for a candidate matrix D to be an element of $\mathcal{D}(k, 1, e)$.

Lemma 2.1: *Let D be a candidate design matrix in $\mathcal{D}(k, 1, e)$. Suppose f_+ and f_- are respectively the frequencies of $+$ and $-$ entries in the vector underlying factor F_1 . Then $|f_+ - f_-| = 1$.*

Proof: We have seen that any element of $\mathcal{D}(k, 1, e)$ is necessarily on the form

$$D = \begin{bmatrix} M & c_1 & M \\ -N & c_2 & N \end{bmatrix},$$

where M and N are $\{-1, 1\}$ -matrices of dimensions $f_+ \times k$ and $f_- \times k$ respectively. c_1 and c_2 are vectors of length f_+ and f_- respectively. Thus the matrix $[M \ c_1]$ has the dimension $f_+ \times (k + 1)$. The matrix D is a square matrix of order $2k + 1$ and $f_+ + f_- = 2k + 1$ which is an odd number. Note that $|f_+ - f_-| = 1$ if and only if $f_+ = k + 1$ or $f_- = k + 1$.

To show that $|f_+ - f_-| = 1$ is a necessary condition for D to be in $\mathcal{D}(k, 1, e)$, we will show that if $f_+ > k + 1$ or $f_- > k + 1$ then the matrix D is a singular matrix which would mean it is not in $\mathcal{D}(k, 1, e)$.

Assume without loss of generality that $f_+ > k + 1$. Then, since $[M \ c_1]$ is of the dimension $f_+ \times (k + 1)$, we have $\text{rank}([M \ c_1])$ is at most $k + 1$. Therefore, the rows of $[M \ c_1]$ that we define as $[m_1^\top \ c_{11}]^\top, \dots, [m_{f_+}^\top \ c_{1f_+}]^\top$ are linearly dependent. We may assume without loss of generality that $[m_1^\top \ c_{11}]^\top$ is linearly dependent on $[m_2^\top \ c_{12}]^\top, \dots, [m_{f_+}^\top \ c_{1f_+}]^\top$, so that $[m_1 \ c_{11}]^\top = \sum_{i=2}^{f_+} c_i [m_i \ c_{1i}]^\top$ with some $c_i \neq 0$, $2 \leq i \leq f_+$. This implies that $[m_1, c_{11}, m_1]^\top = \sum_{i=2}^{f_+} c_i [m_i \ c_{1i} \ m_i]^\top$. It means that the rows $[m_1^\top \ c_{11} \ m_1^\top], \dots, [m_{f_+}^\top \ c_{1f_+} \ m_{f_+}^\top]$ of D are linearly dependent, which would make D a singular matrix. Similarly, one can show that if $f_- > k + 1$ then D is a singular matrix. Thus, it turns out that $|f_- - f_+| = 1$ is a necessary condition for D to be non-singular. ■

Note that Lemma 2.1 sets some conditions on the frequencies of $+$ and $-$ underlying the pivot factor F_1 . In Theorem 2.2 we give the necessary and sufficient conditions on a candidate design matrix D to be an element of $\mathcal{D}(k, 1, e)$. Lemma 2.1 is key for the proof of Theorem 2.2.

Theorem 2.2: A square matrix D of order $2k + 1$ is a design matrix in $\mathcal{D}(k, 1, e)$ if and only if it is in the form

$$D = \begin{bmatrix} M & c_1 & M \\ -N & c_2 & N \end{bmatrix}$$

and one of the following two conditions is satisfied.

- (1) $f_+ = k + 1$, $\begin{bmatrix} M & c_1 \end{bmatrix}$ is an element in $\mathcal{M}_{k+1}\{-1, 1\}$, and N is an element in $\mathcal{M}_k\{-1, 1\}$.
- (2) $f_- = k + 1$, $\begin{bmatrix} N & c_2 \end{bmatrix}$ is an element in $\mathcal{M}_{k+1}\{-1, 1\}$, and M is an element in $\mathcal{M}_k\{-1, 1\}$.

Proof: We have seen that any element of $\mathcal{D}(k, 1, e)$ is necessarily in the form

$$D = \begin{bmatrix} M & c_1 & M \\ -N & c_2 & N \end{bmatrix}.$$

We have also seen from Lemma 2.1 that it is necessary that $f_+ = k + 1$ or $f_- = k + 1$ for D to be element of $\mathcal{D}(k, 1, e)$.

- (1) Suppose $f_+ = k + 1$. Then the block matrix $\begin{bmatrix} M & c_1 \end{bmatrix}$ is a square matrix of order $k + 1$. If $\begin{bmatrix} M & c_1 \end{bmatrix}$ is a singular matrix, then the rows of the block matrix $\begin{bmatrix} M & c_1 & M \end{bmatrix}$ would be linearly dependent by analogy to the argument in the proof of Lemma 2.1. This would make the candidate matrix D a singular matrix.

Suppose $\begin{bmatrix} M & c_1 \end{bmatrix}$ is a non-singular matrix. Then

$$\begin{aligned} |\det(D)| &= \left| \det \begin{bmatrix} M & c_1 & M \\ -N & c_2 & N \end{bmatrix} \right| \\ &= \left| \det \left[N - \begin{bmatrix} -N & c_2 \end{bmatrix} \begin{bmatrix} M & c_1 \end{bmatrix}^{-1} M \right] \right| |\det(\begin{bmatrix} M & c_1 \end{bmatrix})|. \end{aligned}$$

Note that $\begin{bmatrix} M & c_1 \end{bmatrix}^{-1} \begin{bmatrix} M & c_1 \end{bmatrix} = I_{k+1}$. Thus, by deleting the last column of the identity matrix I_{k+1} , we obtain the $(k + 1) \times k$ matrix $\begin{bmatrix} M & c_1 \end{bmatrix}^{-1} M$.

It is easy to see that $\begin{bmatrix} M & c_1 \end{bmatrix}^{-1} M = \begin{bmatrix} I_k & \vec{0}^\top \end{bmatrix}$, where I_k is the identity matrix of order k and $\vec{0}$ is the zero vector of length k . This implies that

$$\begin{bmatrix} -N & c_2 \end{bmatrix} \begin{bmatrix} M & c_1 \end{bmatrix}^{-1} M = \begin{bmatrix} -N & c_2 \end{bmatrix} \begin{bmatrix} I_k \\ \vec{0}^\top \end{bmatrix} = -NI_k + c_2 \vec{0}^\top = -N.$$

We deduce that

$$\begin{aligned} |\det(D)| &= |\det[N - (-N)]| |\det(\begin{bmatrix} M & c_1 \end{bmatrix})| = |\det[2N]| |\det(\begin{bmatrix} M & c_1 \end{bmatrix})| \\ &= 2^k |\det[N]| |\det(\begin{bmatrix} M & c_1 \end{bmatrix})|. \end{aligned}$$

Note that D is non-singular only if $|\det(D)| = 2^k |\det[N]| |\det(\begin{bmatrix} M & c_1 \end{bmatrix})| \neq 0$. This happens if and only if both N and $\begin{bmatrix} M & c_1 \end{bmatrix}$ are non-singular matrices. That is $\begin{bmatrix} M & c_1 \end{bmatrix}$ is an element in $\mathcal{M}_{k+1}\{-1, 1\}$, and N is an element in $\mathcal{M}_k\{-1, 1\}$.

- (2) Suppose $f_- = k + 1$. Then by analogy of the argument above, we can show that D is non-singular if and only if $\begin{bmatrix} N & c_2 \end{bmatrix}$ is an element in $\mathcal{M}_{k+1}\{-1, 1\}$, and M is an element in $\mathcal{M}_k\{-1, 1\}$. ■

Corollary 2.3: A design matrix D^* is a D-optimal saturated design in $\mathcal{D}(k, 1, e)$ if and only if it can be written as

$$D^* = \begin{bmatrix} M^* & c_1^* & M^* \\ -N^* & c_2^* & N^* \end{bmatrix}$$

and one of the following two conditions is satisfied.

- (1) $f_+ = k + 1$, $\begin{bmatrix} M^* & c_1^* \end{bmatrix}$ is an element in $\mathcal{M}_{k+1}\{-1, 1\}$ with maximal absolute value determinant, and N^* is an element in $\mathcal{M}_k\{-1, 1\}$ with maximal absolute value determinant.
- (2) $f_- = k + 1$, $\begin{bmatrix} N^* & c_2^* \end{bmatrix}$ is an element in $\mathcal{M}_{k+1}\{-1, 1\}$ with maximal absolute value determinant, and M^* is an element in $\mathcal{M}_k\{-1, 1\}$ with maximal absolute value determinant.

Proof: Using Theorem 2.2, there are exactly two ways to obtain a D-optimal design matrix in $\mathcal{D}(k, 1, e)$.

- (1) For $f_+ = k + 1$, choose $\begin{bmatrix} M^* & c_1^* \end{bmatrix}$ from $\mathcal{M}_{k+1}\{-1, 1\}$ with maximal absolute value determinant Θ_{k+1} , and N^* from $\mathcal{M}_k\{-1, 1\}$ with maximal absolute value determinant Θ_k . In that case $|\det(D)| = 2^k \Theta_k \Theta_{k+1}$ which is the maximum absolute value of determinant for an element in $\mathcal{D}(k, 1, e)$.
- (2) For $f_- = k + 1$, choose $\begin{bmatrix} C^* & c_2^* \end{bmatrix}$ from $\mathcal{M}_{k+1}\{-1, 1\}$ with maximal absolute value determinant Θ_{k+1} , and M^* from $\mathcal{M}_k\{-1, 1\}$ with maximal absolute value determinant Θ_k . In that case $|\det(D)| = 2^k \Theta_k \Theta_{k+1}$ which is the maximum absolute value of determinant for an element in $\mathcal{D}(k, 1, e)$.

■

2.4. Algorithm for construction D-optimal design in $\mathcal{D}(k, 1, e)$

Corollary 2.3 yields an algorithm for the construction of a D-optimal saturated design matrix of $\mathcal{D}(k, 1, e)$.

Step 1: For $f_+ = k + 1$, select two matrices $\begin{bmatrix} M & c_1 \end{bmatrix}$ and N from $\mathcal{M}_{k+1}\{-1, 1\}$ $\mathcal{M}_k\{-1, 1\}$ respectively with maximal absolute valued determinant. Set $c_2 = \vec{0}$.

Step 2: The design matrix

$$D = \begin{bmatrix} M & c_1 & M \\ -N & c_2 & M \end{bmatrix}$$

obtained through *Step 1* is a D-optimal design matrix in $\mathcal{D}(k, 1, e)$.

3. Concluding remarks

In this paper, we developed an algorithm for the construction of a D-optimal saturated design matrix for $k + 1$ main effects, the second-order interactions of one factor with $k - 1$ factors, and the mean. Note that in the example given in Section 2.1, the experimenter started with eleven factors A, B, C, D, E, F, G, H, I, J, and K. He then omitted factors C, G, and K since he had prior information that those factors do not affect the response variable. As explained in Section 2.1, the main effect model yielded the wrong conclusion about the important effects

and interactions. By taking into account the interactions, the analysis showed three important main effects (E, F, and H) and one important interaction (EF). Here, note that having prior information about the factors involved in your experiment can be crucial for saving resources and improving the accuracy of the analysis. Suppose, for instance, that the experimenter has the prior information that factor F is the only one that potentially interacts with all the remaining factors. Then he may conduct the experiment with 16 runs for the estimation of the mean, the main effects A, B, D, E, F, H, I, and J, along with the interactions FA, FB, FD, FE, FH, FI, and FJ. An algorithm for constructing a D-optimal saturated design for such a problem is developed in Domagni et al. (2024). In addition, suppose the experimenter, for one reason or another, knows beforehand that one of the interactions FA, FB, FD, FE, FH, FI, and FJ is negligible. Then, if we assume without loss of generality that FJ is the negligible interaction, we need a design for the estimation of the mean, the main effects A, B, D, E, F, H, I, and J, along with the interactions FA, FB, FD, FE, FH, and FI. Under these assumptions, factor J is the only free factor, and the algorithm in Section 2.4 can be used to construct a D-optimal saturated design for the problem. However, when several factors are free, it is challenging to construct a D-optimal design for the problem. Concretely, the problem of constructing a D-optimal design in $\mathcal{D}(k, 1, e)$, where $e > 1$, is challenging. Our team is still investigating this. Finally note that in the proof of Theorem 2.2, we have seen that for $f_+ = k + 1$ the determinant of the design matrix D does not depend on the vector c_2 underlying the extra factor F^e . Thus, the experimenter can save resources by discarding the factor F^e from the runs of the experiment that involve the vector c_2 without compromising the D-optimality of the design matrix. This means even though we are dealing with a two-level factorial experiment, we can replace each entry of c_2 with 0 without losing any information in terms of D-optimality. This is important, especially if it is expensive in terms of cost or resources to keep the factor F^e at its high or low levels for each run of the experiment. Note that if saving the resource underlying the factor F^e is not a goal, the experimenter can keep factor F^e as balanced as possible in the runs of the experiment involving vector c_2 . In the Appendix, we give two examples of D-optimal design matrices in $\mathcal{D}(15, 1, e)$. Note that in those examples $c_2 = \vec{0}$ and $c_1 = \vec{0}$. This is illustrated in Figures A5 and A6 with the bunch of zero entries appearing in the D-optimal design matrices. This indicates that the experimenter does not necessarily need resources from the extra factor F^e for the runs involving c_2 .

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Appendix. D-optimal design matrices in $\mathcal{D}(15, 1, e)$

$$M_{15}^* = \begin{bmatrix} - & - & - & - & + & + & + & + & - & + & + & + & + & - \\ - & - & - & + & - & + & + & - & + & + & + & + & - & + & + \\ - & - & - & + & + & - & + & + & - & + & + & - & + & + & + \\ - & + & + & - & - & + & + & + & - & + & + & - & - & - & - \\ + & + & - & + & - & - & + & + & + & - & + & - & - & - & - \\ + & - & + & - & + & - & + & - & + & + & + & - & - & - & - \\ + & + & + & + & + & + & - & + & + & + & + & - & - & + & - \\ - & + & + & - & - & - & - & - & + & - & + & - & + & + & + \\ + & + & + & - & - & - & + & + & + & + & - & + & + & + & + \\ + & - & + & - & - & - & - & + & - & - & + & + & - & + & + \\ + & + & - & - & - & - & - & - & + & + & + & + & + & - & - \\ + & + & - & - & + & + & + & - & - & - & - & - & + & + & + \\ + & - & + & + & - & + & + & - & - & - & - & - & + & + & - \\ - & + & + & + & + & - & + & - & - & - & - & + & - & + & - \\ + & + & + & + & + & + & + & - & - & - & + & + & + & - & + \end{bmatrix}$$

Figure A1. Maximal determinant matrix in $\mathcal{M}_{15}\{-1, 1\}$. A result of the work of Smith (1988), Cohn (1989), Cohn (2000), and Orrick (2005).

$$M_{15}^{*+} = \begin{bmatrix} + & + & + & + & - & - & - & - & - & + & - & - & - & - & + \\ + & + & + & - & + & - & - & + & - & - & - & - & + & - & - \\ + & + & + & - & - & + & - & - & + & - & - & + & - & - & - \\ + & - & - & + & + & - & - & - & + & - & - & + & + & + & + \\ + & + & - & + & - & - & + & + & + & - & + & - & - & - & - \\ + & - & + & - & + & - & + & - & + & + & + & - & - & - & - \\ + & + & + & + & + & + & - & + & + & + & + & - & - & + & - \\ + & - & - & + & + & + & + & + & - & + & - & + & - & - & - \\ + & + & + & - & - & - & + & + & + & + & - & + & + & + & + \\ + & - & + & - & - & - & - & + & - & - & + & + & - & + & + \\ + & + & - & - & - & - & - & - & - & + & + & + & + & + & - \\ + & + & - & - & + & + & + & - & - & - & - & - & - & + & + \\ + & - & + & + & - & + & + & - & - & - & - & - & + & + & - \\ + & - & - & - & - & + & - & + & + & + & + & - & + & - & + \\ + & + & + & + & + & + & + & - & - & - & + & + & + & - & + \end{bmatrix}$$

Figure A2. Normalized maximal determinant matrix in $\mathcal{M}_{15}\{-1, 1\}$ obtained from M_{15}^* .

$$M_{15}^{*-} = \begin{bmatrix} - & - & - & - & + & + & + & + & + & - & + & + & + & + & - \\ - & - & - & + & - & + & + & - & + & + & + & + & - & + & + \\ - & - & - & + & + & - & + & + & - & + & + & - & + & + & + \\ - & + & + & - & - & + & + & + & - & + & + & - & - & - & - \\ - & - & + & - & + & + & - & - & - & + & - & + & + & + & + \\ - & + & - & + & - & + & - & + & - & - & - & + & + & + & + \\ - & - & - & - & - & - & + & - & - & - & - & + & + & - & + \\ - & + & + & - & - & - & - & - & + & - & + & - & + & + & + \\ - & - & - & + & + & + & - & - & - & - & + & - & - & - & - \\ - & + & - & + & + & + & + & - & + & + & - & - & + & - & - \\ - & - & + & + & + & + & + & + & - & - & - & - & - & + \\ - & - & + & + & - & - & - & + & + & + & + & + & + & - & - \\ - & + & - & - & + & - & - & + & + & + & + & + & - & - & + \\ - & + & + & + & + & - & + & - & - & - & - & + & - & + & - \\ - & - & - & - & - & - & - & + & + & + & - & - & - & + & - \end{bmatrix}$$

Figure A3. The opposite matrix of M_{15}^{*+} .

$$H_{16} = \begin{bmatrix} + & + & + & + & + & + & + & + & + & + & + & + & + & + & + & + \\ + & - & + & - & + & - & + & - & + & - & + & - & + & - & + & - \\ + & + & - & - & + & + & - & - & + & + & - & - & + & + & - & - \\ + & - & - & + & + & - & - & + & + & - & - & + & + & - & - & + \\ + & + & + & + & - & - & - & - & + & + & + & + & - & - & - & - \\ + & - & + & - & - & + & - & + & + & - & + & - & - & + & - & + \\ + & + & - & - & - & - & + & + & + & + & - & - & - & - & + & + \\ + & - & - & + & - & + & + & - & + & - & - & + & - & + & + & - \\ + & + & + & + & + & + & + & + & + & - & - & - & - & - & - & - \\ + & - & + & - & + & - & + & - & - & + & - & + & - & + & - & + \\ + & + & - & - & + & + & - & - & - & - & + & + & - & - & + & + \\ + & - & - & + & + & - & - & + & - & + & + & - & - & + & + & - \\ + & + & + & + & - & - & - & - & - & - & - & - & + & + & + & + \\ + & - & + & - & - & + & - & + & - & + & - & + & + & - & + & - \\ + & + & - & - & - & - & + & + & - & - & + & + & + & + & - & - \\ + & - & - & + & - & + & + & - & - & + & + & - & + & - & - & + \end{bmatrix}$$

Figure A4. Hadamard matrix of order 16.

+	+	+	+	-	-	-	-	-	+	-	-	-	-	+	0	+	+	+	-	-	-	-	-	+	-	-	-	-	+
+	+	+	-	+	-	-	+	-	-	-	-	-	+	-	-	0	+	+	-	+	-	-	+	-	-	-	-	+	-
+	+	+	-	-	+	-	-	+	-	-	+	-	-	-	0	+	+	-	-	+	-	-	+	-	-	+	-	-	-
+	-	-	+	+	-	-	-	+	-	-	+	+	+	+	0	+	-	+	+	-	-	-	+	-	-	+	+	+	+
+	+	-	+	-	-	+	+	+	+	-	-	-	-	-	0	+	+	-	+	-	-	+	+	+	+	-	+	-	-
+	-	+	+	+	+	+	-	+	+	+	+	-	-	+	-	0	+	+	+	+	+	-	+	+	+	+	-	-	+
+	-	-	+	+	+	+	+	-	+	-	+	-	-	-	0	+	-	+	+	+	+	+	-	+	-	+	-	-	-
+	+	+	-	-	-	+	+	+	+	-	+	+	+	+	0	+	+	-	-	-	+	+	+	+	-	+	+	+	+
+	-	+	-	-	-	-	+	-	-	+	+	-	+	+	0	+	-	+	-	-	-	+	-	-	+	+	-	+	+
+	+	-	-	-	-	-	-	-	+	+	+	+	+	-	0	+	+	-	-	-	-	-	-	+	+	+	+	+	-
+	+	-	-	+	+	+	-	-	-	-	-	-	-	+	+	0	+	-	-	+	+	+	-	-	-	-	-	+	+
+	-	+	+	-	+	+	-	-	-	-	-	-	+	+	-	0	+	-	+	+	-	+	+	-	-	-	-	+	+
+	-	-	-	-	+	-	+	+	+	+	+	-	+	-	+	0	+	-	-	-	+	-	+	+	+	+	-	+	+
+	+	+	+	+	+	+	+	-	-	-	+	+	+	-	+	0	+	+	+	+	+	+	-	-	-	+	+	+	+
-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
-	+	-	+	-	+	-	+	-	+	-	+	-	+	-	-	+	-	+	-	+	-	+	-	+	-	+	-	+	-
-	-	+	+	-	-	+	+	-	-	+	+	-	-	+	-	+	+	-	-	+	+	-	-	+	+	-	-	+	+
-	+	+	-	-	+	+	-	-	+	+	-	-	+	+	+	-	-	+	+	-	-	+	+	-	-	+	+	-	-
-	-	-	-	+	+	+	+	-	-	-	-	+	+	+	-	+	+	+	-	-	-	+	+	+	+	-	-	-	-
-	+	-	+	+	-	+	-	-	+	-	+	+	-	+	+	-	+	-	-	+	-	+	+	-	+	-	-	+	-
-	-	+	+	+	+	-	-	-	-	+	+	+	+	-	+	+	-	-	-	-	+	+	+	+	-	-	-	-	+
-	+	+	-	+	-	-	+	-	+	+	-	+	-	-	-	+	-	-	+	-	+	+	-	+	-	-	+	-	+
-	-	-	-	-	-	-	+	+	+	+	+	+	+	+	-	+	+	+	+	+	+	+	-	-	-	-	-	-	-
-	+	-	+	-	+	-	+	+	-	+	-	+	-	+	+	-	+	-	+	-	+	-	+	-	+	-	+	-	+
-	-	+	+	-	-	+	+	+	+	-	+	+	-	+	+	-	+	+	-	-	+	+	-	-	+	+	-	+	+
-	+	+	-	-	+	+	-	+	-	+	+	-	-	+	-	-	+	-	-	+	-	+	+	-	+	+	-	+	+
-	-	-	-	+	+	+	+	+	+	+	+	+	+	-	+	+	+	+	-	-	-	-	-	-	-	-	-	+	+
-	+	-	+	+	-	+	-	+	-	+	-	-	+	-	-	+	+	-	-	+	-	+	-	+	-	+	+	-	+
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Figure A6. D-optimal saturated design matrix for $F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, F_9, F_{10}, F_{11}, F_{12}, F_{13}, F_{14}, F_{15}, F^e$, $F_0, F_{1,2}, F_{1,3}, F_{1,4}, F_{1,5}, F_{1,6}, F_{1,7}, F_{1,8}, F_{1,9}, F_{1,10}, F_{1,11}, F_{1,12}, F_{1,13}, F_{1,14}$, and $F_{1,15}$ with $f_- = 15 + 1$.