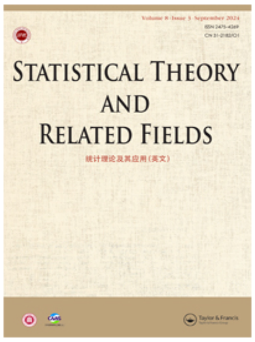

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D-optimal saturated designs for main effects and interactions in 2^k-factorial experiments

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ABSTRACT
In a 2^k-factorial experiment with limited resources, when practitioners can identify the non-negligible effects and interactions beforehand, it is common to run an experiment with a saturated design that ensures the unbiased estimation of the non-negligible parameters of interest. We propose a method for the construction of D-optimal saturated designs for the mean, the main effects, and the second-order interactions of one factor with the remaining factors. In the process, we show the problem is just as hard as the Hadamard determinant problem.

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Saturated designs; D-optimal designs; hadamard matrices; maximal determinant problem

1. Introduction

A saturated design (SD) in a two-level factorial experiment is a design with the minimum number of runs that ensures the unbiased estimation of the effects and interactions of interest given the remaining parameters are negligible. The number of runs n retained in an SD is equal to the total number of parameters of interest. Thus a saturated design matrix is a square non-singular matrix of order n with entries from $\{-1, 1\}$ that is chosen to satisfy the conditions of the parameters of interest. Saturated designs are one of the most important designs in practice. They are desirable to practitioners mainly when the important effects and interactions to be estimated are known beforehand. In general, the statistical model retained for an SD is the regular linear model $Y = X\beta + \epsilon$, 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. Once X is chosen, the ordinary least square method (OLS) can be used to obtain the unbiased estimation of the parameters of interest. That is $\hat{\beta} = (X^\top X)^{-1}X^\top Y = X^{-1}Y$. As a result of the estimator $\hat{\beta} = X^{-1}Y$, the determinant of the Fisher information $X^\top X$ of an SD is maximal if the absolute value of the determinant of X is maximal. Such an SD is known as a D-optimal saturated design. Since the determinant of the Fisher information is inversely proportional to the volume of the confidence ellipsoid of the vector parameter β, the D-optimality criterion is one of the key criteria used to search for a design because it guarantees that the volume of the confidence ellipsoid of the vector parameter β is minimized. See (Wald, 1943) and Kiefer (1959). However, it turns out that the construction of a D-optimal SD is not a trivial problem. There has been a vast literature as well as ongoing investigation about the construction of SD under certain conditions. Hedayat and Pesotan in Hedayat and Pesotan (1992) and Hedayat and Pesotan (2007) have discussed how to construct a saturated design that includes the estimation of the mean, the main effects, and a selected number of second-order interactions. Furthermore, various computer algorithms have been developed to search for SDs for two-level factorial experiments, some of which are SPAN, and DETMAX. As a case in point, see Hedayat and Zhu (2011).

In this paper, we propose methods for the construction of D-optimal saturated design matrices for the estimation of the mean, the main effects, and the second-order interaction(s) of one factor with the remaining factors. Specifically, we consider a two-level factorial experiment with k factors $F_1, \ldots, F_k$ and we develop algorithms for the construction of a saturated design matrix as well as a D-optimal saturated design matrix that includes the estimation of the main effects $F_1, \ldots, F_k$, the second-order interactions of factor F_1 with each of the remaining factors namely $F_1F_2, F_1F_2, \ldots, F_1F_k$, and the mean that we denote by F_0. For simplicity, in the rest of the paper, $F_1F_2, F_1F_2, \ldots, F_1F_k$ will be called F_1-two-factor interactions and we write them as $F_{12}, \ldots, F_{1k}$. We also define $\mathcal{D}(k, 1)$ as the set of all saturated designs that ensure the unbiased estimation of the mean, k main effects, and the F_1-interactions for a given k.

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Table 1. Experiment reported by Vander 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

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

2.1. Motivation

In Table 1, Vander Heyden et al. (1999) used high-performance liquid chromatography (HPLC) to conduct an experiment that studied the assay of ridogrel and its related compounds in ridogrel oral film-coated tablet simulations. In the original experiment, multiple responses were of interest. One of the responses was the percentage recovery of the main compound. For scientific reasons, only eight factors were considered in the experiment that assessed the importance of the factors on the response which in this case is the percentage recovery of the main compound (MC). The eight factors retained 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). For this specific experiment factors C, G, and K in Table 1 were not used in the experiment. It is worth pointing out that in Table 1, each factor has two levels coded as $+1$ and -1 that are represented by $+$ and $-$ respectively. The 12-run Plackett-Burman design in Table 1 was used to assess the importance of the eight factors on the response variable. Fitting a main effects model to the data yields

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

This model has an $R^2 = 0.78$ with $\hat{\sigma} = 1.045$ on 3 degrees of freedom. The most significant factors are E and F with p-values of 0.16 and 0.24 respectively. The experimenters decided the test was not significant and concluded there was no significant relationship between any of the factors and the response variable because, at the 10% significance level, none of the effects is significant. Phoa et al. (2009) reanalyzed the experiment in Table 1 taking into account interactions, and found the following model

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

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. Here, the takeaway message is that in Plackett-Burman designs, the main effects are partially aliased with second-order interactions. Thus, since one or more second-order interactions are not negligible, some effects in the main-effect model in Equation (1) are biased. This misled the experimenters to draw the wrong conclusion that none of the effects is important. On the other hand, by taking into account second-order interactions, the experimenters were able to identify the important main effects and the second-order interaction given by the model in Equation (2). In general, if for scientific reasons, the experimenter can identify the potential main effects and interactions, he may cut down the number of runs and conduct a saturated design for the experiment. That is the main purpose of the remainder of this paper.

2.2. Preliminaries

In the rest of this paper, we consider a two-level factorial experiment with k factors $F_1, \ldots, F_k$. We investigate the class of saturated design matrices for a vector parameter β that includes the mean, the k main effects, and the second-order interactions of factor F_1 with the remaining factors $F_2, \ldots, F_k$. More precisely, for such a problem there are k main effects $F_1, \ldots, F_k$, the mean F_0 and $k-1$ second-order interactions $F_{12}, \ldots, F_{1k}$. The total number of parameters to estimate is $2k$. A saturated design would therefore require $2k$ runs. The corresponding linear model is on the form

$$Y_i = \beta_0(F_0)_i + \beta_1(F_1)_i + \cdots + \beta_k(F_k)_i + \beta_{12}(F_{12})_i + \cdots + \beta_{1k}(F_{1k})_i + \epsilon_i \tag{3}$$

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

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 6, namely, $F_0, F_1, F_2, F_3, F_{12}, F_{13}$. It follows that a saturated design would require 6 runs. Suppose we choose the candidate design with the runs $\{(+ + +), (+ - -), (+ - +), (- - +), (- + +), (- + -)\}$. Then the candidate saturated design matrix would be a square matrix of order 6 that is obtained by converting the runs into the underlying design matrix. As illustrated below, the first matrix underlies the main effects plus mean F_1, F_2, F_3 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 candidate saturated design matrix obtained by combining the first and second matrices. 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.

$$\begin{array}{cccc} F_1 & F_2 & F_3 & F_0 \end{array}\quad \begin{array}{cc} F_{12} & F_{13}\end{array}\quad \begin{array}{cccccc} F_1 & F_2 & F_3 & F_0 & F_{12} & F_{13}\end{array}$$
$$\begin{bmatrix} + & + & + & + \\ + & - & - & + \\ + & - & + & + \\ - & - & + & + \\ - & + & + & + \\ - & + & - & + \end{bmatrix} \Rightarrow \begin{bmatrix} + & + \\ - & - \\ - & + \\ + & + \\ - & - \\ - & + \end{bmatrix} \Rightarrow \left[\begin{array}{ccc|ccc} + & + & + & + & + & + \\ + & - & - & + & - & - \\ + & - & + & + & - & + \\ \hline - & - & + & + & + & - \\ - & + & + & + & - & - \\ - & + & - & + & - & + \end{array}\right]$$

It is important to observe that for the given candidate design matrix given above, F_1 is of the form $F_1 = \begin{bmatrix} 1_3 \\ -1_3 \end{bmatrix}$, where the Schür product of F_1 by itself (F_{11}) yields

$$F_{11} = \begin{bmatrix} 1_3 * 1_3 \\ -1_3 * (-1_3) \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = F_0 \quad F_{12} = \begin{bmatrix} 1_3 \\ -1_3 \end{bmatrix} * F_2 = \begin{bmatrix} 1_3 \\ -1_3 \end{bmatrix} * \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

and $F_{13} = \begin{bmatrix} 1_3 \\ -1_3 \end{bmatrix} * F_3 = \begin{bmatrix} 1_3 \\ -1_3 \end{bmatrix} \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix} = \begin{bmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$.

Furthermore, the Schür product of F_1 with F_2 and F_3 leaves the first 3 entries of F_2 and F_3 unchanged and negates the last 3 entries. It turns out from the above observations that the candidate saturated design can be written as:

$$\begin{array}{cccccc} F_1 & F_2 & F_3 & F_{11} & F_{12} & F_{13}\end{array}$$
$$\left[\begin{array}{ccc|ccc} + & + & + & + & + & + \\ + & - & - & + & - & - \\ + & - & + & + & - & + \\ \hline - & - & + & + & + & - \\ - & + & + & + & - & - \\ - & + & - & + & - & + \end{array}\right] = \begin{bmatrix} M & M \\ -N & N \end{bmatrix}$$

where $M = \begin{bmatrix} + & + & + \\ + & - & - \\ + & - & + \end{bmatrix}$ and $N = \begin{bmatrix} + & + & - \\ + & - & - \\ + & - & + \end{bmatrix}$.

Remark 2.1: A few remarks can be made as follows.

(1) 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) For any choice of candidate saturated design the corresponding candidate saturated design matrix is necessarily of the form $\left[\begin{smallmatrix} M & M \\ -N & N \end{smallmatrix}\right]$ as shown above. In the example F_1 has as many $+1$ entries as -1 entries which means F_1 is balanced. Therefore M and N are square matrices of order k.
(3) The candidate design matrix as displayed above will be a valid design matrix if it is a non-singular matrix. We shall see in the remainder of this paper that in general, a candidate design matrix is a valid design matrix if and only if the design is chosen so that F_1 is balanced and that M and N are non-singular matrices.

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

In the remainder of this section, we explore the construction of a D-optimal design matrix for mean, main effects, and the F_1-second-order interactions from a general perspective. We assume without loss of generality that the vector parameter of interest is of the form $\beta = [\beta_1, \ldots, \beta_k, \beta_0, \beta_{12}, \ldots, \beta_{1k}]^\top$. For convenience, we make the following definitions.

Definition 2.1: We make the following definitions:

(1) We define $\mathcal{D}(k, 1)$ to be the set of all the saturated design matrices that ensure the unbiased estimation of the vector parameter of interest β. We purposely use the notation $\mathcal{D}(k, 1)$ to indicate that the vector parameter of interest β includes the k main effects, the mean, and all the F_1-second-order interactions.
(2) 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.
(3) We define Θ_k to be the maximal value of the absolute value of the determinant of matrices in $\mathcal{M}_k\{-1, +1\}$.

The factor F_1 plays a key role in the construction of a saturated design for the vector parameter β as specified above because it is the only factor that interacts with all the remaining factors. Therefore, we define the factor F_1 as the pivot factor. Since the entries of F_1 takes values from $\{-1, 1\}$ we assume without loss of generality that F_1 is of the form $F_1 = \begin{bmatrix} 1_{f_+}^\top & -1_{f_-}^\top \end{bmatrix}^\top$, where f_+ and f_- are respectively the frequencies of 1 and -1 entries in the vector F_1 with $f_+ + f_- = 2k$. For convenience we write $F_2, \ldots, F_k$ as block vectors $F_2 = \begin{bmatrix} m_2^\top & n_2^\top \end{bmatrix}^\top, \ldots, F_k = \begin{bmatrix} m_k^\top & n_k^\top \end{bmatrix}^\top$, where $m_2, \ldots, m_k$ are vectors of length f_+ and $n_2, \ldots, n_k$ are vectors of length f_- with entries from $\{-1, 1\}$. We enumerate the following key observations.

(1) The F_1-second-order interactions $F_{12}, \ldots, F_{1k}$ are obtained by the Schür product of F_1 with $F_2, \ldots, F_k$ as follows.
$$F_{12} = \begin{bmatrix} (1_{f_+} * m_2)^\top & (-1_{f_-} * n_2)^\top \end{bmatrix}^\top = \begin{bmatrix} m_2^\top & -n_2^\top \end{bmatrix}^\top$$
$$\vdots \quad \vdots \quad \vdots$$
$$F_{1k} = \begin{bmatrix} (1_{f_+} * m_k)^\top & (-1_{f_-} * n_k)^\top \end{bmatrix}^\top = \begin{bmatrix} m_k^\top & -n_k^\top \end{bmatrix}^\top.$$
(2) The mean F_0 which is a 1_{2k} column vector can be written as $F_0 = \begin{bmatrix} 1_{f_+}^\top & 1_{f_-}^\top \end{bmatrix}^\top = \begin{bmatrix} (1_{f_+} * 1_{f_+})^\top & (-1_{f_-} * (-1_{f_-})^\top \end{bmatrix}^\top = F_1 * F_1$. That is the mean F_0 can be obtained by the Schür product of F_1 with itself.

By preserving the order in which the parameters in the vector $\beta = [\beta_1, \ldots, \beta_k, \beta_0, \beta_{12}, \ldots, \beta_{1k}]^\top$ appear, each element of $\mathcal{D}(k, 1)$ can be written as
$$\begin{bmatrix} 1_{f_+} & m_2 & \cdots & m_k & 1_{f_+} & m_2 & \cdots & m_k \\ -1_{f_-} & n_2 & \cdots & n_k & 1_{f_-} & -n_2 & \cdots & -n_k \end{bmatrix} = \begin{bmatrix} M & M \\ -N & N \end{bmatrix},$$
where $M = \begin{bmatrix} 1_{f_+} & m_2 & \cdots & m_k \end{bmatrix}$ and $N = \begin{bmatrix} 1_{f_-} & n_2 & \cdots & n_k \end{bmatrix}$ with dimensions $f_+ \times k$ and $f_- \times k$ respectively. Thus each element of $\mathcal{D}(k, 1)$ is necessarily on the block matrix form $\begin{bmatrix} M & M \\ -N & N \end{bmatrix}$. Now just because we have the block matrix form $\begin{bmatrix} M & M \\ -N & N \end{bmatrix}$ doesn't mean that we have obtained an element of $\mathcal{D}(k, 1)$. The question one may ask is " What are the necessary and sufficient conditions on the matrix $\begin{bmatrix} M & M \\ -N & N \end{bmatrix}$ to be an element of $\mathcal{D}(k, 1)$? ".

Our goal in what follows is to provide necessary and sufficient conditions to construct an element of $\mathcal{D}(k, 1)$. In the theorem below we provide the necessary and sufficient conditions to construct an element of $\mathcal{D}(k, 1)$.

Theorem 2.1: *A square matrix D of order $2k$ is a design matrix in $\mathcal{D}(k,1)$ if and only if it is in the form $D = \begin{bmatrix} M & M \\ -N & N \end{bmatrix}$ where M and N are elements of $\mathcal{M}_k\{-1,1\}$.*

Proof: We have seen that any element of $\mathcal{D}(k,1)$ is necessarily on the form $F = \begin{bmatrix} M & M \\ -N & N \end{bmatrix}$, where M and N are $\{-1,1\}$-matrices of dimensions $f_+ \times k$ and $f_- \times k$ respectively. We will first show that if $f_+ \neq f_-$ then the matrix F is a singular matrix. In that case, F is not an element of $\mathcal{D}(k,1)$. We then show that M and N have to be both non-singular matrices of order k for F to be an element of $\mathcal{D}(k,1)$.

(1) Assume without loss of generality that $f_+ > k$. Then, since M is of dimensions $f_+ \times k$ we have rank(M) is at most k. Therefore, the rows of M that we define as $m_1^\top, \ldots, m_{f_+}^\top$ are linearly dependent. We may assume without loss of generality that $m_1^\top$ is linearly dependent on $m_2^\top, \ldots, m_{f_+}^\top$, so that $m_1 = \sum_{i=2}^{f_+} c_i m_i$ with some $c_i \neq 0$, $2 \leq i \leq f_+$. This implies that $\begin{bmatrix} m_1 \\ m_1 \end{bmatrix} = \sum_{i=2}^{f_+} c_i \begin{bmatrix} m_i \\ m_i \end{bmatrix}$. It means that the rows $\begin{bmatrix} m_1^\top & m_1^\top \end{bmatrix}, \ldots, \begin{bmatrix} m_{f_+}^\top & m_{f_+}^\top \end{bmatrix}$ of F are linearly dependent, which would make F a singular matrix. In a similar manner, one can show that if $f_- > k$ then F is a singular matrix. Thus, it turns out that $f_- = f_+ = k$ is a necessary condition for F to be non-singular. It follows that any element F of $\mathcal{D}(k,1)$ is on the form $F = \begin{bmatrix} M & M \\ -N & N \end{bmatrix}$, where M and N are $\{-1,1\}$-matrices of order k.
Now, if the matrix M is singular the rows of F would be linearly dependent and F would be a singular matrix by the analogy of the argument above. By the same argument, if N is singular, F would be a singular matrix.

(2) Now suppose both M and N are non-singular matrices, that is M and N are elements of $\mathcal{M}_k\{-1,1\}$. Then, $\det(F) = \det \begin{bmatrix} M & M \\ -N & N \end{bmatrix} = \det(N)\det(M + MN^{-1}N) = 2^k \det(N)\det(M) \neq 0$. It follows that F is an element of $\mathcal{D}(k,1)$ if and only if $F = \begin{bmatrix} M & M \\ -N & N \end{bmatrix}$, where M and N are elements of $\mathcal{M}_k\{-1,1\}$.

■

Corollary 2.1: *A design matrix D^* is a D-optimal saturated design in $\mathcal{D}(k,1)$ if and only if it can be written as $D^* = \begin{bmatrix} M^* & M^* \\ -N^* & N^* \end{bmatrix}$ where M^* and N^* are elements of $\mathcal{M}_k\{-1,1\}$ with maximal absolute value determinant. Furthermore* $|\det(D^*)| = 2^k \Theta_k^2$.

Proof: By Theorem 2.1 for any element D of $\mathcal{D}(k,1)$, $\det(D) = 2^k \det(N)\det(M)$ for some N and M elements $\mathcal{M}_k\{-1,1\}$. This determinant is maximal in absolute value when both M and N have maximal absolute value determinants in $\mathcal{M}_k\{-1,1\}$. ■

2.4. Algorithm for the construction of an element of $\mathcal{D}(k,1)$

We use Theorem 2.1 and Corollary 2.1 to develop an algorithm for the construction of a saturated and a D-optimal saturated design matrix of $\mathcal{D}(k,1)$.

- *Step 1*: Select two matrices M and N from $\mathcal{M}_k\{-1,1\}$ (For a D-optimal design select the matrices M and N with maximal absolute value of determinant).
- *Step 2*: The design matrices $D_1 = \begin{bmatrix} M & M \\ -M & M \end{bmatrix}$ and $D_2 = \begin{bmatrix} M & M \\ -N & N \end{bmatrix}$ obtained through the above steps are saturated design matrices for the estimation of the mean F_0, the k main effects $F_1, \ldots, F_k$ and the interactions $F_{12}, \ldots, F_{1k}$. D_1 is a D-optimal design matrix in $\mathcal{D}(k,1)$ if $|\det(M)|$ is maximal in $\mathcal{M}_k\{-1,1\}$. D_2 is a D-optimal design matrix in $\mathcal{D}(k,1)$ if both $|\det(M)|$ and $|\det(N)|$ have maximal determinant in $\mathcal{M}_k\{-1,1\}$.

In the appendix we give two examples of D-optimal design matrices in $\mathcal{D}(15,1)$ and $\mathcal{D}(16,1)$.

3. Concluding remarks

The construction of saturated design matrices for two-level factorial experiments has gained a lot of interest over a long period of time by both mathematicians and statisticians. In general, mathematicians are interested in finding a matrix with maximal determinant in $\mathcal{M}_k\{-1,1\}$, as well as investigating the spectrum of the determinant function which is the set of the value(s) taken by the $|\det(D_k)|/2^{k-1}$ for D_k element of $\mathcal{M}_k\{-1,1\}$. Thus, numerous papers have been written about the classification of saturated design matrices of fixed order via the spectrum of the determinant function. The spectra of the determinant function S_k for $\{-1,+1\}$-matrices of order k are well known in the literature for orders up to 11. The spectrum of order $k=8$ is due to Metropolis (1969). For $k=9$ and $k=10$, the spectra were computed by Živković (2006) and the spectrum for $k=11$ is due to Orrick (2005). Furthermore, many other papers have investigated D-optimal saturated design matrices for a fixed order. Orrick (2005) constructed a D-optimal design matrix of order 15. Chadjipantelis et al. (1987) came up with a D-optimal design of order 21. The D-optimal design matrix discussed by these papers is a matrix with the maximal absolute value of the determinant in $\mathcal{M}_k\{-1,1\}$. Statisticians on the other hand are not only interested in the global D-optimal design matrices in $\mathcal{M}_k\{-1,1\}$ but also they are interested in the local D-optimal design matrices that satisfy certain restrictions on the columns of matrices in $\mathcal{M}_k\{-1,1\}$. In fact, more than often it is desirable for design statisticians to find a D-optimal design matrix to estimate the mean, the main effects, and a selected number of two-factor interactions. The restriction imposed by the interactions on the columns of saturated design matrices makes it impossible to construct a saturated design matrix that achieves the maximal determinant in $\mathcal{M}_k\{-1,1\}$ under certain conditions. The work we did in the current paper is a good illustration. We showed that the construction of saturated D-optimal design matrices in $\mathcal{D}(k,1)$ is equivalent to finding matrices with maximal determinant in $\mathcal{M}_k\{-1,1\}$. Thus, this problem is just as hard as the Hadamard determinant problem discussed in the introduction.

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Appendix

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

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).

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

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.

+	+	+	+	−	−	−	−	−	+	−	−	−	−	+	+	+	+	+	−	−	−	−	−	+	−	−	−	−	+
+	+	+	−	+	−	−	+	−	−	−	−	+	−	−	+	+	+	−	+	−	−	+	−	−	−	−	+	−	−
+	+	+	−	−	+	−	−	+	−	−	+	−	−	−	+	+	+	−	−	+	−	−	+	−	−	+	−	−	−
+	−	−	+	+	−	−	−	+	−	−	+	+	+	+	+	−	−	+	+	−	−	−	+	−	−	+	+	+	+
+	+	−	+	−	−	+	+	+	−	+	−	−	−	−	+	+	−	+	−	−	+	+	+	−	+	−	−	−	−
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+	+	−	−	−	−	−	−	−	+	+	+	+	+	−	+	+	−	−	−	−	−	−	−	+	+	+	+	+	−
+	+	−	−	+	+	+	−	−	−	−	−	−	+	+	+	+	−	−	+	+	+	−	−	−	−	−	−	+	+
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−	−	−	−	−	−	−	+	+	+	−	−	−	+	−	+	+	+	+	+	+	+	−	−	−	+	+	+	−	+

Figure A5. Saturated D-optimal design matrix for $F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, F_9, F_{10}, F_{11}, F_{12}, F_{13}, F_{14}, F_{15}, F_0, F_{1,2}, F_{1,3}, F_{1,4}, F_{1,5}, F_{1,6}, F_{1,7}, F_{1,8}, F_{1,9}, F_{1,10}, F_{1,11}, F_{1,12}, F_{1,13}, F_{1,14}$, and$F_{1,15}$.

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Figure A6. Saturated D-optimal design matrix for $F_1, F_2, F_3, F_4, F_5, F_6, F_7, F_8, F_9, F_{10}, F_{11}, F_{12}, F_{13}, F_{14}, F_{15}, F_{16} F_0, F_{1,2}, F_{1,3}, F_{1,4}, F_{1,5}, F_{1,6}, F_{1,7}, F_{1,8}, F_{1,9}, F_{1,10}, F_{1,11}, F_{1,12}, F_{1,13}, F_{1,14}, F_{1,15},$ and $F_{1,16}$.