Chapter 1

D-optimal saturated designs: a simulation study

Roberto Fontana, Fabio Rapallo and Maria Piera Rogantin

Abstract In this work we focus on saturated D-optimal designs. Using recent results, we identify D-optimal designs with the solutions of an optimization problem with linear constraints. We introduce new objective functions based on the geometric structure of the design and we compare them with the classical D-efficiency criterion. We perform a simulation study. In all the test cases we observe that designs with high values of D-efficiency have also high values of the new objective functions.

1.1 Introduction

The optimality of an experimental design depends on the statistical model that is assumed and is assessed with respect to a statistical criterion. Among the different criteria, in this chapter we focus on D-optimality.

Widely used statistical systems like SAS and R have procedures for finding an optimal design according to the user’s specifications. Proc Optex of SAS/QC searches for optimal experimental designs in the following way. The user specifies an efficiency criterion, a set of candidate design points, a model and the size of the design to be found, and the procedure generates a subset of the candidate set so that the terms in the model can be estimated as efficiently as possible.
There are several algorithms for searching for $D$-optimal designs. They have a common structure. Indeed, they start from an initial design, randomly generated or user specified, and move, in a finite number of steps, to a better design. All of the search algorithms are based on adding points to the growing design and deleting points from a design that is too big. Main references to optimal designs include [1], [4], [7], [8], [9] and [11].

In this work, we perform a simulation study to analyze a different approach for describing $D$-optimal designs in the case of saturated fractions. Saturated fractions, or saturated designs, contain a number of points that is equal to the number of estimable parameters of the model. It follows that saturated designs are often used in place of standard designs, such as orthogonal fractional factorial designs, when the cost of each experimental run is high. We show how the geometric structure of a fraction is in relation with its $D$-optimality, using a recent result in [3] that allows us to identify saturated designs with the points with coordinates in \{0, 1\} of a polytope, being the polytope described by a system of linear inequalities. The linear programming problem is based on a combinatorial object, namely the circuit basis of the model matrix. Since the circuits yield a geometric characterization of saturated fractions, we investigate here the connections between the classical $D$-optimality criterion and the position of the design points with respect to the circuits.

In this way the search for $D$-optimal designs can be stated as an optimization problem where the constraints are a system of linear inequalities. Within the classical framework the objective function to be maximized is the determinant of the information matrix. In our simulations, we define new objective functions, which take into account the geometric structure of the design points with respect to the circuits of the relevant design matrix. We study the behavior of such objective functions and we compare them with the classical $D$-efficiency criterion.

The chapter is organized as follows. In Sect. 1.2 we briefly describe the results of [3] and in particular how saturated designs can be identified with \{0, 1\} points that satisfy a system of linear inequalities. Then in Sect. 1.3 we present the results of a simulation study in which, using some test cases, we experiment different objective functions and we analyze their relationship with the $D$-optimal criterion. Concluding remarks are made in Sect. 1.4.

1.2 Circuits and saturated designs

As described in [3], the key ingredient to characterize the saturated fractions of a factorial design is its circuit basis. We recall here only the basic notions about circuits in order to introduce our theory. For a survey on circuits and its connections with Statistics, the reader can refer to [6].

Given a model matrix $X$ of a full factorial design $\mathcal{D}$, an integer vector $f$ is in the kernel of $X'$ if and only if $X'f = 0$. We denote by $A$ the transpose of $X$. Moreover, we denote by $\text{supp}(f)$ the support of the integer vector $f$, i.e., the set of indices $j$ such that $f_j \neq 0$. Finally, the indicator vector of $f$ is the binary vector $(f_j \neq 0)$,
where \((\cdot)\) is the indicator function. An integer vector \(f\) is a circuit of \(A\) if and only if:

1. \(f \in \ker(A)\);
2. there is no other integer vector \(g \in \ker(A)\) such that \(\text{supp}(g) \subset \text{supp}(f)\) and \(\text{supp}(g) \neq \text{supp}(f)\).

The set of all circuits of \(A\) is denoted by \(\mathcal{C}_A\), and is named as the circuit basis of \(A\). It is known that \(\mathcal{C}_A\) is always finite. The set \(\mathcal{C}_A\) can be computed through specific software. In our examples, we have used 4ti2 [10].

Given a model matrix \(X\) on a full factorial design \(D\) with \(K\) design points and \(p\) degrees of freedom, we recall that a fraction \(F \subset D\) with \(p\) design points is saturated if \(\det(X_F) \neq 0\), where \(X_F\) is the restriction of \(X\) to the design points in \(F\).

With a slight abuse of notation, \(F\) denotes both a fraction and its support. Under these assumptions, the relations between saturated fractions and the circuit basis \(\mathcal{C}_A = \{f_1, \ldots, f_L\}\) associated to \(A\) is illustrated in the theorem below, proved in [3].

**Theorem 1.** \(F\) is a saturated fraction if and only if it does not contain any of the supports \(\{\text{supp}(f_1), \ldots, \text{supp}(f_L)\}\) of the circuits of \(A = X'\).

### 1.3 Simulation study

The theory described in Sect. [12] allows us to identify saturated designs with the feasible solutions of an integer linear programming problem. Let \(C_A = (c_{ij}, i = 1, \ldots, L, j = 1, \ldots, K)\) be the matrix, whose rows contain the values of the indicator functions of the circuits \(f_1, \ldots, f_L\), \(c_{ij} = (f_i \neq 0), i = 1, \ldots, L, j = 1, \ldots, K\) and \(Y = (y_1, \ldots, y_K)\) be the \(K\)-dimensional column vector that contains the unknown values of the indicator function of the points of \(F\). In our problem the vector \(Y\) must satisfy the following conditions:

1. the number of points in the fractions must be equal to \(p\);
2. the support of the fraction must not contain any of the supports of the circuits.

In formulae, this fact translates into the following constraints:

\[
\begin{align*}
1_K^t Y &= p, \\
C_A Y &< b, \\
y_i &\in \{0, 1\}
\end{align*}
\]

where \(b = (b_1, \ldots, b_L)\) is the column vector defined by \(b_i = \#\text{supp}(f_i), i = 1, \ldots, L,\) and \(1_K\) is the column vector of length \(K\) and whose entries are all equal to 1.

Since \(D_F = \det(V(Y)) = \det(X_F^t X_F)\) is an objective function, it follows that a \(D\)-optimal design is the solution of the optimization problem

\[
\begin{align*}
\text{maximize } & \det(V(Y)) \\
\text{subject to } & (1.1), (1.2) \text{ and } (1.3).
\end{align*}
\]
In general the objective function to be maximized \( \det(V(Y)) \) has several local optima and the problem of finding the global optimum is part of current research. Instead of trying to solve this optimization problem in this work we prefer to study different objective functions that are simpler than the original one but that could generate the same optimal solutions. By analogy of Theorem 1 our new objective functions are defined using the circuits of the model matrix.

For any \( Y \), we define the vector \( b_Y = C_A Y \). This vector \( b_Y \) contains the number of points that are in the intersection between the fraction \( \mathcal{F} \) identified by \( Y \) and the support of each circuit \( f_i \in C_A, i = 1, \ldots, L \). From (1.2) we know that each of these intersections must be strictly contained in the support of each circuit. For each circuit \( f_i, i = 1, \ldots, L \) it seems natural to minimize the cardinality \( b_Y \) of the intersection between its support \( \text{supp}(f_i) \) and \( Y \) with respect to the size of its support, \( b_i \).

Therefore, we considered the following two objective functions:

- \( g_1(Y) = \sum_{i=1}^{L} (b - b_Y)_i \);
- \( g_2(Y) = \sum_{i=1}^{L} (b - b_Y)^2 \).

From the examples analyzed in Sect. 1.3.1 we observe that the \( D \)-optimality is reached with fractions that contain part of the largest supports of the circuits, although this fact seems to disagree with Thm. 1. In fact, Thm. 1 states that fractions containing the support of a circuit are not saturated, and therefore one would expect that optimal fractions will have intersections as small as possible with the supports of the circuits. On the other hand, our experiments show that optimality is reached with fractions having intersections as large as possible with such supports. For this reason we consider also the following objective function:

- \( g_3(Y) = \max(b_Y) \).

As a measure of \( D \)-optimality we use the \( D \)-efficiency. The \( D \)-efficiency of a fraction \( \mathcal{F} \) with indicator vector \( Y \) is defined as

\[
E_Y = \left( \frac{1}{\#\mathcal{F} \cdot D_Y} \right) \times 100
\]

where \( \#\mathcal{F} \) is the number of points of \( \mathcal{F} \) that is equal to \( p \) in our case, since we consider only saturated designs.

### 1.3.1 First case. \( 2^4 \) with main effects and 2-way interactions

Let us consider the \( 2^4 \) design and the model with main factors and 2-way interactions. The design matrix \( X \) of the full design has 16 rows and 11 columns, the number of estimable parameters. As the matrix \( X \) has rank 11, we search for fractions with 11 points. A direct computation shows that there are \( \binom{16}{11} = 4,368 \) fractions with 11 points: among them 3,008 are saturated, and the remaining 1,360 are not. Notice that equivalences up to permutations of factor or levels are not considered here.
The circuits are 140 and the cardinalities of their supports are 8 in 20 cases, 10 in 40 cases, 12 in 80 cases. For more details refer to [3]. This example is small enough for a complete enumeration of all saturated fractions. Moreover, the structure of that fractions reduces to few cases, due to the symmetry of the problem.

For each saturated fraction \( \mathcal{F} \) with indicator vector \( Y \) we compute the vector \( b_Y \), whose components are the size of the intersection between the fraction and the support of all the circuits, \( \mathcal{F} \cap \text{supp}(f_i), i = 1, \ldots, 140, \) and we consider \( b - b_Y \). Recall that \( b \) is the vector of the cardinalities of the circuits. The frequency table of \( b - b_Y \) describes how many points need to be added to a fraction in order to complete each circuit. All the frequency tables are displayed in the left side of Table 1.1 while on the right side we report the corresponding values of \( D \)-efficiency.

| \( b - b_Y \) | \( E_Y \) |
|-----------------|------|
| 1 2 3 4 5 | 68.29 77.46 83.38 |
| 5 15 50 60 10 | 192 0 0 |
| 5 18 48 55 14 | 1,040 0 0 |
| 5 21 46 50 18 | 960 0 0 |
| 5 24 44 45 22 | 480 0 0 |
| 5 27 42 40 26 | 0 320 0 |
| 5 30 40 35 30 | 0 0 16 |
| **Total** | **2,672** **320** **16** |

For instance, consider one of the 192 fractions in the first row. Among the 140 circuits, 5 of them are completed by adding 1 point to the fraction, 15 of them by adding 2 points, and so on. We observe that there is a perfect dependence between the \( D \)-efficiency and the frequency table of \( b - b_Y \).

However, analyzing the objective functions \( g_1(Y) \), \( g_2(Y) \) and \( g_3(Y) \), we argue that the previous finding has no trivial explanation. The values of all our objective functions are displayed in Table 1.2.

From Table 1.2 we observe that both \( g_2(Y) \) and \( g_3(Y) \) are increasing as \( D \)-efficiency increases. Notice also that \( g_1(Y) \) is constant over all the saturated fractions. This is a general fact for all no-m-way interaction models.

**Proposition 1.** For a no-m-way interaction model, \( g_1(Y) \) is constant over all saturated fractions.

**Proof.** We recall that \( C_A = (c_{ij}, i = 1, \ldots, L, j = 1, \ldots, K) \) is the \( L \times K \) matrix, whose rows contain the values of the indicator functions of the supports of the circuits \( f_1, \ldots, f_L \). \( c_{ij} = (f_{ij} \neq 0), i = 1, \ldots, L, j = 1, \ldots, K. \) We have

\[
g_1(Y) = \sum_{i=1}^{L} (b - b_Y)_i = \sum_{i=1}^{L} (b)_i - \sum_{i=1}^{L} (b_Y)_i.
\]
Table 1.2 Classification of all saturated fractions for the $2^4$ design with main effects and 2-way interactions.

| $g_1(Y)$ | $g_2(Y)$ | $g_3(Y)$ | $E_Y$ | $n$  |
|----------|----------|----------|-------|------|
| 475      | 1,725    | 9        | 68.29 | 192  |
| 475      | 1,739    | 10       | 68.29 | 960  |
| 475      | 1,753    | 10       | 68.29 | 960  |
| 475      | 1,739    | 11       | 68.29 | 80   |
| 475      | 1,767    | 11       | 68.29 | 480  |
| 475      | 1,781    | 11       | 77.46 | 320  |
| 475      | 1,795    | 11       | 83.38 | 16   |
|          |          |          |       | Total 3,008 |

The first addendum does not depend on $Y$, and for the second one we get

$$\sum_{i=1}^{L} (b_Y)_i = \sum_{i=1}^{L} \sum_{j=1}^{K} c_{ij} Y_j = \sum_{j=1}^{K} Y_j \sum_{i=1}^{L} c_{ij}.$$  

Now observe that a no-$m$-way interaction model does not change when permuting the factors or the levels of the factors. Therefore, by a symmetry argument, each design point must belong to the same number $q$ of circuits, and thus $\sum_{i=1}^{L} c_{ij} = q$. It follows that

$$\sum_{i=1}^{L} (b_Y)_i = q \sum_{j=1}^{K} Y_j = pq.$$

\square

In view of Prop. 1 in the remaining examples we will consider only the functions $g_2$ and $g_3$.

1.3.2 Second case. $3 \times 3 \times 4$ with main effects and 2-way interactions

Let us consider the $3 \times 3 \times 4$ design and the model with main factors and 2-way interactions. The model has $p = 24$ degrees of freedom. The number of circuits is 17,994. In this case the number of possible subsets of the full design is \( \binom{36}{24} = 1,251,677,700 \). It would be computationally unfeasible to analyze all the fractions. We use the methodology described in [2] to obtain a sample of saturated $D$-optimal designs. It is worth noting that this methodology finds $D$-optimal designs and not simply saturated designs. This is particularly useful in our case because allows us to study fractions for which the $D$-efficiency is very high. The sample contains 500 designs, 380 different.
The results are summarized in Table 1.3 where the fractions with minimum $D$-efficiency $E_Y$ have been collapsed in a unique row in order to save space. We observe that for 138 different designs the maximum value of $D$-efficiency, $E_Y = 24.41$ is obtained for both $g_2(Y)$ and $g_3(Y)$ at their maximum values $g_2(Y) = 970,896$ and $g_3(Y) = 24$.

### Table 1.3 Classification of 380 random saturated fractions for the $3 \times 3 \times 4$ design with main effects and 2-way interactions.

| $g_2(Y)$ | $g_3(Y)$ | $E_Y$   | $n$ |
|----------|----------|---------|-----|
| $\leq 963,008$ | $\leq 21$ | 22.27   | 37  |
| 962,816   | 21       | 23.6    | 7   |
| 962,816   | 22       | 23.6    | 12  |
| 963,700   | 22       | 23.6    | 34  |
| 965,308   | 22       | 23.6    | 46  |
| 966,760   | 22       | 23.6    | 9   |
| 967,676   | 22       | 23.6    | 6   |
| 970,860   | 24       | 23.6    | 91  |
| 970,896   | 24       | 24.41   | 138 |
| **Total** |          |         | 380 |

#### 1.3.3 Third case. $2^5$ with main effects

Let us consider the $2^5$ design and the model with main effects only. The model has $p = 6$ degrees of freedom. The number of circuits is 353,616. As in the previous case we use the methodology described in [2] to get a sample of 500 designs, 414 different.

The results are summarized in Table 1.4. We observe that for 194 different designs, the maximum value of $D$-efficiency, $E_Y = 90.48$ is obtained for both $g_2(Y)$ and $g_3(Y)$ at their maximum values $g_2(Y) = 11,375,490$ and $g_3(Y) = 6$.

### Table 1.4 Classification of 414 random saturated fractions for the $2^5$ design with main effects.

| $g_2(Y)$ | $g_3(Y)$ | $E_Y$   | $n$ |
|----------|----------|---------|-----|
| 11,360,866 | 6       | 76.31   | 31  |
| 11,342,586 | 6       | 83.99   | 9   |
| 11,371,834 | 6       | 83.99   | 126 |
| 11,375,490 | 5       | 83.99   | 54  |
| 11,375,490 | 6       | 90.48   | 194 |
| **Total** |          |         | 414 |
1.4 Concluding remarks

The examples discussed in the previous section show that the \( D \)-efficiency of the saturated fractions and the new objective functions based on combinatorial objects are strongly dependent. The three examples suggest to investigate such connection in a more general framework, in order to characterize saturated \( D \)-optimal fractions in terms of their geometric structure. Notice that our presentation is limited to saturated fractions, but it would be interesting to extend the analysis to other kinds of fractions. Moreover, we need to investigate the connections between the new objective functions and other criteria than \( D \)-efficiency.

Since the number of circuits dramatically increases with the dimensions of the factorial design, both theoretical tools and simulation will be essential for the study of large designs.

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