CONSTRUCTION OF SUPERSATURATED DESIGNS THROUGH PARTIALLY ALIASED INTERACTIONS

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ABSTRACT

An N x N Hadamard matrix can be used to construct a saturated two-level design with N runs and N - 1 factors. Furthermore, if an interaction column of the matrix is not fully aliased with any of the N - 1 columns of the matrix, it can be used as a supplementary column for studying an additional factor. For some small Hadamard matrices studied by Plackett & Burman (1946), the number of such interaction columns is very large, thus allowing the construction of supersaturated designs whose number of factors far exceeds the run size. A general method of construction along these lines is proposed. Efficiency of the constructed designs is studied by using three criteria.

Key Words: A-efficiency; D-efficiency; Effect sparsity; Plackett-Burman designs; Screening designs.

1. INTRODUCTION

Supersaturated designs allow more factors than the run size to be studied. For an $N \times M$ design matrix to simultaneously estimate the effects of M factors, we must have $N - 1 \geq M$, where N is the run size. In some practical situations runs may be expensive and the number of factors to be studied can be large. It may then be desirable to use a supersaturated design for screening purpose. In many experiments, particularly those in engineering investigations, the number of factors with relatively large effects is small, often not exceeding 5 or 6. Under this assumption of effect sparsity, supersaturated designs can be used effectively for studying a large number of factors and still allowing the important ones to be estimated simultaneously. Booth & Cox (1962) first adopted this approach in constructing systematic supersaturated designs. Previously Satterthwaite (1959) suggested the use of random balance designs, which were criticized in the accompanying discussion. Watson (1961) suggested an alternative idea by grouping the factors into sets of factors. A much smaller design is used to study the grouped factors. If a grouped factor is found significant in the analysis, then the factors in the group will be studied in a subsequent experiment. Otherwise they will be screened out. Although it is more acceptable than the random balance design, it requires strong assumptions to ensure that a grouped factor is significant if and only if at least one of its factors is significant. In practice such assumptions are often much stronger and more difficult to verify than the effect sparsity assumption.

In this paper we construct supersaturated designs by utilizing *partially aliased* interactions. The efficiencies of the constructed designs are high when effect sparsity holds. A good example of partially aliased interactions is given by the 12-run Plackett-Burman design in Table 1. Let ij denote the column obtained by multiplying entry-wise the i^{th} and j^{th} columns. It is not equal to any of the 11 columns of the matrix and has $1/3$ or $-1/3$ correlation with each of the 11 columns. In factorial experiments ij is called the interaction between factors i and j. If ij has a correlation 1 or -1 with one of the 11 columns, say column k, then it is said to be fully aliased with factor k. Otherwise it is partially aliased. Note that for 2-level designs defined by a group of defining contrasts (Kempthorne, 1973), any interaction is either orthogonal or fully aliased with any other main effect or interaction.

(Table 1)

The idea of the proposed construction is simple: supplement a saturated design with columns defined by its partially aliased interactions. The difficulty is what partially aliased interactions should be chosen. In §3 we give one such method and in §4 we elaborate and improve the method in the construction of 12-run and 20-run design that can accommodate up to 66 and 124 factors respectively. Three criteria for design efficiencies are given in §2. In §5 we compare our designs with those constructed by Booth & Cox (1962) and Lin (1992). Analysis of data from such experiments is briefly discussed in §6.

2. DESIGN CRITERIA

To compare different supersaturated designs, Booth & Cox (1962) proposed the following criterion. Let s_{ij} be the sum of cross products between columns i and j of a design. Define $E(s^2)$ to be the average of s_{ij}^2 over all pairs (i,j). Since $E(s^2) = 0$ for orthogonal designs, it is a measure of non-orthogonality under the strong assumption that only two out of the M factors are active. In this paper we prefer to use $E(s^2)/N^2$ since it is the average of squared correlations over all pairs of columns. This criterion is equivalent to a determinant criterion commonly used in optimal designs. Let X_{ij} be the $N \times 2$ matrix consisting of columns i and j. If the entries of each column are either 1 or -1, then $\left|X_{ij}^T X_{ij}\right| = (N^2 - s_{ij}^2)$ and its average over all pairs equals $(N^2 - E(s^2))$. Therefore $E(s^2)/N^2$ can be interpreted as a measure of D-efficiency loss relative to orthogonal designs.

We can extend this criterion to situations with more than two active factors. Let f be the number of active factors. Define the D-criterion

$$D_f = \sum_i \left|\frac{1}{N} X_i^T X_i\right|^{1/f} / \binom{M}{f}, \tag{2.1}$$

where the summation is over all possible $N \times f$ submatrices X_i of the full design matrix and M is the total number of columns in the design matrix. Taking the f^{th} root in (2.1) makes D_f a more realistic measure of efficiency. An alternative to (2.1) is the A-criterion given by

$$A_f = \sum_i \frac{1}{f} tr\left(\frac{1}{N} X_i^T X_i\right)^{-1} / \binom{M}{f}. \tag{2.2}$$

Since $A_f \geq 1$ in general and equals 1 for orthogonal designs, we can also use $A_f - 1$ to measure nonorthogonality. If one $X_i^T X_i$ is singular, A_f becomes infinite while D_f is still well-defined. Since in reality only some subsets of f factors are active, D_f is a more reasonable criterion in case one or more $X_i^T X_i$ are singular.

Booth & Cox (1962) observed an interesting connection between the A_f and the $E(s^2)$ criteria. Assuming that $|s_{ij}|/N$ are sufficiently smaller than 1 for all i and j, they showed that, in our notation, $A_f \approx 1 + (f-1)E(s^2)/N^2$. A significant implication of this approximation is that, although the $E(s^2)$ criterion is based on $f = 2$, $(f-1)E(s^2)/N^2$ can be used as a measure of A-efficiency loss for any f. However, as demonstrated in §4, this approximation can be poor when some $|s_{ij}|/N$ are not small, which is more likely to occur for larger f.

3. A GENERAL CONSTRUCTION METHOD

A Hadamard matrix is an $N \times N$ orthogonal matrix of 1 and -1, where N must be a multiple of four. Without loss of generality, one of its columns consists of all 1's. Since this column cannot be used for studying factors, for design purposes it is removed from the matrix. We call the remaining $N \times (N-1)$ matrix a Hadamard design. Denote its $N-1$ columns by c_1, c_2, ..., c_{N-1}. An interaction column c_{ij} is defined to be the entry-wise product of c_i and c_j, which we use as a column of a supersaturated design. Plackett & Burman (1946) gave Hadamard designs for various values of N and discussed their use in factorial experiments. We will refer to them as PB designs. The smaller ones with $N = 12$, 20, 24 and 28 are more

popular among experimenters. Many of the PB designs can be obtained by cyclic generation of the first row. Take the 12-run design in Table 1. Rows 2 to 11 are obtained from cyclically permuting the signs in the first row. Then add the row of -1's as the last row. Similarly the 20-run PB design can be constructed by cyclic generation from its first row $(+--++---+-+-++++--+)$.

Among the c_i and c_{jk}, the pairs $(c_i,\ c_j)$, $(c_i,\ c_{ij})$, $(c_{ij},\ c_{ik})$ are orthogonal, where $i \neq j \neq k$. For computing the $E(s^2)$ value, we have to evaluate $c_i^T c_{k\ell}$ and $c_{ij}^T c_{k\ell}$, where $i \neq j \neq k \neq \ell$. For cyclic designs, there is a cross balance among the c_i's. Therefore we need to compute these values only for $i = 1$.

From an $N \times (N-1)$ Hadamard design, we can construct an $N \times M$ supersaturated design for $N \leq M \leq 2N-3$, which consists of $c_1,\ ...,\ c_{N-1}$ and $(M-N+1)$ columns chosen from the $N-2$ interaction columns $c_{i_o j}$, where $j \neq i_o$ and i_o is fixed. For cyclic designs, we can choose $i_o = 1$ without loss of generality. For noncyclic designs, we can choose i_o to minimize $\max \left| c_i^T\ c_{i_o j} \right| N^{-1}$ over i and j. See the discussion after (3.2). From the previous discussion the only pairs of columns that may be non-orthogonal are $(c_i,\ c_{i_o j})$ where $i \neq i_o \neq j$. The $E(s^2)$ value of the proposed design has a simple formula based on the following fact:

$$\sum_{i=1}^{N-1} (c_i^T\ c_{jk})^2 = N^2 \quad \text{for any} \quad j \neq k\ . \tag{3.1}$$

Its proof is simple. Since the c_i's form an orthogonal basis, the left expression is equal to $N||c_{jk}||^2 = N^2$.

Since the other pairs of columns are orthogonal, we have

$$\frac{E(s^2)}{N^2} = (M - N + 1)/\binom{M}{2} \tag{3.2}$$

for the proposed designs with $N \leq M \leq 2N-3$. Even for $M = 2N-3$, $E(s^2)/N^2 = (2N-3)^{-1}$, which indicates a small loss of efficiency.

Since $E(s^2)$ is a constant independent of the choice of design, further discrimination may be made by examining the maximum of $\left|c_i^T\ c_{i_o j}\right| N^{-1}$ over all possible i and j. If N is a power of two and the columns c_i's form a subgroup, i.e., any c_{jk} is equal to one of the c_i's, the maximum value is N. Since $c_{i_o j}$ is fully aliased with one of the c_i's in this case, they cannot be used to construct supersaturated designs. Among designs with $\max\left|c_i^T\ c_{i_o j}\right| N^{-1} < 1$, in view of (3.1), we want the values of $\left|c_i^T\ c_{i_o j}\right|$ with $i \neq i_o \neq j$ to be as evenly distributed as possible. The most extreme case is the 12-run PB design which has $N^{-1}\left|c_i^T\ c_{i_o j}\right| = \frac{4}{12} = \frac{1}{3}$ for any $i \neq i_o \neq j$. For the 20-run PB design, out of the 19 $N^{-1}\left|c_i^T\ c_{i_o j}\right|$ values, $i = 1,\ ...,\ 19$, one is $\frac{3}{5}$, sixteen are $\frac{1}{5}$, and two are 0. Although the maximum is $\frac{3}{5}$, it only occurs once. The rest take $\frac{1}{5}$ or 0. There are two more Hadamard matrices of order 20 constructed by M. Hall Jr. From them we can construct supersaturated designs with $N = 20$ and $20 \leq M \leq 37$. It turns out that each of them has the same distribution of the $N^{-1}\left|c_i^T\ c_{i_o j}\right|$ values as the 20-run PB design. For the 24-run PB design, out of the 23 values of $N^{-1}\left|c_i^T\ c_{i_o j}\right|$, nine are $\frac{1}{3}$ and the rest are 0. For other PB designs, these values can be found in an unpublished paper by Lin and Draper.

To accommodate more than $2N-3$ columns, we must understand the correlation

structure between c_{ij} and $c_{k\ell}$, $i \neq j \neq k \neq \ell$. Since this can be quite tedious for general designs, we will not consider it here. Only the 12-run and 20-run designs are studied in detail in the next section because of their nice correlation structures.

4. SUPERSATURATED DESIGNS OF 12 and 20 RUNS

For the 12-run PB design, it is easy to show that $\left|c_i^T\ c_{jk}\right| = \left|c_{ij}^T\ c_{k\ell}\right| = 4$ for any $i \neq j \neq k \neq \ell$, and $= 0$ otherwise. Therefore any supersaturated design consisting of the c_i's and some of the c_{jk}'s has its $E(s^2)$ value equal to $16p$, where p is the percentage of non-orthogonal pairs of columns. A good design should minimize the value of p. The following construction appears to give the best values of p for designs with M columns, $12 \leq M \leq 66$. Arrange the 66 columns by taking c_1, ..., c_{11} as the first 11 columns and lexicographically ordering the remaining 55 interaction columns c_{ij}, i.e., c_{ij} precedes $c_{k\ell}$ if $i < k$, or $i = k$ and $j < \ell$. For $12 \leq M \leq 21$, it coincides with the general construction in §3 and $p = 9(M-11)/\binom{M}{2}$. For $22 \leq M \leq 30$, the columns consist of three groups: (i) c_i, $i = 1$, ..., 11, (ii) c_{1i}, $i = 2$, ..., 11, (iii) c_{2i}, $i = 3$, ..., $M - 19$. Each column in (ii) and (iii) is non-orthogonal to nine columns in (i). Each column in (iii) is also non-orthogonal to eight columns in (ii). The total number of non-orthogonal pairs is $(10 + M - 21) \times 9 + (M - 21) \times 8$ and $p = \{90 + 17(M-21)\}/\binom{M}{2}$. Similarly, for $31 \leq M \leq 38$, the columns consist of four groups: (i) and (ii) as before, (iii) c_{2i}, $i = 3$, ..., 11, (iv) c_{3i}, $i = 4$, ..., $M-27$. By using the same argument, the total number of non-orthogonal pairs is $(10+9+M-30)\times 9+(9+M-30)\times 8+(M-30)\times 7$

and $p = \{243 + 24(M - 30)\}/\binom{M}{2}$. The p values for the remaining cases can be obtained similarly.

The ordering of interaction columns can be justified by a simple argument. Consider the 22^{nd} factor c_{23}. Once it is introduced, we should bring in the other c_{2i}'s because they are orthogonal to each other, and the correlation structure of c_{2i} with those in (i) and (ii) is the same as any other c_{ij}. If, instead, c_{45} were used as the 23^{rd} factor, it would introduce one additional nonorthogonal pair between c_{23} and c_{45}. The same argument applies to the subsequent factors.

In Figure 1 we plot the efficiency loss $E(s^2)/N^2 = \frac{1}{9}\, p$ for $12 \leq M \leq 66$. It is surprisingly small. For $M = 66$, it is less than 8%. We also plot the A-efficiency loss $A_f - 1$ and its approximation $(f-1)E(s^2)/N^2$ for $f = 4$ and 5. The approximation consistently underestimates the $A_f - 1$ value and the error becomes larger as f and M increase. For $f = 3$ which is omitted in Figure 1, the approximation is more satisfactory and the error never exceeds 23%. Since A_5 is finite, any five columns of the designs are linearly independent. In Figure 2 we plot the D_f efficiency for $f = 3, 4$ and 5. The D_f-efficiency loss is smaller than the A_f-efficiency loss. Recall that the A_f or D_f efficiency is relative to a hypothetical orthogonal design which does not exist for $M \geq N$. Therefore either measure of efficiency loss is an upper bound. As remarked in §1, the number of active factors f is usually small in practice. Therefore the small efficiency loss of the proposed design strongly suggests its effectiveness in screening.

(Figures 1 & 2)

Next we consider the construction of supersaturated designs with 20 runs. As in §3 we use $I_o = \{c_i,\ i = 1,\ \ldots,\ 19\}$ and

$$I_1 = \{c_{1i},\ i = 2,\ \ldots,\ 19\} \tag{4.1}$$

for the first 37 columns, where c_i are the columns of the 20-run PB design. To choose the remaining columns, we need to understand the correlation structure among the c_i's and c_{jk}'s. As pointed out in §3, the distribution of $\left|c_I^T c_{jk}\right|$ over $i = 1,\ ...,\ 19$ is independent of j and k. Therefore we need only to examine the value of $\left|c_{1i}^T c_{jk}\right|$ for $i \neq j \neq k \neq 1$. The cyclic property of the 20-run PB design ensures that we can choose the first subscript of c to be 1. Out of the $\binom{18}{3} = 816$ triplets (i, j, k), 48 take the value 12 and the remaining ones take the value 4. These 48 triplets are:

$237, 249, 25t_6, 26t_9, 28t_2, 2t_0t_5, 2t_1t_8, 2t_4t_7, 34t_3, 35t_2, 36t_6, 38t_9, 39t_5, 3t_0t_8, 3t_1t_4, 45t_7,$

$478, 4t_0t_2, 4t_1t_6, 4t_4t_8, 4t_5t_9, 569, 57t_0, 58t_5, 5t_3t_4, 5t_8t_9, 67t_5, 68t_4, 6t_0t_3, 6t_1t_2, 6t_7t_8,$

$79t_7, 7t_1t_9, 7t_2t_4, 7t_3t_8, 8t_0t_1, 8t_3t_7, 8t_6t_8, 9t_0t_6, 9t_1t_3, 9t_2t_8, 9t_4t_9, t_0t_7t_9, t_1t_5t_7, t_2t_3t_5,$

$t_2t_6t_7, t_3t_6t_9, t_4t_5t_6$, where t_i denotes the $(10 + i)^{\text{th}}$ column of the 20-run PB design. They provide the solution to the following question: find jk such that $\left|c_{1i}^T c_{jk}\right| = 4$ for all i. There are only nine of them: $2t_3, 3t_7, 46, 5t_1, 7t_6, 89, t_0t_4, t_2t_9, t_5t_8$. Based on this information we are ready to construct designs with $M \geq 38$. As in the 12-run case we can use $c_{2i},\ i = 3,\ ...,\ 19$, for $38 \leq M \leq 54$, but unlike the former, the ordering of c_{2i} matters. It is obvious that $2t_3$ should be the 38^{th} column since it has

the smallest correlations with the columns in (4.1). For simplicity we will drop c and only retain the subscript in the following definition of groups of columns. So we use

$$II = \{2t_3,\ 2i,\ i \neq t_3,\ i \geq 3\} \tag{4.2}$$

for the 38^{th} to 54^{th} columns. For the next 16 columns we can use

$$III = \{3t_7,\ 3t_4,\ \text{remaining } 3i\text{'s }\}.$$

The choice of $3t_7$ as the first column in III is obvious. We choose $3t_4$ as the next column because it has the smallest correlations with the columns in II, which follows from $|c_{3t_4}^T c_{2i}| = |c_{2t_3}^T c_{1(i-1)}| = 4$ for all $i \geq 3$. By elaborating on this argument, we can choose the remaining columns up to $M = 124$ in four groups:

$$\begin{aligned}
IV &= \{46, 4t_8, 4t_5,\ \text{remaining } 4i\text{'s}\},\\
V &= \{5t_1, 57, 5t_9, 5t_6,\ \text{remaining } 5i\text{'s}\},\\
VI &= \{89, 8t_7, 86, 8t_4, 8t_0,\ \text{remaining } 8i\text{'s}\},\\
VII &= \{t_2t_9, t_26, t_2t_6, t_2t_1, t_2t_3, t_2t_8,\ \text{remaining } t_2i\text{'s}\}.
\end{aligned}$$

In VII the first six columns are chosen so that the i^{th} column has the smallest correlations with the columns in the i^{th} group. The same criterion is used for choosing the first five columns in VI and so forth.

By exploiting the correlation structure we can further improve these designs. Take, for example, $M = 39$. Choosing $3t_7$ for the 39^{th} column gives a smaller $E(s^2)$ value than choosing 23 or other $2i$'s as in (4.2). Although 23 is orthogonal to $2t_3$, it

has correlation 3/5 with 17 in the group I_1. On the other hand, $3t_7$ has correlation $1/5$ or $-1/5$ with the columns in I_1 and with $2t_3$. By following the same argument, we can choose $7t_6, t_0t_4, 23$ for the 40^{th} to 42^{nd} columns. The resulting designs for $M \leq 42$ are better than the designs given in (4.1) and (4.2) in terms of the $E(s^2)$, A_f and D_f criteria with $f = 3, 4, 5$. In Figure 3 we plot the values of A_f and D_f for $f = 3, 4, 5$. The efficiency loss appears to be very small.

(Figures 3)

5. COMPARISON WITH OTHER DESIGNS

Lin (1992) proposed an ingenious method for constructing supersaturated designs of order $N \times M$ with $M \leq 2N-2$. Starting with a $2N \times (2N-1)$ Hadamard design, choose a column as the branching column and retain only the N rows that have $+1$ in the branching column. Then the $2N-2$ columns other than the branching column form a supersaturated design of order $N \times (2N-2)$. If the original Hadamard design is obtained from cyclic generation, any column can be used as the branching column. Otherwise a complete search is warranted. For $M < 2N-2$, the best M columns can be found by computer search. By comparison, Lin's designs are more flexible in the choice of run size because our construction requires the existence of Hadamard matrix of order N while his requires the same for $2N$. On the other hand ours can accommodate more than $2N-2$ factors as illustrated in §4.

In Table 2 we compare these two classes of designs and those by Booth & Cox (1962) using the $E(s^2)$ criterion. We do not use $E(s^2)/N^2$ for comparison since $E(s^2)$ values are given in the tables of Booth & Cox and Lin. The table does not include designs with $N = 20$ since they are not given in either paper. For $N = 12$ the designs in the last column (under "Wu") are those constructed in §4. For $N = 24$ and $M = 30$ and 45, the designs under "Wu" are those constructed in §3 based on the 24-run PB design and $c_o = 1$. For $M = 46$, we use the 2×5 interaction column as the 46^{th} column.

(Table 2)

The designs by Booth & Cox have larger $E(s^2)$ values than the other two classes. For $M \leq 2N - 3$, our designs are at least as good as Lin's designs. For smaller M ours are better. The most interesting findings are: (i) Lin's design for $M = 2N - 2$ has the smallest value, (ii) Lin's designs for $M = 2N - 2$ and $2N - 3$ have the same $E(s^2)$ value. Both deserve further investigation. The interior performance of our designs for $M = 2N - 2$ can be explained in part by its construction. The $(2N-2)^{\text{th}}$ column uses a $2 \times k$ intervention for some $k > 2$, which has nonzero correlations with the majority of the $1 \times j$ interactions in the N^{th} to $(2N - 3)^{\text{th}}$ columns.

6. ANALYSIS

Columns of a supersaturated design are not mutually orthogonal. Therefore standard analysis techniques for orthogonal designs, e.g., half-normal plots and analysis of variance are not applicable. Although we cannot estimate all the factor effects simultaneously, we can use forward selection in regression analysis to select a model (or several models) consisting of a smaller number of factors. Alternatively we can use subset selection procedures such as C_p. Knowledge on the dependency of columns of the supersaturated design will put an upper bound on the subset size.

If only a small number of factors are identified as important, we can go beyond screening by entertaining some interactions among the factors identified. One such analysis strategy is suggested by Hamada & Wu (1992). However, by the nature of our construction some interactions cannot be entertained. Take, for example, the 12×21 design in §3 and §4, whose columns consist of $1, \ldots, 11$ and $1i, i = 2, \ldots, 11$. Suppose that factors 1 and 2 turn out to be significant and it is desired to study their interaction. It would not be possible because it is fully aliased with the 12th factor. To minimize the chance of full aliasing, it is advisable to assign column 1 to a factor least likely to be important. Similarly, if as in §4, $2i, i = 3, \ldots, 11$ are introduced as the next 9 factors, column 2 should be assigned to a factor thought to be less important.

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Table 1. *A 12-run Plackett-Burman design*

1	2	3	4	5	6	7	8	9	10	11
1	1	−1	1	1	1	−1	−1	−1	1	−1
−1	1	1	−1	1	1	1	−1	−1	−1	1
1	−1	1	1	−1	1	1	1	−1	−1	−1
−1	1	−1	1	1	−1	1	1	1	−1	−1
−1	−1	1	−1	1	1	−1	1	1	1	−1
−1	−1	−1	1	−1	1	1	−1	1	1	1
1	−1	−1	−1	1	−1	1	1	−1	1	1
1	1	−1	−1	−1	1	−1	1	1	−1	1
1	1	1	−1	−1	−1	1	−1	1	1	−1
−1	1	1	1	−1	−1	−1	1	−1	1	1
1	−1	1	1	1	−1	−1	−1	1	−1	1
−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1

Table 2. $E(s^2)$ **values of some designs due to Booth & Cox (1962), Lin (1992), and the author.**

(When no design is available, it is indicated by – in the table.)

$N = 12$

M	BC	Lin	Wu
16	7.06	6.27	6.00
18	9.68	6.59	6.59
21	–	6.86	6.86
22	–	6.86	7.40
24	10.26	–	8.17

$N = 24$

M	BC	Lin	Wu
30	12.06	11.59	9.27
45	–	12.80	12.80
46	–	12.80	13.29

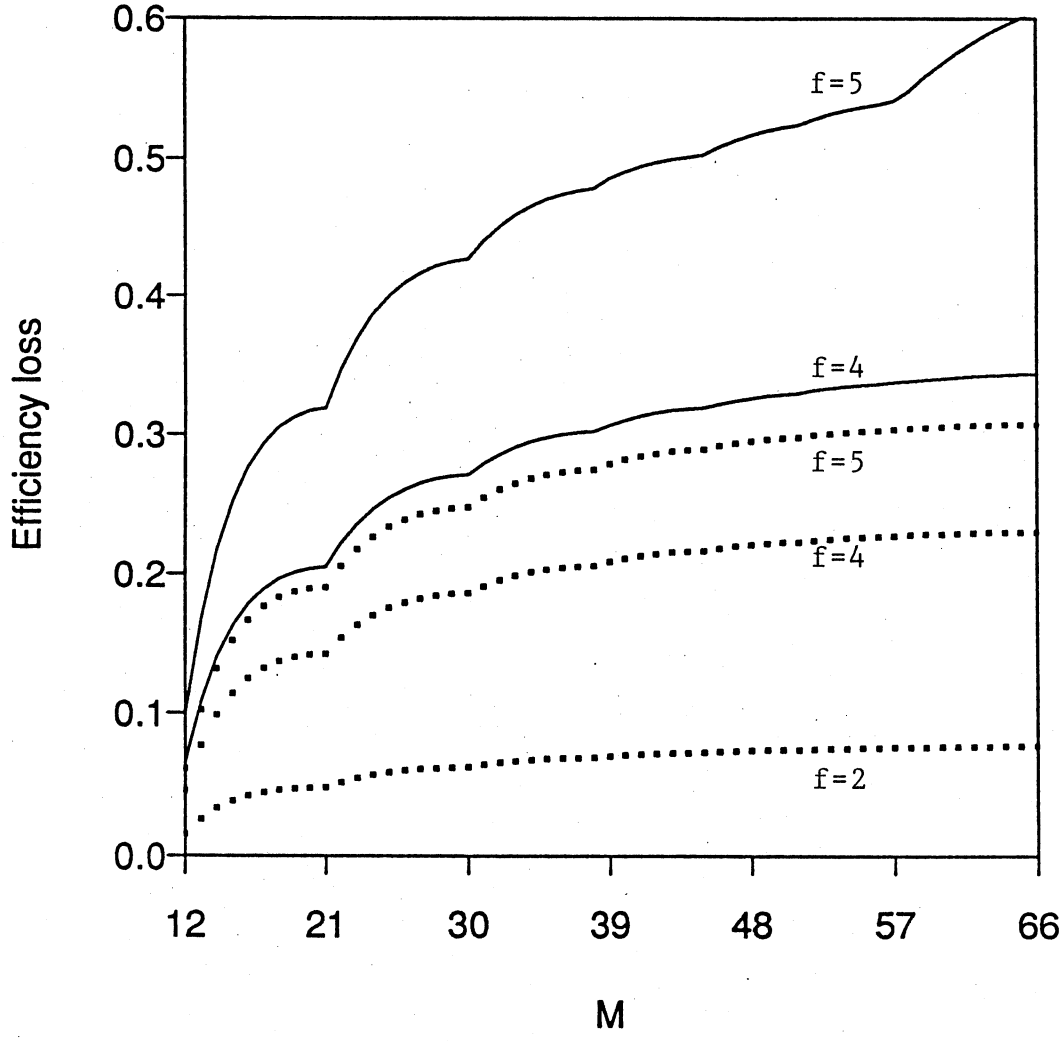

Figure 1. A_f-efficiency loss (indicated by ———) of 12-run designs with M factors and its approximation $(f-1)E(s^2)/N^2$ (indicated by . . .).

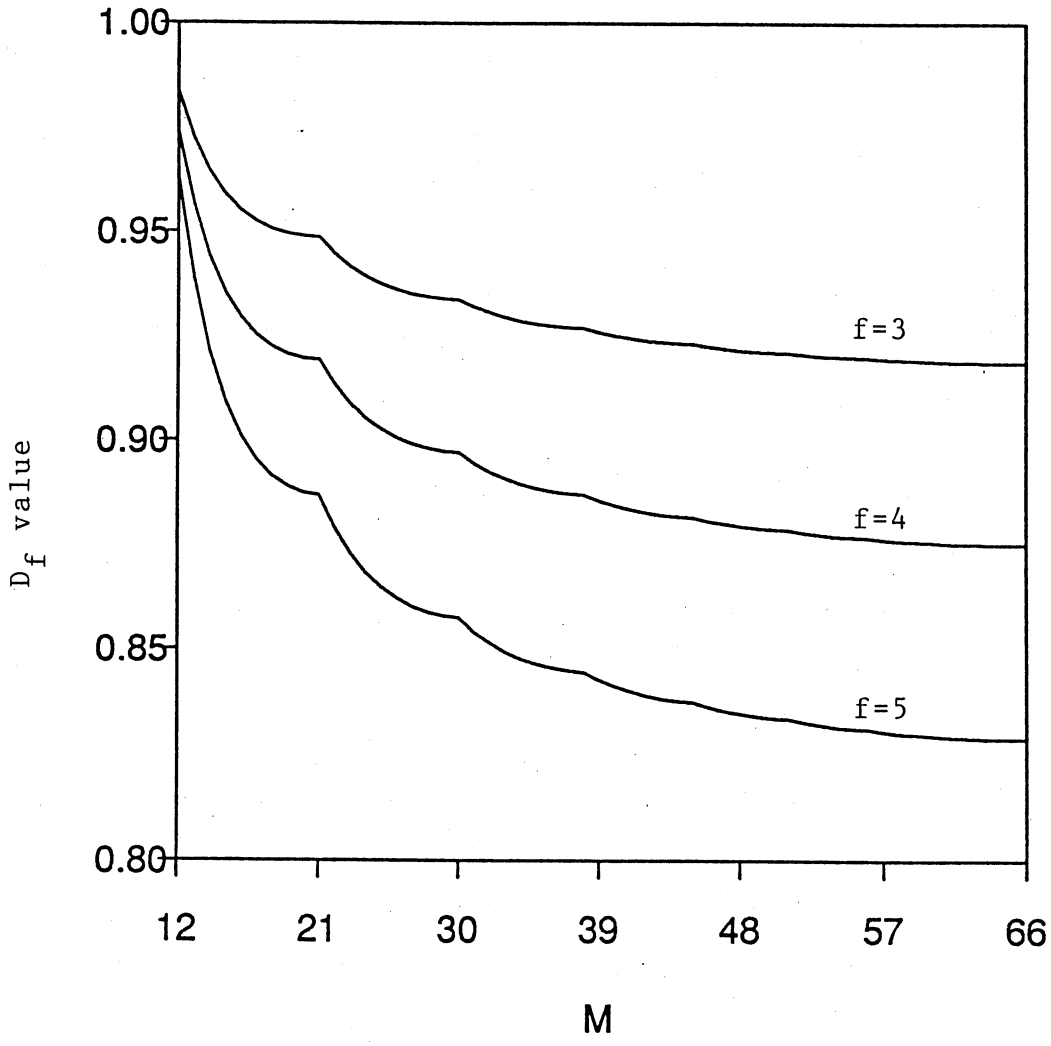

Figure 2. D_f-values of 12-run designs with M factors.

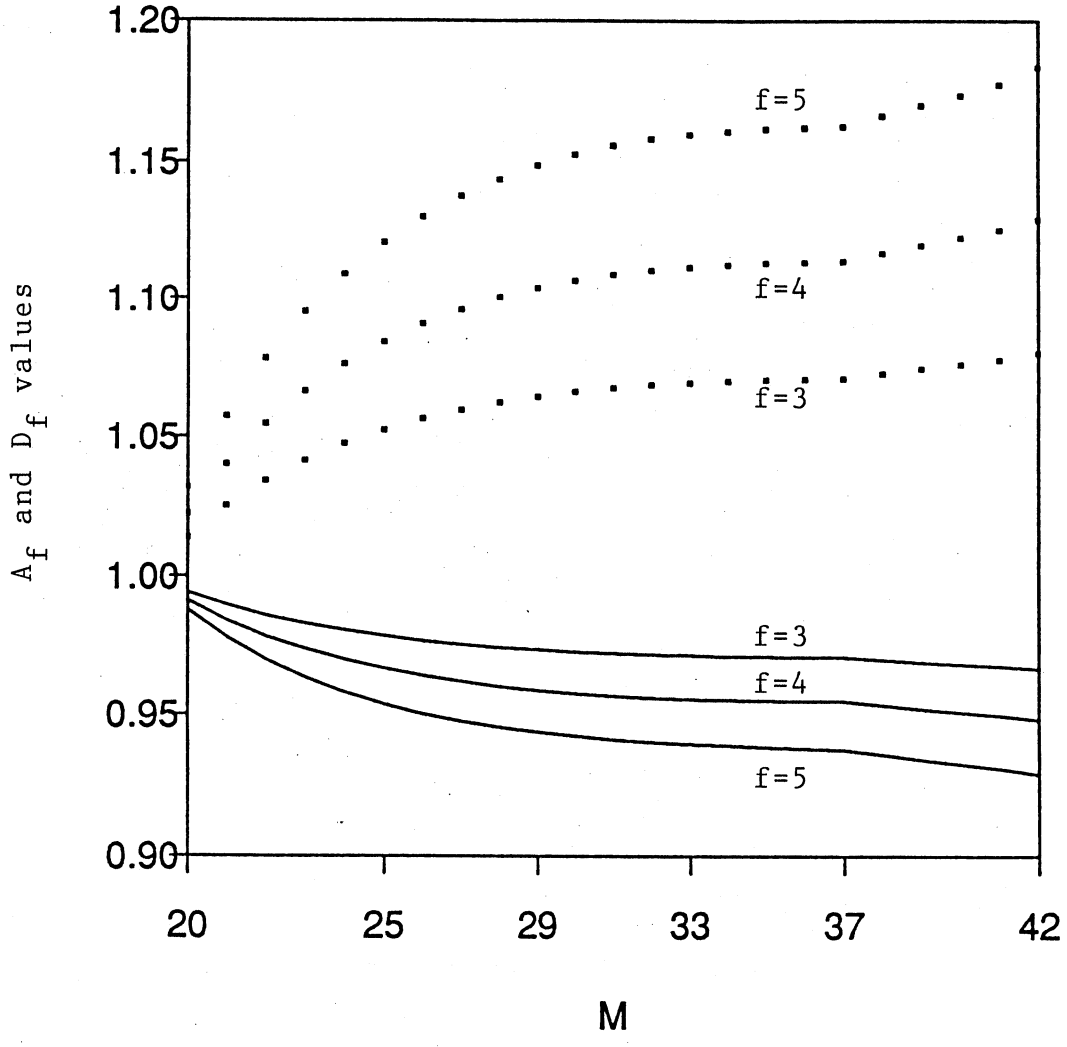

Figure 3. A_f-values (indicated by ...) are D_f-values (indicated by ——) of 20-run designs with M factors.