D-OPTIMUM WEIGHING DESIGNS

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For the problem of weighing k objects in n weighings ($n \ge k$) on a chemical balance, and certain related problems, we obtain new results and list the designs which have been proved D-optimum up to this time. While some of these optimality results have been known for some time, others are fairly recent. In particular, in the most difficult case $n = 3 \pmod{4}$ we prove a result characterizing optimum designs when $n \ge 2k - 5$. In addition, by a combination of theoretical bounds and computer search we find previously unknown optimum designs in the cases (k, n) = (9, 11), (11, 15), and (12, 15), and establish the optimality of Mitchell's (10, 11) design. In some cases the optimum X'X is not unique. Thus, we find two optimum X'X's for the (6, 7), (8, 11), (10, 11), and (10, 15) cases. As a consequence of these results and other constructions, D-optimum designs are now known in all cases $k \le 12$ (for all $n \ge k$), and in many other cases. Essentially complete listings for all $n \ge k$ had been given previously only for $k \le 5$.

1. Introduction. Let k and n be positive integers with $k \le n$, and let $\mathcal{X} = \mathcal{X}(k, n)$ denote the set of all $n \times k$ matrices $X = \{x_{ij}\}$ consisting entirely of entries ± 1 . If \bar{X} maximizes $\det(X'X)$ over \mathcal{X} , then \bar{X} or $\bar{X}'\bar{X}$ is said to be D-optimum.

The problem of characterizing such \bar{X} arises in two statistical settings, both with uncorrelated homoscedastic observations. In both cases $1/\det(X'X)$ is proportional to the generalized variance of the least squares estimators of the parameters $\theta_1, \theta_2, \dots, \theta_k$ of interest.

Firstly, there is the setting of finding the weights θ_j ($1 \le j \le k$) of k objects with n weighings. In one model, in which a chemical balance is used with each object present on each weighing, we let $x_{ij} = 1$ or -1 depending on whether the jth object is on the left or right pan in the ith weighing. That weighing model may be altered to allow the x_{ij} to be 1, -1, or 0; i.e., all k objects need not be present in each weighing. The development of the next paragraph shows that every \bar{X} optimum for the previous model is optimum for this one. Also, when k = n = r the optimality results for $x_{ij} = \pm 1$ are well-known to correspond to optimality results for k = n = r - 1 with $x_{ij} = 0$ or 1, the "spring-balance" model; see Mood (1946). The equivalences of the various D-optimality problems for the two settings is also treated by Hedayat and Wallis (1978), pages 1206 and 1220, when k = n.

Secondly, there is the setting of estimating the parameters of the first order regression model on the p-dimensional cube $[-1, 1]^p$ with p = k - 1, the ith observation being at $(z_{i1}, z_{i2}, \dots, z_{ip})$ with expectation $\theta_k + \sum_{1}^p z_{ij}\theta_j$, which we can write $\sum_{1}^k z_{ij}\theta_j$ by defining $z_{ik} = 1$. Expanding $\det(Z'Z)$ into a sum of $\binom{n}{k}$ squares of $k \times k$ determinants (Cauchy-Binet expansion) each linear in its entries, we conclude that, as a function of a single z_{i_0,j_0} ($j_0 < k$) for all other z_{ij} fixed, $\det(Z'Z)$ is quadratic in z_{i_0,j_0} with nonnegative coefficient of $(z_{i_0,j_0})^2$. Hence, z_{i_0,j_0} can be changed to one of the values 1 or -1 without decreasing $\det(Z'Z)$. Making such changes, one by one, for each \overline{z}_{i_0,j_0} of a D-optimum \overline{Z} , we conclude that there is a D-optimum \overline{Z} in \mathscr{X} . Conversely, each X in \mathscr{X} can be transformed, by multiplication of each row by 1 or -1, into an element of \mathscr{X} with the same determinant and all $x_{ik} = 1$. (The reduction to \mathscr{X} need not yield all \overline{Z} ; thus, for p = 2, p = 3, the three points (1, 1), (1, -1), $(-1, z_{3,2})$ constitute a D-optimum design for every $z_{3,2}$ in [-1, 1], with $\det(X'X) = 16$.)

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If $[-1, 1]^p$ is replaced by $\{-1, 1\}^p$ in the above, we obtain the even simpler correspondence of the weighing problem to the first order (resolution III) fractional 2^p -factorial problem.

The cases k = n are called *saturated*.

The problem of finding an \bar{X} is the subject of many papers, two early ones being those of Hotelling (1944) and Mood (1946). For reference to the many contributions of Kishen, Banerjee, Raghavarao, and others, see Raghavarao (1971), who also gives typical results. Many of the known results characterize a *D*-optimum \bar{X} subject to the restriction to X's in \mathcal{X} for which X'X is permutation invariant (has all diagonal elements equal and all off-diagonal elements equal). The imposition of this restriction simplifies the optimization problem considerably, but for many k and n it yields designs that, although often fairly efficient, are not optimum in \mathcal{X} . This is known, for example, from the saturated cases n = 6 or 7 in Mood (1946) and $n \equiv 2 \pmod{4}$ in Ehlich (1964a). The matter is discussed in Cheng (1980) and Kiefer (1978). In the present paper we are concerned with finding a D-optimum \bar{X} in \hat{X} without any such restriction.

We note that recent combinatorial literature often refers to "weighing matrices" as square orthogonal matrices with entries from $\{0, 1, -1\}$. This should not be confused with our weighing designs X.

Other optimality criteria, such as $tr(X'X)^{-1}$, have also been considered, and we shall refer in Subsections 2.0 and 2.1 to some results on them; but our main concern here is with det(X'X).

There are some commonly employed rules, discussed by various authors such as Mood (1946) and Mitchell (1974b), for augmenting or reducing Hadamard matrices to yield designs in cases other than the saturated case of Case 0 of (2.0). However, the optimality or nonoptimality of the designs produced by such recipes is not always clear in the literature. The paper of Payne (1974) clarified and vastly expanded the state of knowledge of optimality of such designs. In Section 2 (in terms of n) and in Section 5 (in terms of k) we summarize the current state of knowledge, incorporating some new constructive devices and optimality results of the present paper. We shall occasionally refer to the searches, more extensive than those of Mitchell (1974b), which have been carried out using our modification of his pioneering technique. Details were reported in Galil and Kiefer (1980).

Results of this and previous papers imply that certain forms of X and X'X, both of which forms we term "regular", are optimum if they exist. Previous work, including Payne's for $n \ge 5$, assumes the existence of Hadamard matrices for constructions. Although we are able to avoid assuming such matrices always exist, and to extend constructions to such cases as k = n - 1 of Case 2 of (2.0) not previously considered, other existence questions are generally more difficult, and are not much treated here. We show that easily constructed optimum designs are regular except in certain saturated instances of Case 1 and in Case 3 for n < 2k - 5, for all "practical" values (k, n). The (9, 9) and (11, 11) optimum designs gave difficulty because they are not of this regular nature, and their optimality was proved, respectively, by Ehlich and Zeller (1962) and by Ehlich in unpublished work mentioned in Subsections 2.1 and 2.3, using a combination of theoretical and computer developments. Regular optimum designs for (9, 11), (11, 15), (12, 15) were found by us by extensive computer search and (with Mitchell's (10, 11) design) are proved optimum herein by means of our development that stems from the work of Ehlich (1964b).

Ehlich is the pioneer and chief contributor of ideas to this subject of finding D-optimum designs in the non-Hadamard cases. We are grateful for the inspiration of his work and for the communication of Ehlich (1978).

2. Listing of D-optimum designs. For further discussion, we divide the values of n into four cases:

(2.0) Case 0:
$$n \equiv 0 \pmod{4}$$
;
Case 1: $n \equiv 1 \pmod{4}$;
Case 2: $n \equiv 2 \pmod{4}$;
Case 3: $n \equiv 3 \pmod{4}$.

We denote by \mathcal{N} the nonnegative integers and by \mathcal{N}_j the set of all integers in \mathcal{N} that fall in Case j. We have included n=0 in Case 0 to shorten the discussion, below. Although X'X is $k \times k$, the value of n appears to be more critical than that of k in determining optimality structure, since n has more important influence on the values of the entries of X'X. This accounts for the classification (2.0). (The case k=2 is separated by its triviality: every D-optimum X has orthogonal columns if n is even and columns with inner product ± 1 if n is odd.)

The term "normalization" will be used herein to refer to the following operations on X: multiplying on the left by a diagonal matrix of ± 1 's and/or a permutation matrix (which permutes or reflects the points of $\{-1, 1\}^k$ that are rows of X, but does not affect X'X); the same operations on the right, which permutes rows and corresponding columns of X'X and multiplies some entries of X'X by -1, but leaves $\det(X'X)$ unchanged. The optimum structure of X'X is generally listed in a convenient form "after normalization". For example, in the regular case in Subsection 2.1 all off-diagonal elements of an optimum X'X can be taken as -1 after normalization. Without normalization, some could be of each sign.

2.0 Case 0. An $n \times n$ Hadamard matrix H_n is a member of $\mathcal{X}(n, n)$ with $H'_n H_n = nI_n$. A necessary condition for H_n to exist is that n be 1, 2, or $\equiv 4$ in Case 0, and we also include the empty matrix H_0 for use in further discussion. There is much more literature on the existence of H_n than on all other aspects of the subject of weighing designs; see, e.g., Hedayat and Wallis (1978). By now H_n are known to exist in Case 0 for all $n \le 200$, and for infinitely many other n. There is an \bar{X} in $\mathcal{X}(k, n)$ with $\bar{X}'\bar{X} = nI_k$ if H_n exists (namely, k columns of H_n), and such \bar{X} can in fact often be found much more easily, as we describe in the next paragraph. Such an \bar{X} is not only well known to be D-optimum, but also minimizes $\Phi(X'X)$ over \mathcal{X} for every nonincreasing convex orthogonally invariant extended real-valued Φ defined on the nonnegative definite symmetric $k \times k$ matrices; see Kiefer (1975). It also minimizes the individual variances of best unbiased estimators of the θ_k (diagonal element of $(X'X)^{-1}$), as was shown by Hotelling (1944).

In Case 0 the "regular" \tilde{X} 's in $\mathcal{X}(k,n)$ are those with $\tilde{X}'\tilde{X}=nI_k$, for which $\det(\tilde{X}'\tilde{X})=n^k$. We now make a simple observation about the existence of such designs. For fixed k it is unnecessary to assume the Hadamard conjecture of existence of an H_n for all n in \mathcal{N}_0 as Payne and others do, in order to give optimality results for all such n. (Payne mentions that the assumption can be avoided when $k \leq 4$.) For, we only need k orthogonal n-vectors for the columns of \tilde{X} , not n of them. One way of constructing such an \tilde{X} is to adjoin vertically sufficiently many $n_i \times k$ submatrices of H_{n_i} 's. If $n_1 + n_2 + \cdots + n_L = n$ and $n_i \geq k$ and H_{n_i} exists for $1 \leq i \leq L$, such an \tilde{X} can obviously be constructed. A convenient sufficient condition for this to be possible for given k and all $n \geq k$ is the

PROPOSITION. For $k \ge 4$, let $n_k = \min\{j: j \ge k, j \in \mathcal{N}_0\}$. Suppose H_j exists for all j in \mathcal{N}_0 satisfying $n_k \le j < 2n_k$. Then, for all $n \ge k$ with $n \in \mathcal{N}_0$, there is an \tilde{X} in $\mathcal{X}(k, n)$ with $\tilde{X}'\tilde{X} = nI_k$. (A construction can similarly be given in terms of orthogonal arrays of strength 2.)

Thus, for example, when k = 6 our knowledge of H_8 and H_{12} suffices, and for $k \le 100$ (which presumably includes all "practical" values) the proposition may be used.

The other three cases of (2.0) are not so simple, and their investigation in the saturated case was pioneered by Ehlich (1964a, b). (See also Wojtas (1964).)

2.1 Case 1. Ehlich showed that an X in $\mathcal{X}(n, n)$ with $\tilde{X}'\tilde{X} = (n-1)I_n + J_n$ (where J_n consists entirely of 1's) is D-optimum. Unfortunately, such an \tilde{X} can exist only if 2n-1 is the square of an integer. Such designs are known for the "practical" values n=1, 5, 13, 25.

It is perhaps somewhat surprising at first glance that the unsaturated case of Case 1 is easier to handle than the saturated case. It was shown by Cheng (1980) that any \tilde{X} in $\mathcal{X}(k, n)$ with $\tilde{X}'\tilde{X} = (n-1)I_k + J_k$ and $\det(\tilde{X}'\tilde{X}) = (n-1)^{k-1}(n-1+k)$ (the "regular" designs of Case 1) is not only *D*-optimum, but also optimum with respect to a large subclass of the Φ 's of the previous paragraph, including all those of common interest. (The *D*-optimality in the unsat-

urated case, obtained by Payne (1974), can also be obtained by a simple modification of Ehlich's saturated case proof; but the more general results require Cheng's analysis.) Moreover, for k < n such an \tilde{X} can always be obtained when the regular design of Case 0 in $\mathcal{X}(k, n-1)$ exists, by adjoining a row of 1's to that design, whose construction can often be obtained from the Proposition of the previous paragraph even if an H_{n-1} is not known. Although such an adjoining is a common practice in the literature of weighing designs, the D-optimality over \mathscr{X} (without the additional symmetry restriction) of the resulting \tilde{X} was evidently unknown before Payne's paper. Thus, Mitchell (1974b) made computer searches in several of these cases, always obtaining such an \tilde{X} , and remarking that Mood had suggested such designs would be "very efficient." For values of $n \le 20$ in Case 1, we are left without knowledge of an optimum design only in the saturated cases k = n = 9, 17. Ehlich and Zeller (1962) state that for k = n= 9 the nonregular design obtained by them, for which the above-diagonal elements of X'Xare all I except for a single 5, can be proved optimum. A normalization of the design given in Table 4b of Mitchell (1974b) is of this form, and such a design can also be constructed using a method of Williamson (1946, page 433). Ehlich (1978) has indicated to us that the method of proof of optimality is similar to, but simpler than, that mentioned in Subsection 2.3 below for the k = n = 11 case. The method also shows no other form of X'X can be optimum for k = n = 9. While the k = n = 11 case required machine help, the calculations by Ehlich and Zeller (1962) in the k = n = 9 case were done by hand.

2.2 Case 2. Here Ehlich (1964a) and Wojtas (1964) showed in the saturated case that any X for which $X'X = \begin{pmatrix} M & 0 \\ 0 & M \end{pmatrix}$, where $M = (k-2)I_{k/2} + 2J_{k/2}$, is D-optimum. Ehlich constructed such X of the form $\begin{pmatrix} A & B \\ -B' & A \end{pmatrix}$ with A and B circulants, in all cases $k \le 38$ except k = 22 and 34. Other optimum designs in these cases were obtained by Yang (1968), who in references cited by him there also obtained optimum X for k = 42, 46, 48, 52.

For general $k \le n \in \mathcal{N}_2$, we define the regular \tilde{X} in $\mathcal{X}(k, n)$ to be those for which $\tilde{X}'\tilde{X} = \begin{pmatrix} L & 0 \\ 0 & M \end{pmatrix}$, where for k even $L = M = (n-2)I_{k/2} + 2J_{k/2}$, and for k odd L and M are $(n-2)I_{(k\pm 1)/2} + 2J_{(k\pm 1)/2}$; thus, $\det(\tilde{X}'\tilde{X}) = (n-2)^{k-2}(n-2+k)^2$ or $(n-2)^{k-2}(n-1+k)(n-3+k)$, for k even or odd. These designs were proved D-optimum by Payne for $k \le n-2$ using the work of Wojtas, and one can also see that Ehlich's proof requires only simple modifications to apply to Case 2 for $n \ge k$. (In fact, Payne's proof also applies for $n \ge k$, but he does not say so because he gives constructive methods only when $k \le n-2$ and H_{n-2} exists.)

When $k \le n-2$ and one knows an H_{n-2} or, more generally, a regular \bar{X} in $\mathcal{X}(k, n-2)$ constructed from the Proposition of Case 0, a regular optimum \bar{X} for Case 2 is achieved by using one of Mood's devices, discussed and employed by Mitchell and by Payne. This \bar{X} is obtained by adjoining to \bar{X} two rows, one consisting entirely of ones and the other consisting of k/2 (respectively, (k-1)/2) 1's following by k/2 (respectively, (k+1)/2) -1's, depending on whether k is even or odd. It seems not to have been observed by the cited authors that, when k = n - 1 with $n \in \mathcal{N}_2$, removing a column from an optimum saturated regular X of Ehlich in $\mathcal{X}(n, n)$ (mentioned two paragraphs above) yields an optimum regular design in $\mathcal{X}(n-1, n)$. Thus, just as the construction problem in Case 1 was much simpler for k < n than in the saturated case, so in Case 2 it is simpler for k < n - 1 than in the saturated or near-saturated (k = n - 1) case.

That these results seem unknown is indicated by the fact that Mitchell's computer search for optimal designs included the cases (k, n) = (5, 6), (9, 10) (also excluded in Payne's work), in which cases the previous paragraph implies that such search could be dispensed with. Unlike the *D*-optimum designs of Case 1, those of Case 2 are not yet known to have other optimum properties, except that Cheng (1980) has shown they are among the *E*-optimum designs (that is, they maximize the minimum eigenvalue of X'X), not all of which need have this X'X structure.

2.3 Case 3. This is well known to be the most difficult case, and we devote the next two sections to new results for it. We first summarize, here, the previously known results. If one knows an H_{n+1} or, more generally, a regular \bar{X} in $\mathcal{X}(k, n+1)$ from the Proposition of Case 0, deletion of one row of \bar{X} yields an \bar{X} in $\mathcal{X}(k, n)$ with $\bar{X}'\bar{X} = (n+1)I_k - J_k$. However, such an \bar{X} was until recently known to be optimum for k > 2 only when n = 3 (e.g., Mood (1946)). For k = n = 7, the optimum design X is not of this form. It was found by Williamson (1946) and discussed by Mood (1946), and the exceptional above-diagonal elements (3's) of that X'X other than -1 can be put into positions (1, 2), (3, 4), (5, 6) by normalization. Designs for the cases k < n = 7 have been obtained through computer search by Mitchell (1974b) but their optimality was not previously verified theoretically. His computer search yielded, after normalization, the \bar{X} described just above, and Payne (1964) proved these optimum for $k \le 5$. The optimality for k = 6 is proved herein.

For n = k = 11 (not treated by Mitchell), an X'X was obtained through computer search combined with some algebra by Ehlich and Zeller (1962), in which paper the optimality of the design was indicated to be questionable. This design was subsequently verified by Ehlich to be optimum, as described to us in Ehlich (1978). This X'X has exceptional above-diagonal elements 3 rather than -1 in positions that (by normalization) can be taken to be (1, 2), (2, 3), (3, 4), (4, 5), (6, 7), (8, 9), (10, 11). An X of this character, obtained by the computer search method of Galil and Kiefer (1978), is listed in Table 9a herein.

Not knowing this X'X had been proved optimum in earlier unpublished work of Ehlich, and viewing this evidently "nonregular" case as a good example on which to investigate properties of variations of our computing method, we ran several thousand trials in this case and found other designs that gave the same value of $\det(X'X)$ but two other forms of X'X. Two such designs are listed in Tables 9b and 9c. The first of these has an X'X that differs from that described above only in having an additional above-diagonal 3 in position (1, 3). The second has an X'X that is a "block matrix" whose description is deferred until that concept is defined. (All three forms of X'X were obtained several times, in a total of about 1% of the computer trials. Thus, the designs are not "easy" to find in this case by use of our general search method, which does not make use of the special theoretical devices used by Ehlich in this case.)

Subsequently, Professor Ehlich (1978) very kindly sent us a description of the ingenious combination of theoretical developments and computer search by means of which he obtained designs with all three of these structures of X'X, proved them optimum, and proved no other structures of X'X could be optimum. Thus, the design of Table 9a should be viewed as that of Ehlich and Zeller, and those of Tables 9b and 9c as Ehlich's, but we list them here because there is no indication that they are to appear elsewhere in print. These X'X all have determinant $B = (5 \times 2^{16})^2$.

Ehlich's indication of the proof of optimality is that a simple inequality eliminates all X'X with off-diagonal elements other than -1, -5, or 3. The computer program searches among all normalized 11×11 matrices C with such elements (and diagonal elements 11) and shows none with a -5 can have det $C \ge B$. Using the upper bound of Ehlich (1964b) listed in Table 1 herein, and further computer search, only 7 possible C's with det $C \ge B$ are found to within normalization. Finally, a systematic search for X's that realize one of these seven C's as X'X yields the three structures of Table 9.

Designs for k < n = 11 have not previously been proved optimum theoretically except for Payne's treatment when $k \le 5$. Of the designs found by Mitchell (1974b, Tables 4d and 4e) for k = 9 and 10, the former is improved upon by the design of Table 5 herein, found in our more extensive search. Both the design of Table 5 and Mitchell's design for k = 10, as well as \tilde{X} with $\tilde{X}'\tilde{X} = 12I_k - J_k$ for $k \le 8$, are proved optimum herein. The size of these designs is such that computer search using our modifications of the Detmax procedure invented by Mitchell (1974a), which of course requires more computing for these larger values of k and k, is also decreasingly successful. For example, as stated above, only about 1% of the starts (involving some random element) reached an optimum solution when k = n = 11.

Payne (1974) showed that an \tilde{X} with $\tilde{X}'\tilde{X} = (n+1)I_k - J_k$ (and determinant $(n+1)^{k-1}(n+1)^{k-1}$)

+1-k)) is D-optimum provided n is sufficiently large compared with k. He gives $n > (5/2)3^k k^2 \binom{k}{[k/2]}$ as a crude sufficient bound for which his proof works, and remarks that numerical evidence suggests that n > 7k/2 might suffice, and that the proof is likely to fail in general for $k \le n < 3k$. Our own early numerical investigations indicated that $n \ge 2k$ might suffice, so that the evidence cited by Payne is a commentary on his method of proof rather than on the definitive results. In Section 3 we show $n \ge 2k - 5$ suffices.

Because of this complex situation, we have chosen not simply to define \tilde{X} of the above form as "regular" in Case 3. Rather, we are guided by a development of Ehlich (1974b), which we now describe. Thus material through (2.5) is also used in proving the Theorem of the next section.

Let $\mathscr{C} = \mathscr{C}_{k,n}$ be the class of all symmetric $k \times k$ matrices with diagonal entries n and off-diagonal entries -1 or 3, where $n \in \mathscr{N}_3$. Let

(2.1)
$$\Psi(k, n) = \max_{A \in \mathcal{C}_{k,n}} \det A.$$

Ehlich shows $\max_{X \in \mathcal{X}} \det(X'X) \leq \Psi(k, n)$ in Case 3.

A block of size r is an $r \times r$ matrix with diagonal elements n and off-diagonal elements 3. A block matrix in $\mathcal{C}_{k,n}$ with block sizes $r_1, r_2, \dots r_s$ satisfying $\sum_{i=1}^{s} r_i = k$ is a $k \times k$ matrix with diagonal blocks of those sizes and with all other elements equal to -1. As Ehlich shows, any such block matrix C has

(2.2)
$$\det C = (n-3)^{k-s} \{1-G\} \prod_{i=1}^{s} (n-3+4r_i),$$

$$G = \sum_{i=1}^{s} r_i / (n-3+4r_i).$$

Ehlich also shows that there is a block matrix in $\mathscr{C}_{k,n}$ which has maximum determinant in $\mathscr{C}_{k,n}$ and which is a member of the subset $\mathscr{B}_{k,n}$ of $\mathscr{C}_{k,n}$ which consists of block matrices with blocks of only one size or blocks of only two contiguous sizes, u of size r and v of size r+1, where consequently

(2.3)
$$u + v = s$$
, $ur + v(r + 1) = sr + v = k$.

For any block matrix C_s in $\mathcal{B}_{k,n}$ with s blocks, (2.2) and (2.3) yield

$$\det C_s \equiv D_{k,n}(s) = (n-3)^{k-s}(n-3+4r)^u(n+1+4r)^v\{1-G\}$$

$$= (n-3)^{k-s}(n-3+4r)^{(r+1)s-k}(n+1+4r)^{k-sr}\{1-G\},$$

$$G = [k(n-3)+4sr(r+1)]/(n+4r+1)(n+4r-3).$$

Ehlich's last-cited result is thus $\Psi(k, n) = \max_s D_{k,n}(s)$. Of course, s uniquely determines r except when $s \mid k$. In that case, the block matrix with $r = r_0$, $u = u_0$, v = 0 is identical to that with $r = r_0 - 1$, u = 0, $v = u_0$, and either yields the same result in (2.4). The $\tilde{X}'\tilde{X} = (n+1)I_k - J_k$ discussed earlier has s = k.

In Case 3 we call X in $\mathcal{X}(k, n)$ "regular" if $X'X = C_s^*$ is of the form C_s in $\mathcal{B}_{k,n}$ described in (2.3) and (2.4) and

(2.5)
$$\det C_s^* = D_{k,n}(s) = \max_t D_{k,n}(t).$$

If s = k maximizes $D_{k,n}(s)$, we call the resulting X and $X'X = (n+1)I_k - J_k$ "very regular." As we shall see, the s maximizing $D_{k,n}(s)$ need not be unique.

In Section 3 we characterize cases where very regular designs maximize $D_{k,n}(s)$, and the construction problem of D-optimum designs in $\mathcal{X}(k, n)$ is then handled in all practical cases by the simple construction described at the outset of the discussion of Case 3, above. For other k with $n \in \mathcal{N}_3$, we encounter difficult construction problems of whether C_s^* is realizable as an X'X. If not, we have no optimality characterization. Many saturated or near-saturated cases give evidence that such C_s^* are not realizable as X'X. As we mention in Section 4, that is always so when k = n < 91. In Section 4 we discuss $D_{k,n}(s)$ further and give a few positive results in regular cases that are not very regular. As more becomes known about the form of D-optimum designs in Case 3, it may become convenient to alter the definition of regularity.

2.4 UNIQUENESS. In Case 0, if an optimum X'X exists that is regular, then it is well known that every D-optimum X'X must have that same form. The same conclusion holds (with possible normalization) in Case 1 and Case 2, as can be seen by examining the modification of the uniqueness part of the proofs of Ehlich (1964a) needed to make them apply when k < n. Finally, when n > 2k - 5 in Case 3, the same conclusion applies if a D-optimum X'X exists that is very regular, as one can see by tracing through the inequalities in the reductions in Ehlich (1964b) that are described in the development of (2.1)–(2.4) relating to $\mathcal{C}_{k,n}$ and $\mathcal{B}_{k,n}$, together with the proof of Section 3 below, as these apply when n > 2k - 5.

When $n \le 2k - 5$, no general Case 3 uniqueness results for X'X are known, and we now describe examples of nonuniqueness. (Uniqueness for the optimum X'X for k = n = 7 may be obtainable from Williamson's development.) Table 1 and Section 4 describes the lack of uniqueness that is possible among regular block designs that are optimum in $\mathcal{X}(k, n)$. In the borderline case n = 2k - 5 of case 3, the theorem of Section 3 shows that an optimum design can have the very regular X'X consisting entirely of blocks of size 1 (s = k) or can have one block of size 2 and the rest of size 1 (s = k - 1). The smallest possible example is (k, n) = (6, 7), and in Table 2 we give an optimum X for which X'X has s = 5, the above-diagonal 3 being in position (1, 2). We remark herein that our theorem obviates the need for Payne's longer proof of optimality of the very regular X'X in this case. In addition, we have settled his question about uniqueness in the negative. In the next case (k, n) = (8, 11), we also obtained, and list in Table 3, an optimum X(X'X) with s = 7, above-diagonal 3 in position (1, 2) other than the very regular one. For the case (10, 15), we list in Table 4 an optimum X whose X'X has s = 9, the above-diagonal 3 again being in position (1, 2).

For n < 2k - 5, there are four cases of (k, n) in which we know a regular optimum X'X at the current writing. For the case (9, 11), Table 1 shows that s = 6 or 7 is possible, and the first of these (Table 5) was found frequently in our search. However, the second of these was not obtained in 1500 trials. (Mitchell's Table 4d gives a block design with s = 5, not optimum.) For (10, 11), where Mitchell's design (proved optimum in our Section 4) has s = 5, we have also found an alternate with s = 6, given in Table 6. (Mitchell states that he did not attempt to list more than one maximizer of det(X'X).) For (11, 15), Table 1 shows that s = 8 (Table 7) gives the unique block design optimum in $\mathcal{X}(11, 15)$. For (12, 15) we have only found an optimum X'X with s = 6 (Table 8), not one with s = 7. Ehlich (1978) indicates that he has found the latter.

Perhaps most interesting is the presence of three different forms X'X mentioned in Subsection 2.3 as being optimum in the case k = n = 11. Two of these, not block matrices, were described earlier (Tables 9a and 9b). The third, yielded by the X of Table 9c, is a block matrix with one block of size 5 and three of size 2.

Thus, lack of uniqueness of the optimum X'X is quite possible, and we do not yet know the general situation. It is well known from simple examples that the uniqueness of the D-optimum "information matrix" (analogue of X'X) in "approximate" design theory does not persist in the exact theory, as has been illustrated in the example of k = n = 3 on $[-1, 1]^2$ in Section 1. Still, these first examples of nonunique D-optimum X'X in the simple standard weighing design setting are somewhat surprising. (For nonuniqueness of the E-optimum design, even possible in the approximate setting, see Cheng (1980) and also his references to earlier work of Takeuchi.) We emphasize that we are not treating here the more detailed consideration of nonisomorphic X with the same X'X—for example, of nonisomorphic H_n .

3. Optimum very regular designs in Case 3. We now prove

THEOREM. If $k \le n \in \mathcal{N}_3$ and $n \ge 2k - 5$, then $\max_t D_{k,n}(t) = D_{k,n}(k) = (n+1)^{k-1}(n-k+1)$, and hence any very regular X (with $X'X = (n+1)I_k - J_k$) is D-optimum in $\mathcal{X}(k,n)$. If n > 2k - 5, the value t = k uniquely maximizes $D_{k,n}(t)$, while if n = 2k - 5 the one other maximizing value is t = k - 1, for which X'X (if it exists) differs from $(n+1)I_k - J_k$ by having 3's in positions (1, 2) and (2, 1) after normalization. If n < 2k - 5, $D_{k,n}(t)$ is not maximized by t = k.

PROOF. Suppose $k \le n \in \mathcal{N}_3$ and $n \ge 2k - 5$, and that t = s < k maximizes $D_{k,n}(t)$.

Continuing with the nomenclature and developments of (2.1)–(2.4), we adopt the second representation just after (2.4) in the cases $s \mid k$. This means we may assume $\nu > 0$ for all s, and hence

$$(3.1) sr \le k - 1.$$

With this choice, the parameters u, v, r, s, G hereafter refer to C_s^* satisfying (2.5) with s < k and hence r > 0.

Let C^{**} be obtained from C^{*} by replacing one block of length r+1 (recall $\nu>0$) by a block of length r and a block of length 1 (perhaps now yielding blocks of three lengths in C^{**}). We shall show the resulting contradiction det $C^{**}>$ det C^{*} except in the single case r=1, $\nu=1$, n=2k-5, when det $C^{**}=$ det C^{*} . Writing L=n+4r+1 to simplify calculations, we have from (2.2) after some simple arithmetic,

$$L^{1-v}(L-4)^{-u}(L-4r-4)^{s+1-k}[\det C^{**} - \det C^{*}]$$

$$(3.2) = (L-4)(L-4r)\left\{1 - G + \frac{r+1}{L} - \frac{1}{L-4r} - \frac{r}{L-4}\right\} - (L-4r-4)L\{1-G\}$$

$$= 16r\{1-G\} + 8r\{-1 + 2(r+1)L^{-1}\} = 8r\{1 - 2G + 2(r+1)L^{-1}\}.$$

From (2.4) and (3.1),

$$L(L-4)\{1-2G+2(r+1)L^{-1}\}$$

$$(3.3) \geq L(L-4)-2[k(L-4r-4)+4(k-1)(r+1)]+2(r+1)(L-4)$$

$$=L[L-2-2k+2r]=L[n+6r-1-2k] \geq L[n+5-2k].$$

This last, and hence (3.2), is nonnegative provided $n \ge 2k - 5$.

We also see that the left side of (3.3) can be zero only if r = 1, v = 1, and n = 2k - 5. In all other cases we have obtained the contradiction det $C^{**} > \det C^{*}$. In the single case n = 2k - 5, we have also proved that s = k is optimum in $\mathcal{C}_{k,n}$, and have also shown that s = k - 1 (r = 1, v = 1) is optimum (and no other s is) in that case.

Finally, if C^* has s = k - 1 and r = 1, so that C^{**} has s = k, the left side of (3.3) is L(L - 2k), which is <0 if n < 2k - 5. \square

4. Case 3 with n < 2k - 5. When $k \le n \le 3$ the optimum design is always very regular. When n = 7, the only value $k \le 7$ not covered by the theorem above is k = 7. In particular, Payne's intricate proof in the case k = 5 is unnecessary. The saturated case k = 7 was treated by Williamson: As mentioned earlier, an optimum X is not regular since $\Psi(7, 7)$ is not a square. It is of interest that Ehlich's inequality det $X'X \le \max_s D_{k,n}(s)$ (see just below (2.1) and (2.4)) can be used to give a much shorter proof of Williamson's result: One computes easily that $\Psi(7, 7) = D_{7,7}(5) = 84 \times 2^{12}$, but since $\det(X'X)$ is trivially seen to be a square divisible by 2^{12} in this case, we must have $\det(X'X) \le 81 \times 2^{12}$. Williamson's design attains this bound, and is thus D-optimum. The upper bound of Ehlich's inequality is actually achieved for k = n = 3, but the method just used obviously fails for the X's proved optimum by Ehlich when k = n = 11.

Before going on to the case n = 11, we list in Table 1 the values s_{max} of s that maximize $D_{k,n}(s)$, together with $\Psi(k, n)$ for $k \le 15$ and n < 2k - 5. (A printout for larger k, is available to interested readers.)

The values $D_{n,n}(s)$ were studied extensively by Ehlich. We note that, as was the case for $\Psi(7,7)$ in the previous paragraph, $\Psi(n,n)$ is not a square for n=11 or 15 and thus Ehlich's upper bound is not attainable in $\mathcal{X}(n,n)$ (there is no regular optimum X) in these cases. (When k < n, $\det(X'X)$ need not be a square, and this simple unattainability argument fails.) In fact, an analysis of Ehlich's results for $\Psi(n,n)$ show that it is a square (for $n \in \mathcal{N}_3$) for infinitely many (but sparse) n, the only values <200 being 91 and 47; it seems quite unlikely that the bound is attainable in those large cases. Of course, whenever $\Psi(k,n)$ is not attainable by an X'X, there is no reason for the D-optimum X'X to be a block matrix (with smaller

	"	= 15 (Ca.	
k	n	Smax	$\Psi(k,n)$
7	7	5	$.3441 \times 10^{6}$
9	11	6, 7	$.1359 \times 10^{10}$
10	11	5, 6	$.1288 \times 10^{11}$
11	11	5, 6	$.1203 \times 10^{12}$
11	15	8	$.5617 \times 10^{13}$
12	15	6, 7	$.7644 \times 10^{14}$
13	15	6, 7	$.1032 \times 10^{16}$
13	19	9, 10	$.2899 \times 10^{17}$
14	15	6	$.1387 \times 10^{17}$
14	19	7, 8	$.5130 \times 10^{18}$
15	15	6	$.1855 \times 10^{18}$
15	19	7, 8	$.9029 \times 10^{19}$
15	23	11	$.1906 \times 10^{21}$

TABLE 1

Optimum block matrices for n < 2k - 5, $n \le 15$ (Case 3)

 $D_{k,n}(s)$ than $\Psi(k, n)$). Indeed, when k = n = 11 a *D*-optimum X'X need not even be a block matrix (Tables 9a and 9b) as it was in the nonregular case k = n = 7.

The approach of finding new *D*-optimum designs in Case 3 by using a large number of trials with our computational search scheme succeeded in four cases where n < 2k - 5 (in addition to a number of very regular cases before we knew the Theorem of Section 3), as well as in the three cases n = 2k - 5 where it found nonunique optimum X'X. These are the cases (k, n, s) = (9, 11, 6), (10, 11, 6), (11, 15, 8), (12, 15, 6), (6, 7, 5), (8, 11, 7), (10, 15, 9), listed in Table 1, mentioned in Section 2.4, and given in Tables 5, 6, 7, 8, 2, 3, 4. In all of these, our search succeeded in finding a *D*-optimum X in $\mathcal{X}(k, n)$, achieved for a block matrix X'X satisfying det $X'X = \Psi(k, n)$. In these seven tables the designs X have been written so that the blocks of length 2 occur at the beginning, the above-diagonal 3's appearing in positions (1, 2), (3, 4), \cdots , (2v - 1, 2v), where v = 3, 4, 3, 6, 1, 1, 1 in the respective cases. As mentioned in Subsection 2.3, we have also listed, in Table 9, three X's for k = n = 11 obtained by our computer search, which yield matrices X'X for designs X found earlier by Ehlich and Zeller (1962) or Ehlich (1978), and which were proved optimum by the latter.

5. Summary of results for small k. The case k = 2, mentioned at the start of Section 2, is trivial and has been known for many years. For k = 3 and 4, Payne gave detailed calculations that characterize the D-optimum designs for all $n \ge k$. For these values of k, the developments of Sections 2 and 3 also guarantee existence and optimality of a regular X, always very regular in Case 3. The same is true for k = 5, which was treated almost completely by Payne (except for n = 6). Payne did not treat cases k > 5 so completely. For $k \ge 5$ his development assumes all H_n exist in Case 0, an assumption we have seen how to weaken, and to eliminate in all practical cases.

For k = 6, our results again imply existence and optimality of a regular X for all $n \ge k$, always very regular in Case 3. For k = 8 there is a regular X that is optimum for $n \ge k$, always very regular in Case 3. Tables 2 and 3 illustrate the lack of uniqueness of X'X for (k, n) = (6, 7) and (8, 11).

For k = 7 we again have a regular *D*-optimum *X* for all $n \ge k$, except that in the saturated case the Williamson block design with s = 4, not regular (Table 1), is optimum. For all other values n in Case 3 we have very regular designs.

For k = 9 the saturated case was settled by Ehlich and Zeller (1962), as discussed earlier. Our developments yield regular optimum X for all n > 9, the only Case 3 design that is not very regular being that of Table 4 for n = 11.

For k = 10 we always have regular optimum X, always very regular in Case 3 except for n = 11. The design of Table 4e of Mitchell (1974b), after adjunction of a column of +1's and

TABLE 2

D-optimum X for (k, n) = (6, 7)

 $(X'X has s = 5, first block of size 2; very regular X is also optimum; det(X'X) = <math>2^{16}$ = $.6554 \times 10^{5}$.)

+	+	+	_	_	+
_	_	+	_	_	+
+	_	_	_	+	+
_	_	+	+	+	+
_	_	_	+	_	+
_	+	_	_	+	+
+	+	_	+	_	+

TABLE 3
D-optimum X for (k, n) = (8, 11)

 $(X'X \text{ has } s = 7, \text{ first block of size 2; very regular } X \text{ is also optimum; } \det(X'X) = 3^{-7}2^{-16} = .1433 \times 10^{9}.)$

_	_	+	_	_	+	+	+
_	_	_	+	+	+	_	+
+	+	-	+	_	_	+	+
+	-	+	+	-	+	_	+
_	-	-	+	-	_	+	+
_	+	+	+	+	_	_	+
_	+	-	_	-	+	_	+
+	_	_	-	+	_	_	+
+	+	-	_	+	+	+	+
_	_	+	_	+	_	+	+
+	+	+	_	-	_	-	+

TABLE 4
D-optimum X for(k, n) = (10, 15)

(X'X has s = 9, first block of size 2; very regular X is also optimum; $\det(X'X) = 2^{37}3 = .4123 \times 10^{12}.$)

			· ,						
+	_	-	_	_	_	+	+	+	+
_	+	_	_	_	_	+	+	+	+
+	+	_	+	+	+	_	+	+	+
-	_	_	_	+	+	_	+	_	+
+	+	+	+	_	_	_	+	_	`+ +
-	+	_	+	+	_	+	_	_	+
+.	+	+	_	_	+	+	_	_	+
_	_	_	+	_	+	_	_	+	+
+	_	+	_	+	_	_	_	+	+
_	-	+	_	+	+	+	+	_	+
+	+	_	_	+	_	_	_	_	+
_	_	+	+	+	_	+	_	+	+
_	-	+	+	_	_	_	+	_	+
+	_	_	+	-	+	+	_	_	+
-	+	+	-	-	+	_	_	+	+

TABLE 5 $D
-optimum \ X for (k, n) = (9, 11)$

 $(X'X \text{ has } s = 6; \text{ first three blocks have size } 2; \det(X'X)$ = $3^42^{24} = .1359 \times 10^{10}$.)

_	+	+	_	_	_	+	+
_	_	_	+	+	+	_	+
_	_	+	+	_	+	+	+
+	_	-	+	+	_	+	+
_	+	_	+	-	-	_	+
+	+	+	+	+	_	_	+
-	+	_	-	+	+	+	+
+	_	_	-	-	+	_	+
_	_	+	_	+	_	_	+
+	+	+	_	_	+	-	+
+	-	-	-	-	. -	+	+
	+ - + - +	 + - + + + + + + - + + - + +	+ + + + + + + + + + + + + + +	+ + + + + + + - + + + + + + + + + +	+ + + - + + + + + + + + + + + + + +	+ + + + + + + + + + + + + + + + + +	+ + + - + + + + + + + + + + + + + +

TABLE 6

D-optimum X for(k, n) = (10, 11)

(X'X has s = 6, first four blocks have size 2; Mitchell's design with s = 5 is also optimum; $det(X'X) = 3 \times 2^{32} = .1288 \times 10^{11}$.)

+	_	_	_	+	+	+.	_	+	+
_	_	+	_	_	+	+	+	_	+
_	+	_	_	+	+	_	+	+	+
+	+	_	+	_	+	_	_	_	+
_	_	_	_	_	_	_	_	+	+
_	_	_	+	+	_	+	+	_	+
+	+	_	_	_	_	+	+	_	+
+	_	+	+	_	_	_	+	+	+
_	_	+	+	+	+	_	_	_	+
_	+	+	+	_	_	+	_	+	+
+	+	+	_	+	_	_	_	_	+

TABLE 7

D-optimum X for (k, n) = (11, 15)

 $(X'X \text{ has } s = 8; \text{ first three blocks have size } 2; \det(X'X) = 2^{28}5^23^31 = .5617 \times 10^{13}.)$

+	_	_	_	_	+	+	_	+	+	+
+	+	_	+	+	_	_	_	_	+	+
+	+	_	_	_	_	+	_	+	_	+
- +	+	+	_	_	_	+	+	_	+	+
+	_	+	+	_	+	_	+	_		+
- +	+	_	+	_	+	_	+	+	+. - +	+
+	_	+	_	+	_	_	+	+	+	+
_	_	+	+	_	_	+	_	_	+	+
_	+	+	_	+	+	_	_	+	_	+
_	_	_	_	+	+	+	+	_	_	+
_	_	+	+	_	_	_	_	+	_	+
_	_	_	+	+	_	+	+	+	_	+
+	+	_	_	_	_	_	+	_	_	+
_	_	_	_	+	+	_	_	_	+	+
+	+	+	+	+	+	+	_	_	-	+

TABLE 8

D-optimum X for (k, n) = (12, 15)

 $(X'X has s = 6 blocks of size 2; det(X'X) = 3^65^52^{25} = .7644 \times 10^{14}.)$

_	_	+	+	_	_	_	_	+	+	+	+
-	+	_	_	+	_	_	+	-	+	_	+
	_	-	-	_	_	+	+	+	+	+	+
+	_	-	+	_	+	+	+	_	+	_	+
_	-	_	+	+	+	_	+	+	-	+	+
+	.+	_	+	+	_	+	_	_	-	+	+
-	-	+	_	+	+	+	_	_	+	+	+
+	+	+	-	_	+	_	+	-	_	+	+
_	+	_	_	_	+	+	_	+	_	_	+
+	_	+	_	+	_	+	+	+	-	-	+
+	+	_	-	+	+	_	-	+	+	+	+
+	-	_	-	_	_	-	_	_	_	+	+
_	_	+	+	+	+	_	-	_	-	_	+
+	+	+	+	-	-	-	_	+	+	_	+
_	+	+	+	_	_	+	+			+	+

TABLE 9
D-optimum X's for (k, n) = (11, 11); $det(X'X) = 5^22^{32} = .1074 \times 10^{12}$

TABLE 9a. X'X has above-diagonal 3's in positions (1, 2), (2, 3), (3, 4), (4, 5), (6, 7), (8, 9), (10, 11).

+	+	+	+	+	+	+	_	_	_	+
_	+	+	+	-	-	-	+	+	_	+
_	-	-	_	-	+	+	_	_	-	+
-	_	+	-	-	+	+	+	+	+	+
_	_	-	+	+	+		+	-	+	+
+	_	-	-	+	_	-	+	+	_	+
_	+	+	-	+	_	-	_	-	+ '	+
+	+	-	_	-	_	+	+	_	+	+
+	+	_	_	_	+	-		+	+	+
+	-	+	+	-	_	_	-	-	+	+
-	_	-	+	+	_	+	_	+	+	+

TABLE 9b. X'X has above-diagonal 3's in positions (1, 2), (1, 3), (2, 3), (3, 4), (4, 5), (6, 7), (8, 9), (10, 11)

_	_	_	+	_	+	+	+	+	+	+
+	+	+	+	_	-	-	+	_	_	+
_	_	-	_	+	+	+	+	-	-	+
+	+	-	_	+	_	-	+	+	+	+
-	+	+	+	+	_	+	_	-	+	+
+	-	_	_	-	_	+	_	-	+	+
+	+	+	-	-	+	+	_	+	_	+
_	_	_	+	+	_	_	_	+	-	+
+	-	+	+	+	+	-	-	-	+	+
_	+	-	_	-	+	-	_	-	+	+
_	_	+	_	-	-	_	+	+	+	+

TABL 2 in th			a bloc	k mat	rix wit	h s = 4	and b	locks d	of size	5, 2, 2,
_	+	+	+	+	_	_	_	_	+	+

_	+	+	+	+	_	_	_	_	+	+
+	-	+	-	_	+	+	_	-	+	+
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_	-	_	+	_	+	+	+	+	+	+
_	_	_	_	_	+	_	_	+	_	+
+	_	_	+	_	_	-	_	-	+	+
_	+	-	_	+	+	+	_	-	+	+
_	-	+	-	_	_	_	+	+	+	+
+	+	+	+	+	_	+	_	+	_	+
+	+	+	+	+	+	_	+	_	_	+
_	_	_	_	_		+	+	_	_	+

normalization, is proved by our developments to be optimum, since it is a block design with (k, n, s) = (10, 11, 5) (see Table 1). Our search found Mitchell's design frequently, but also succeeded in finding a design with the alternate value s = 6, given in Table 6. Table 4 illustrates the lack of uniqueness of X'X for (k, n) = (10, 15).

For k = 11 there are the three X'X's proved optimum by Ehlich, as described in Subsection 2.3 (see Table 9). For all n > k we have a regular optimum X, the only Case 3 design that is not very regular being that for n = 15 given in Table 7.

For k = 12 our development yields regular optimum X for all $n \ge 12$, the only Case 3 value of n for which there is no very regular design being 15. An optimum design for n = 15 with s = 6 is given in Table 8. Ehlich (1978) has found the optimum design with s = 7 in this case.

For larger values of k of practical interest, the Proposition of Section 2 and our other developments yield regular D-optimum designs in all cases except $n \in \mathcal{N}_3$ with $k \le n < 2k - 5$. The last 7 lines of Table 1 list these unknown cases for k = 13, 14, 15.

Added in proof. Additional Case 3 results obtained by us, to appear in the *Proceedings 1979 Tokyo Conference*, include *D*-optimum designs for the cases (12, 15, 7) and (2k - 5, k, k - 1) for all k; and unattainability of $\Psi(k, n)$ for the cases (13, 15), (14, 15), (9, 11, 7).

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