

Computing D-Optimum Weighing Designs:  
where Statistics, Combinatorics,  
and Computation Meet

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August 1983

\*Research supported by NSF Grant MCS-83-03139. This paper was also delivered at a Statistical Research Conference dedicated to the memory of Jack Kiefer and Jacob Wolfowitz. The conference was held at Cornell University, July 6-9, 1983. It was a special meeting of the Institute of Mathematical Statistics cosponsored by the American Statistical Association. Financial support was provided by the National Science Foundation, Office of Naval Research the Army Research Office--Durham and units of Cornell University.

Abstract: This paper surveys results and techniques for computing D-optimum weighing designs.

## 1. Introduction.

In this paper we survey results and techniques for computing D-optimum weighing designs. The paper summarizes the results of my work with Jack Kiefer ([1]-[6]), and describes some related results. This paper is written with two hopes in mind. We hope that the work on D-optimum design will be continued. Although we know now much more than before, the picture is far from complete. We also hope that some of the techniques we developed will be found useful elsewhere: for finding optimum designs using other optimality criteria or for solving other optimization problems.

Let  $k$  and  $n$  be positive integers with  $k \leq n$ , and let  $\mathcal{X} \equiv \mathcal{X}(k,n)$  denote the set of all  $n \times k$  matrices  $X = \{x_{ij}\}$  consisting entirely of entries  $\pm 1$ . 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  $\theta_j$  ( $1 \leq j \leq k$ ) 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  $j$ th object is on the left or right pan in the  $i$ th 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. It can easily be shown 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), 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  $i$ th observation being at  $(z_{i1}, z_{i2}, \dots, z_{ip})$  with expectation  $\alpha_k + \sum_1^p z_{ij} \theta_j$ , which we can write  $\sum_1^k z_{ij} \theta_j$  by defining  $z_{ik} = 1$ . It can easily be shown that there is a D-optimum  $\bar{X}$  in  $\mathcal{X}$ . Conversely, each  $X$  in  $\mathcal{X}$  can be transformed into an element of  $\mathcal{X}$  with the same determinant and all  $x_{ik} = 1$ .

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 Kischen, 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 (1980). In the present paper we are concerned with finding a D-optimum  $\bar{X}$  in  $\mathcal{X}$  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

$\text{tr}(X'X)^{-1}$ , have also been considered, but our main concern here is with  $\det(X'X)$ .

Our work on finding D-optimum designs touched five different fields:

1. Statistics,
2. Combinatorics,
3. Number Theory,
4. Computation, and
5. Complexity.

Statistics, in particular experimental design, was the source of our problem, as described above. Once the problem is defined as maximizing  $\det(X'X)$  no statistics is used. We are basically solving an optimization problem, or more precisely an infinite family (with parameters  $k$  and  $n$ ) of optimization problems. We will see below how techniques from the other four fields are used.

Since five different fields are involved, it can be valuable to consider the varied interplay between some of them. Kiefer (1981) describes the interplay of optimality and combinatorics in experimental design: there are two approaches for defining "good" designs. The first which was developed by R.A. Fisher and his followers often used combinatorial structures that yielded simple calculation of estimates or of

symmetric variances and covariances. Examples include block designs with balance and regression experiments with equally spaced observations. This approach was justified at the time when inverting a  $10 \times 10$  matrix (by hand) was a formidable computational task.

The second approach was to choose an optimality criterion (or criteria) and to find designs which are optimal or almost optimal according to the criteria chosen. Jack Kiefer was a pioneer (perhaps the leader) in developing this second approach. Using this approach, it was sometimes possible to justify the simple symmetric designs found by the former approach. But in many cases this was not so. Followers of the second approach discovered new designs which, though they displayed some symmetry, were not as "nice" as the symmetric designs found by the former approach. This led to the use of new combinatorial structures and to a "back and forth" between design criteria and combinatorial constructions. In his paper, Kiefer gives two examples of this interplay: construction of D-optimum weighing designs and of incomplete block designs. The interplay in the first case will be indicated below.

In this paper we will emphasize another interplay between analytical methods and computational methods for finding D-optimum designs. There are two pure strategies for finding

D-optimal or almost D-optimal designs. The first is to use analytical methods in order to prove that certain designs are optimal (or almost optimal). Unfortunately, in many cases we do not know how to do this. The second is to use the computer to search for an optimum search strategy, employing simple heuristic, usually yielding a local maximum with very little information on how good this local maximum is.

We now describe <sup>three</sup>  $\wedge$  mixed strategies for finding D-optimum designs. Later in the paper we will give examples, where these mixed strategies were successful.

Sometimes the computational results suggest a theorem. For this to hold we often need that our search be so good that it finds a global optimum. What makes our task difficult is that we do not know when this has occurred. Once a candidate for a theorem emerges from our computations, we of course, try to prove it.

Occasionally, using analytical methods we only prove an upper bound for the maximum. We then try to use our search strategies to match this bound; i.e. to find a design with  $\det(X'X)$  equal to the upper bound. This strategy can work only if our upper bound was actually the value of the optimum. In all cases, the upper bound yields a lower bound for the ratio of the best design we have found so far to the optimal design.

Sometimes, by using analytical methods we considerably restrict the search space. In the resulting (much smaller) space it is sometimes possible to search exhaustively for the optimum. In any case, search procedures perform much better on a smaller space. The "proof" of the Four Color Theorem (Appel and Haken (1976)) uses this type of strategy.

The next sections summarize four cases of our problem: Case  $i$ ,  $i = 0, 1, 2, 3$ . Case  $i$  consists of all  $(k, n)$  such that  $k \leq n \in \mathcal{N}_i \equiv \{n | n \equiv i \pmod{4}\}$ . We also point out several examples of the two interplays mentioned above.

## 2. 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  $n \in \mathcal{N}_0$ , 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  $n \leq 200$ , and for infinitely many other  $n$ . There is an  $\tilde{X}$  in  $\mathcal{X}(k, n)$  with  $\tilde{X}' \tilde{X} = nI_k$  if  $H_n$  exists (namely  $k$  columns of  $H_n$ ), and such  $\tilde{X}$  can in fact often be found much more easily. In particular such  $\tilde{X}$  exists for all  $(k, n)$   $k \leq 100$ ,  $n \in \mathcal{N}_0$  (see [1]). Such an  $\tilde{X}$  is not only well known to be D-optimum, but also minimizes  $\phi(\tilde{X}' \tilde{X})$  over  $\mathcal{X}$



for every nonincreasing convex orthogonally invariant extended real-valued  $\phi$  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  $\theta_i$  (diagonal element of  $(X'X)^{-1}$ ), as was shown by Hotelling (1944).

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

### 3. Case 1.

Ehlich showed that an  $\tilde{X}$  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 a  $\tilde{X}$  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  $\tilde{X}'\tilde{X} = (n-1)I_k + J_k$  is not only D-optimum, but also optimum with respect to a large subclass of the  $\phi$ 's,  $\mathcal{A}$ , of the previous section, including all those of common interest. (The D-optimality in the unsaturated 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 design of Case 0 in  $\mathcal{X}(k, n - 1)$  exists, by adjoining a row of 1's to that design. Although such an adjoining is a common practice in the literature of weighing designs, the D-optimality over  $\mathcal{X}$  (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  $n \leq 20$  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 design obtained by them 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). Ehlich (1978) has indicated to us that the method of proof of optimality is similar to, but simpler than, that mentioned in Section 5 below for the  $k = n = 11$  case. The method also shows no other form of  $X'X$  can be optimum for  $k = n = 9$ . Recently, Moyssiadis and Kounids (1982) computed the case  $k = n = 17$  by applying analytic methods that restricted the number of possible optimal designs, followed by an exhaustive search. Consequently,

the smallest unknown instances of Case 1 are  $k = n = 21, 29$ . We do not know the solution for  $k = n > 30, n \in \eta_1$ .

#### 4. 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  $k \leq 38$  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  $k = 42, 46, 50, 54$ .

For general  $k \leq n \in \eta_2$ , we consider those  $\tilde{X}$  in  $\mathcal{X}(k, n)$  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  $(n - 2)I_{(k+1)/2} + 2J_{(k+1)/2}$ . These designs were proved D-optimum by Payne for  $k \leq n - 2$  using the work of Wojtas, and one can also see that Ehlich's proof requires only simple modifications to apply to Case 2 for  $n \geq k$ . (In fact, Payne's proof also applies for  $n \geq k$ , but he does not say so because he gives constructive methods only when  $k \leq n - 2$  and  $H_{n-2}$  exists.)

When  $k \leq n - 2$  and a design  $\bar{X}$  in  $\mathcal{X}(k, n - 2)$  of Case 0

exists, an optimum  $\tilde{X}$  for Case 2 is achieved by using one of Mood's devices, discussed and employed by Mitchell and by Payne. This  $\tilde{X}$  is obtained by adjoining to  $\tilde{X}$  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  $X$  of Ehlich or Yang in  $\mathcal{X}(n, n)$  (mentioned two paragraphs above) yields an optimum 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. The only four instances of Case 2, with  $n \leq 52$  in which we do not know the optimum are  $n \in \{22, 34\}$ ,  $k \in \{n-1, n\}$ .

It is interesting to note that restricting attention to a symmetric solution in the intuitive Fisherian spirit in which all of the off-diagonal elements are equal is quite poor, especially for small  $n$ ; thus, in the case  $n = k = 6$  the determinant of Ehlich's information matrix is 56% larger than for the best matrix with all off-diagonal elements equal.

Like the D-optimum designs of Case 1, those of Case 2 have been shown to have other optimum properties. Cheng (1980) showed they are among the E-optimum designs. Jacroux, Masaro

and Wong (1983), have recently shown that they are also optimum with respect to the class  $\mathcal{A}$  that we mentioned in Section 3.

### 5. Case 3.

This is well known to be the most difficult (and the most interesting) case. If one knows an  $H_{n+1}$  or, more generally, an  $\bar{X}$  in  $\mathcal{X}(k, n+1)$  of Case 0, deletion of one row of  $\bar{X}$  yields an  $\tilde{X}$  in  $\mathcal{X}(k, n)$  with  $\tilde{X}'\tilde{X} = (n+1)I_k - J_k$ . We denote  $\tilde{X}$  by  $X_e$  (e for easy). However such an  $\tilde{X}$  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). 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  $\tilde{X}$  described just above, and Payne (1964) proved these optimum for  $k \leq 5$ .

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). Ehlich used an ingenious combination of theoretical developments and computer search, by means of which he obtained designs with three structures of  $X'X$ , proved them optimum, and proved no other structures of  $X'X$  could be optimum.

Before [1], designs for  $k < n = 11$  had not been proved optimum theoretically except for Payne's treatment when  $k \leq 5$ . Of the designs found by Mitchell for  $k = 9$  and  $10$ , the former was not optimal, Payne (1974) showed that an  $X_e$  is D-optimum provided  $n$  is sufficiently large compared with  $k$ . He gives  $n > (5/2)3^{k-2} \binom{k}{\lfloor k/2 \rfloor}$  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  $k \leq n < 3k$ . Our own early numerical investigations indicated that  $n \geq 2k$  might suffice, so that the evidence cited by Payne is a commentary on his method of proof rather than on the definitive results. In [1] we showed that  $n \geq 2k - 5$  suffices.

The entire treatment of Case 3 is based on Ehlich work. Ehlich (1964b) considers only the saturated case. But minor modifications yield the development below.

Let  $\mathcal{C} = \mathcal{C}_{k,n}$  be the class of all symmetric  $k \times k$  matrices with diagonal entries  $n$  and off-diagonal entries

-1 or 3, where  $n \in \mathfrak{M}_3$ . Let

$$(1) \quad \psi(k, n) = \max_{A \in \mathcal{C}_{k, n}} \det A.$$

Ehlich shows that  $\max_{X \in \mathcal{X}} \det(X'X) \leq \psi(k, n)$  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  $\sum_1^s r_i = k$  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

$$(2) \quad \det C = (n - 3)^{k-s} \{1 - G\} \prod_1^s (n - 3 + 4r_i),$$

$$G = \sum_1^s r_i / (n - 3 + 4r_i).$$

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

$$(3) \quad u + v = s, \quad ur + v(r+1) = sr + v = k.$$

For any block matrix  $C_s$  in  $\mathfrak{M}_{k, n}$  with  $s$  blocks (2) and (3) yield

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

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

Ehlich's last-cited result is thus  $\psi(k,n) = \max_s D_{k,n}(s)$ .

Of course,  $s$  uniquely determines  $r$  except when  $s|k$ . 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 (4). The  $x_e$  discussed earlier has  $s = k$ .

As a result of the discussion above, one approach of solving our problem (of maximizing  $\det(X'X)$ ) is to solve the following two subproblems:

(1) to find  $s^*$ ,  $1 \leq s^* \leq k$ , such that

$$D_{k,n}(s^*) = \psi(k,n) (= \max_s D_{k,n}(s)), \text{ and then}$$

(2) to find an  $X$  in  $\mathcal{X}$  such that  $\psi(k,n) = \det(X'X)$ .

As indicated above for  $n \geq 2k - 5$ ,  $s^* = k$  and  $X = X_e$  is D-optimum. Thus we are left with those subcases of Case 3 with  $n < 2k - 5$ . For solving some instances of the two subproblems above we used the computer extensively. The next section digresses momentarily to describe briefly our computational methods.



## 6. Computation.

In a pathbreaking sequence of papers, Mitchell (1974a,b) developed and implemented a general technique, termed DETMAX, for obtaining D-optimum experimental designs in a wide variety of settings. It is a search technique. Exhaustive search in typical applications involves too many ( $2^{nk}$ ) possible design matrices  $X$ . Moreover, in attempting to maximize  $\det(X'X)$ , all known usable techniques that move from an  $X$  to a nearby "better"  $X$  can get trapped in a neighborhood of a local maximum that is not the desired global maximum, and perhaps not even moderately efficient. One therefore introduces some randomization into the search technique, both in the initial guess, and also in later "tie-breaking", so that different "tries" can lead to different  $X$ 's; thus, with enough tries, one can hope to find an  $X$  that is optimum or close to it. Mitchell's technique seems to us by far the most successful general method that has appeared for solving such problems.

We had hoped, over a period of several years, to improve upon DETMAX, e.g., by finding a way of "jumping" far enough out of a local maximum to escape from it in a usually favorable direction; or by adding, subtracting, or exchanging more than the one point per step that Mitchell does. These hopes proved fruitless, the first from lack of the right idea, the second

because of astronomically increased computer time. Thus, with renewed respect for Mitchell's method, we were led to try to modify it in more modest ways, in terms of the actual computational steps it performs.

This involved a careful analysis of the individual operations it performs, especially in the updating of such entities as  $(X'X)^{-1}$ , that are used in improving the design successively. In [2] we introduced a collection of methods capable of both time and space saving. We called our procedure MDETMAX (M for modified). We tested MDETMAX and found in our examples that it was typically 15 to 50 times faster than the original DETMAX in problems with 5 to 10 parameters and 10 to 20 observations, on each "try" in which a design  $X$  was found. One could therefore perform that many more tries than did DETMAX, for a given expenditure of computer time or money, and thereby increase greatly the chance of finding an improved solution in many problems. We did often achieve such solutions. Alternatively, we could tackle larger problems (larger  $(k,n)$ ) that DETMAX could not.

### 7. Back to Case 3.

As we concluded in Section 5. one way to solve the problem is first to find  $s^*$  which maximizes  $D_{k,n}(s)$  and then to try to find  $X$  such that

$$(5) \quad \det(X'X) = D_{k,n}(s^*) \quad (= \Psi(k,n)),$$

The first subproblem is relatively easy. For specific cases, this is a very simple task, since one has to compute and compare  $k$  values of  $D_{k,n}(s)$ . In [4] we listed the values of  $s^*$  ( $= s^*(k,n)$ ) for all Case 3  $(k,n)$ ,  $k \leq n \leq 100$ .

The general problem of finding  $s^*(k,n)$  is open. We already noted that  $s^*(k,n) = k$  for  $n \geq 2k - 5$ . Ehlich (1964b) showed that  $s^*(n,n) = 7$  for  $n \geq 63$ . In [4] we obtained upper and lower bounds for  $s^*$ . We also found  $s^*$  for several infinite families of  $(n,k)$ , near the two ends: for cases  $n = 2k - d$ ,  $d = 5, 7, \dots, 17$ , we found  $s^* = \alpha_d k + \beta_d$ , <sup>where</sup>  $\alpha_d$  decreases from 1 to  $1/3$ . Near the saturated case, for  $n$  large enough,  $s^*$  is still 7; then as we increase  $n$ ,  $s^*$  grows slowly. More specifically for  $n \rightarrow \infty$  with  $k/n \rightarrow 1 - \lambda$ , we have  $\lim s^* = 7$  if  $0 \leq \lambda \leq .08837$ ,  $= 8$  if  $.08838 \leq \lambda \leq .17027$ ,  $= 9$  if  $.17028 \leq \lambda \leq .22494$ ,  $> 9$  if  $.22495 \leq \lambda$ .

These results were obtained using elementary number theory and manipulation of inequalities. We believe that  $D_{k,n}(s)$  is unimodal. This was indeed verified for  $k \leq n \leq 100$ , but we could not prove it in general.

Once we know  $s^*$  we have to find a design  $X$  with  $\det(X'X) = \Psi(k,n)$ . Unfortunately, such an  $X$  does not always exist. When  $k = n$ , (the case studied by Ehlich) the Ehlich theory is rarely implementable in the sense of

there existing an  $X$  with  $\det(X'X) = \Psi(n,n)$ . Specifically  $\Psi(n,n)$  is infrequently a square, which is necessary for such an  $X$  to exist; the only two values of  $n < 200$  for which  $\Psi(n,n)$  is square, other than the trivial value  $n = 3$ , are 91 and 147 (misprinted 47 in [1]). It is not known whether an  $X$  with  $\det(X'X) = \Psi(n,n)$  is constructible for any  $n > 3$ . When  $k < n$  we do not of course have squareness of  $D_{k,n}(s^*)$  as a condition for constructibility of an  $X$  with  $\det(X'X) = \Psi(k,n)$ .

We now discuss three different methods for solving (5). The first was to search among all  $X$  in  $X$ . This approach is prohibitively expensive. If one were going to use exhaustive search, he should rather use it for the entire problem (maximizing  $\det(X'X)$ ). Nevertheless we used a modified version of this approach to find that for  $k \in \{13,14\}$ ,  $n = 15$  there is no solution to  $X'X = C_{s^*}$  and hence (by Ehlich's theory) no solution to (5). The search was somewhat reduced by observing certain symmetries (see [3]). Consequently, the smallest unknown instances of Case 3 are  $k \in \{13,14,15\}$   $n = 15$ .

The second approach was to use MDETMAX, and compare the best determinant we found with  $\Psi(k,n)$ . This approach proved to be successful in several cases. Also, in the three cases mentioned above, when (5) is not solvable, MDETMAX found designs with determinants close to (the unattainable)  $\Psi(k,n)$ .

It is interesting to note that in all cases but one the modifications introduced in MDETMAX (in [2]) were crucial. The original DETMAX either could not handle these cases or gave much inferior results.

The third approach was to invent combinatorial construction methods for finding  $X$  with  $X'X = C_{s^*}$ . In [5] we invented such methods, yielding  $X$ 's which attain  $\psi(k,n)$  for infinitely many  $(k,n)$ . As a result we now have an infinite family of D-optimum designs for Case 3 with  $n < 2k - 5$ . Our methods used certain Hadamard matrices as building blocks.

More recently Kounian and Hajipantelis (1983) and Kounias and Farmakis (1983) invented new construction methods using circular matrices, and matrices of Goethals-Seidel type.

## 8. Conclusion.

We surveyed results and techniques for computing D-optimum weighing designs. For more details see [1]-[6]. Two topics which appear in these papers and were not discussed here are: 1. More details on our computational experience with MDETMAX, especially its remarkable performance in computing quadratic regressions [3]. 2. The nonuniqueness of  $s^*$  ([1],[2],[4]). In [4] we characterized all these cases

of "ties". There are five families of  $(k,n)$  which are sub-families of the cases  $n = 2k - d$  discussed above. These are all the cases when  $s^*$  is not unique. In these cases two values of  $s$  are optimum. Beginning in [2] and continuing in [6], we used additional criteria to choose between two such values of  $s$ .

The current state of knowledge of our problem is as follows. Considering the (approximately) 5000 cases  $(k,n)$ ,  $k \leq n \leq 100$ , there are 1250 in each Case  $i$ , for  $i = 0,1,2,3$ . All the Case 0 instances are known. For Case 1 (Case 2) less than 20 (30) instances are not solved. For Case 3, slightly more than half have  $n > 2k - 5$ , for which we know the solution. For the remainder of close to 600 instances we know only about 120. As for small values of  $(k,n)$  all instances of Cases 1 (2) are solved for  $n \leq 20$  and only two instances are not known for  $n \leq 30$ . For Case 3, 5 instances are not known for  $n \leq 20$  ( $k \in \{13,14,15\}$   $n = 15$  and  $k \in \{16,19\}$   $n = 19$ ) and 18 instances (including the 5) are not known for  $n \leq 30$ .

We leave as a challenge

1. to find  $\psi(k,n)$  for all  $k$  and  $n$  (one possible step in this direction would be to show that  $D_{k,n}(s)$  is unimodal);
2. to devise new construction methods for cases for

which  $\psi(k,n)$  is known;

3. to find new methods to deal with instances in which (5) is not solvable; (The only such instances for which a solution is known are  $k = n \in \{7,11\}$ .)
4. to consider Case 3 and other optimality criteria. (Initial work in this direction is reported in Cheng, Masaro and Wong (1983).)

We considered here the following problem:

$$\begin{aligned} \text{I} \quad & \max \det(X'X) \\ & X \text{ an } n \times k \text{ matrix} \\ & x_{ij} \in \{-1,1\}. \end{aligned}$$

A special case of Problem I ( $k = n$ ) is

$$\begin{aligned} \text{II} \quad & \max \det(X) \\ & X \text{ an } n \times n \text{ matrix} \\ & x_{ij} \in \{-1,1\}. \end{aligned}$$

A special case of Problem II is

$$\text{III} \quad \text{Is } X'X = nI_n \text{ solvable for all } n \equiv 0 \pmod{4}?$$

Problem III has been studied for more than a hundred years, Problem II for nearly twenty years, and Problem I for nearly ten years. Naturally, we use our vast knowledge on Problem III to make progress on Problems I and II. Possibly, if we know more on problems I and II we will be able to make progress in solving Problem III.

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