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On the Smith Normal Form of *D*-Optimal Designs

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ABSTRACT

The Smith normal forms (SNF) of D-optimal designs of size <100 are determined by a computer search. A theorem is given for the SNF of D-optimal designs of order $4t+2$ when $4t+1$ is square free, and bounds for the minimum number of 2's which can appear in the SNF are derived.

1. INTRODUCTION

The general question that gave rise to the present paper is the question of isomorphism of D-optimal designs. Theoretically it is enough to check $(n!)^2$

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cases to find if two $n \times n$ given incidence matrices are permutation equivalent. In practice it is not feasible in any interesting case, even despite the fact that the number of comparisons can be reduced to $n!$, as was shown by M. Newman [9]. The Smith normal form may be used for a negative answer: if two incidence matrices have different Smith normal forms, then they are not permutation equivalent. It is thus interesting to learn more about the Smith normal form for the D-optimal designs. First we introduce some notation and summarize results on the Smith normal form and D-optimal designs. Let $\mathbf{R}_n$ be the ring of $n \times n$ matrices with entries from $\mathbf{Z}$, the ring of integers. The unit (*or* unimodular) elements of $\mathbf{R}_n$ are those with determinant ± 1.

DEFINITION 1. The matrices A, B of $\mathbf{R}_n$ are equivalent (or $\mathbf{Z}$-equivalent, written $B \sim A$) if $B = PAQ$ for some unimodular matrices P, Q of $\mathbf{R}_n$.

The following theorem is due to Smith [11] and has been reworded from the theorems and proofs in MacDuffee [7, p. 41] and Marcus and Minc [8, p. 44].

THEOREM 1. *If $A = (a_{ij})$ is any integer (or with elements from any Euclidean domain) matrix of order n and rank r, then there is a unique integer (or with elements from any Euclidean domain) matrix*

$$D = \operatorname{diag}(a_1, a_2, \dots, a_r, 0, \dots, 0)$$

such that $A \sim D$ and $a_i \mid a_{i+1}$, where the a_i are nonnegative. The greatest common divisor of the $i \times i$ subdeterminants of A is

$$a_1 a_2 \dots a_i.$$

If $A \sim E$, where

$$E = \operatorname{diag}(a_1, a_2, \dots, a_i) \oplus F$$

then a_{i+1} is the greatest common divisor of the nonzero elements of F.

DEFINITION 2. The a_i of Theorem 1 are called the *invariants* of A, and the diagonal matrix D is called the *Smith normal form*.

In this paper we will study the Smith normal forms of D-optimal designs. If $2v \equiv 2 \bmod 4$ and X, Y are commuting $v \times v$ matrices, with elements

± 1, such that

$$XX^T + YY^T = 2(v-1)I_v + 2J_v, \tag{1}$$

where J_v is an $v \times v$ matrix of 1's, then the $2v \times 2v$ matrix

$$M = \begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix} \tag{2}$$

has the maximum determinant (see [1, 5]) among all $2v \times 2v$ ± 1 matrices. Such matrices are called *D-optimal designs* of order $2v$. A particular case where this construction is used is when X and Y are circulant matrices.

Suppose $R = (r_{ij})$ is the (0, 1) matrix of order v defined by $r_{i,v-i+1} = 1$ and $r_{ij} = 0$ when $j \neq v - i + 1$, and further suppose X and Y are circulant matrices satisfying (1). Then

$$N = \begin{pmatrix} X & Y \\ -YR & XR \end{pmatrix} \tag{3}$$

is also a D-optimal design.

LEMMA 1. *The two basic methods described in* (2) *and* (3) *use circulant matrices X and Y of order v, satisfying*

$$XX^T + YY^T = 2(v-1)I_v + 2J_v,$$

to make a D-optimal design of order $2v$. These have the same Smith normal form, as they are equivalent.

Proof. We first note that $(YR)^T = YR = RY^T$ and $XR = RX^T$. Now we note that

$$\begin{pmatrix} X & Y \\ -YR & XR \end{pmatrix} = \begin{pmatrix} X & Y \\ -RY^T & RX^T \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix}\begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix}.$$

Hence with

$$P = \begin{pmatrix} I & 0 \\ 0 & R \end{pmatrix} \quad \text{and} \quad Q = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$$

we have $PMQ = N$. ∎

Now form the two sets $A = \{a_1, a_2, \dots, a_r\}$ and $B = \{b_1, b_2, \dots, b_s\}$, where a_i, b_j denote the positions of -1's in the first row of X, Y respectively.

If the matrices X, Y are circulant, then they satisfy (1) if and only if (see [3]) they are supplementary difference sets $2 - \{v; r, s; \lambda\}$, where $\lambda = r + s - \frac{1}{2}(v - 1)$ and $s \geqslant r \geqslant 0$ are found from

$$(v - 2r)^2 + (v - 2s)^2 = 2(2v - 1). \tag{4}$$

Hence the construction of the two circulant matrices X, Y satisfying (1) is equivalent to the construction of the corresponding supplementary difference sets. For $n = 22, 34, 58$, D-optimal designs satisfying (1) do not exist, because $2v - 1$ is not the sum of two squares (see [3]).

2. THE MATRIX EQUATION $AA^T = B$

In this section we discuss the matrix equation $AA^T = B$, proceeding as in Ryser [10]. Throughout this discussion, A is a matrix of order v with rational or integral elements, and A^T denotes the transpose of A. The matrix B is of order v and is defined by

$$B = aI + bJ. \tag{5}$$

In (5), I is the identity matrix of order v, and J is the matrix of order v with every element plus one. We assume that a and b are integers such that $0 < a, b \leqslant v - 1$.

Now simple row and column operations can be used to show

$$\det B = \det(aI + bJ) = (a + bv)a^{v-1},$$

and so, since $\det A = \det A^T$,

$$\det A = (a + bv)^{1/2} a^{(1/2)(v-1)}.$$

We assert

$$B^{-1} = \frac{1}{a} I - \frac{b}{a(a + bv)} J.$$

Suppose $AA^T = B$. Then $A(A^TB^{-1}) = I$, and since a matrix and its inverse commute,

$$(B^{T^{-1}})AA^T = I \quad \text{and} \quad (A^TB^{-1})A = I. \tag{6}$$

Hence

$$A^T\left(\frac{1}{a}I - \frac{b}{a(a+bv)}J\right)A = I,$$

and

$$A^TA = aI + \frac{b}{a+bv}A^TJA.$$

We now apply similar reasoning to D-optimal designs. Writing $DD^T = C$ for the D-optimal design D of order $2v$, we have

$$\begin{aligned}\det D &= \det[2(v-1)I + 2J] \times I_2 \\ &= \left(\left[2(2v-1)2^{(v-1)}(v-1)^{(v-1)}\right]^{1/2}\right)^2 \\ &= (2v-1)2^v(v-1)^{v-1}.\end{aligned}$$

As above,

$$C^{-1} = \frac{1}{2(v-1)}I \times I_2 - \frac{1}{2(v-1)(2v-1)}J \times I_2. \tag{7}$$

Similarly,

$$D^TC^{-1}D = I$$

and

$$D^TD = 2(v-1)I_{2v} + \frac{1}{2v-1}D^T(J \times I_2)D. \tag{8}$$

LEMMA 2. *Suppose*

$$D = \begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix}, \tag{9}$$

and $X^TJ = XJ = xJ$, $Y^TJ = YJ = yJ$. *Then*

$$D^T(J_v \times I_2)D = D(J_v \times I_2)D^T.$$

In particular, if $XX^T + YY^T = aI_v + bJ_v$ *then*

$$D^T(J_v \times I_2)D = D(J_v \times I_2)D^T = (a + bv)J_v \times I_2.$$

Proof. $XX^T + YY^T = aI_v + bJ_v$ so $XX^TJ + YY^TJ = (x^2 + y^2)J_v = (a + bv)J_v$. Now consider

$$\begin{pmatrix} X^T & -Y \\ Y^T & X \end{pmatrix}\begin{pmatrix} J & 0 \\ 0 & J \end{pmatrix}\begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix}$$

$$= \begin{pmatrix} (x^2 + y^2)J & 0 \\ 0 & (x^2 + y^2)J \end{pmatrix} = (a + bv)J_v \times I_2.$$

Similarly

$$D(J_v + I_2)D^T = (a + bv)J_v \times I_2. \qquad \blacksquare$$

REMARK 1. We recall here that

$$(XX^T + YY^T)^{-1} = \frac{1}{a} I_v - \frac{b}{a(a + bv)} J_v, \tag{10}$$

so for X, Y from a D-optimal design,

$$(XX^T + YY^T)^{-1} = \frac{1}{2(v - 1)} I_v - \frac{1}{2(v - 1)(2v - 1)} J_v. \tag{11}$$

THEOREM 2. *Let D be a D-optimal design of order $2v$. Then*

$$D^{-1} = (DD^T)^{-1} D^T = \frac{1}{2(v - 1)} D^T - \frac{1}{2(v - 1)(2v - 1)} (J \times I) D^T$$

and

$$D^{-1} = D^T(D^TD)^{-1} = \frac{1}{2(v - 1)} D^T - \frac{1}{2(v - 1)(2v - 1)} D^T(J \times I).$$

Proof. Use Equation (8) and Lemma 2 to obtain

$$D^T D = DD^T = 2(v-1) I_{2v} + 2J_v \times I_2.$$

Hence $D^{-1}(D^T)^{-1} = (D^T)^{-1}D^{-1}$, and from (7)

$$(DD^T)^{-1} = (D^T D)^{-1} = \frac{1}{2(v-1)} I_{2v} - \frac{1}{2(v-1)(2v-1)} J_v \times I_2.$$

This gives the required result. ■

3. THE NUMBER OF SMALL INVARIANTS

It we start to normalize the incidence matrix of a D-optimal design, we find it has exactly one invariant equal to 1 and that the next invariant is 2. We write $[x]$ for the largest integer not exceeding x. We use a result of Wallis quoted in [12, p. 411].

THEOREM 3 (W. D. Wallis). *Suppose E is a $v \times v$ matrix with nonzero determinant whose entries are all* 0 *and* 1, *the identity elements of the Euclidean domain* $\mathbf{Z}$. *Then the number of invariants of E under $\mathbf{Z}$-equivalence which equal* 1 *is at least*

$$[\log_2 v] + 1.$$

Suppose we have a general D-optimal design

$$\begin{pmatrix} X' & Y' \\ Z' & W' \end{pmatrix}. \tag{12}$$

We note that if we multiply any column through by -1, we do not change the D-optimality of the design. So we normalize the design to have its first row all $+1$'s. Write this as

$$\begin{pmatrix} X & Y \\ Z & W \end{pmatrix}. \tag{13}$$

We now add the first row to every other row and obtain a $(2v-1) \times 2v$ matrix with every element 0 or 2. We note that the operation we have just performed has not changed the determinant. Thus, as the determinant of the $2v \times 2v$ matrix was not zero, the $(2v - 1) \times 2v$ matrix still has rank $2v - 1$. It thus satisfies the conditions of Wallis's theorem and has at least $[\log_2(2v - 1)] + 1$ equal elements (here 2) in its normalization over the Euclidean domain $\mathbf{Z}$.

Thus we have

THEOREM 4. *Let D be the incidence matrix of a D-optimal design of order $2v$. Then the Smith normal form of D has one element 1 and at least $[\log_2(2v - 1)] + 1$ elements equal to 2.*

Now the Smith normal form S of

$$D = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_{2v}),$$

is such that $S \sim D$ and $\lambda_i \mid \lambda_{i+1}$, where the λ_i are nonnegative integers. There are no zeros in S, as the determinant is not zero.

Now

$$\prod \lambda_i = 2^v (v - 1)^{v-1} (2v - 1) = \det D,$$

and for $v = 2t + 1$ we have

$$\prod \lambda_i = 2^{4t+1} \cdot t^{2t} \cdot (4t + 1) \tag{14}$$

and so $\lambda_1 = 1, \lambda_2 = 2, \dots, \lambda_{[\log_2(2v-1)]+2} = 2, \dots, \lambda_{2v} = 2t^a(4t + 1)$ for some a.

NOTATION 1. In order to simplify writing we will henceforth use the notation $(x)^t$ to denote t copies of x, or $x, x, \dots, x$ (t times). So

$$\lambda_1 = 1, \quad \lambda_2 = 2, \dots, \quad \lambda_{[\log_2(2v-1)]+2} = 2, \dots, \quad \lambda_{2v} = 2t^a(4t + 1)$$

for some a will be written.

$$\lambda_1 = 1, \quad (\lambda_2 = 2)^{[\log_2(2v-1)]+2}, \dots, \quad \lambda_{2v} = 2t^a(4t + 1) \qquad \text{for some } a.$$

REMARK 2. We note that in general D-optimal designs are not of circulant type.

The previous theorem shows that for $2v = 18$ there must be at least five elements in the Smith normal form which are 2. This leads us to the possibilities

$$\left(1, (2)^{\zeta}, (4)^{\mu}, (8)^{16-\zeta-\mu}, 136\right)$$

for the Smith normal form, where $\zeta = 5, 6, 7, 8$, or 9.

In fact for the case $2v = 18$ we have three different Smith normal forms, i.e. three nonequivalent D-optimal designs, one of which is of circulant type (see also Cohn [2]), so the possibilities $\zeta = 5$ and 6 are not realized.

If we use the matrices

$$X = \begin{pmatrix} - & - & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & - & - & 1 & 1 & 1 & 1 & 1 & 1 \\ - & 1 & - & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & - & - & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & - & - & 1 & 1 & 1 \\ 1 & 1 & 1 & - & 1 & - & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & - & - & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & - & - \\ 1 & 1 & 1 & 1 & 1 & 1 & - & 1 & - \end{pmatrix},$$

$$Y = \begin{pmatrix} 1 & 1 & - & 1 & - & 1 & 1 & - & 1 \\ 1 & - & 1 & - & 1 & 1 & - & 1 & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 & 1 & - \\ 1 & - & 1 & 1 & 1 & - & 1 & - & 1 \\ - & 1 & 1 & 1 & - & 1 & - & 1 & 1 \\ 1 & 1 & - & - & 1 & 1 & 1 & 1 & - \\ 1 & - & 1 & 1 & - & 1 & 1 & 1 & - \\ - & 1 & 1 & - & 1 & 1 & 1 & - & 1 \\ 1 & 1 & - & 1 & 1 & - & - & 1 & 1 \end{pmatrix},$$

where — represents -1, then the SNF of the corresponding D-optimal design $\begin{pmatrix} x & y \\ -y & x \end{pmatrix}$ is

$$\left(1, (2)^{7}, (4)^{4}, (8)^{5}, 136\right).$$

If we use

$$X = \begin{pmatrix} - & - & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & - & - & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & - & - & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & - & - & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & - & - & 1 & 1 & 1 \\ - & 1 & 1 & 1 & 1 & - & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & - & - & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & - & - \\ 1 & 1 & 1 & 1 & 1 & 1 & - & 1 & - \end{pmatrix},$$

$$Y = \begin{pmatrix} - & 1 & - & 1 & 1 & 1 & - & 1 & 1 \\ 1 & - & 1 & 1 & 1 & - & 1 & 1 & - \\ - & 1 & 1 & 1 & - & 1 & 1 & - & 1 \\ 1 & 1 & 1 & - & 1 & - & - & 1 & 1 \\ 1 & 1 & - & 1 & - & 1 & 1 & 1 & - \\ 1 & - & 1 & - & 1 & 1 & 1 & - & 1 \\ - & 1 & 1 & - & 1 & 1 & 1 & 1 & - \\ 1 & 1 & - & 1 & 1 & - & 1 & - & 1 \\ 1 & - & 1 & 1 & - & 1 & - & 1 & 1 \end{pmatrix},$$

then the SNF of the corresponding D-optimal design $\left(\begin{smallmatrix} x & y \\ -y & x \end{smallmatrix}\right)$ is

$$\left(1, (2)^8, (4)^2, (8)^6, 136\right).$$

However, if the circulant matrices

$$X = \begin{pmatrix} - & - & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & - & - & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & - & - & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & - & - & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & - & - & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & - & - & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & - & - & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & - & - \\ - & 1 & 1 & 1 & 1 & 1 & 1 & 1 & - \end{pmatrix},$$

$$Y = \begin{pmatrix} - & 1 & 1 & 1 & - & 1 & 1 & - & 1 \\ 1 & - & 1 & 1 & 1 & - & 1 & 1 & - \\ - & 1 & - & 1 & 1 & 1 & - & 1 & 1 \\ 1 & - & 1 & - & 1 & 1 & 1 & - & 1 \\ 1 & 1 & - & 1 & - & 1 & 1 & 1 & - \\ - & 1 & 1 & - & 1 & - & 1 & 1 & 1 \\ 1 & - & 1 & 1 & - & 1 & - & 1 & 1 \\ 1 & 1 & - & 1 & 1 & - & 1 & - & 1 \\ 1 & 1 & 1 & - & 1 & 1 & - & 1 & - \end{pmatrix}$$

are used in (2), we obtain the SNF

$$\left(1,(2)^9,(8)^7,136\right).$$

LEMMA 3. *The Smith normal form S of a D-optimal design of order* $2v$ *has the form*

$$S = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_{2v})$$

where $\lambda_i \mid \lambda_{i+1}$ *and*

$$\lambda_1 = 1, \quad \lambda_2 = 2, \dots, \quad \lambda_{[\log_2(2v-1)]+2} = 2, \dots, \quad \lambda_{2v} = 2t^a(4t+1)$$

for some a.

In the case where $2v - 1 = 4t + 1$ is square free it cannot be decomposed into two integers α and β such that $\alpha \mid \beta$ and $\alpha \cdot \beta = 4t + 1$. Nor does $t \mid 4t + 1$, so, if t is odd, the only possible decomposition in (14) is for $\lambda_1 = 1, 2 \mid \lambda_i$, $i = 2, \dots, 2v$, and hence λ_{2v} to be a multiple of 2 $(4t + 1)$. Since $\lambda_i \mid \lambda_{i+1}$ for all i, we have:

COROLLARY 1. *The Smith normal form S of a D-optimal design of order* $2v = 4t + 2$ *where* $4t + 1$ *is square free, t odd, has the form*

$$\left(1,(2)^{2t+1},(2t)^{2t-1},2t(4t+1)\right). \tag{15}$$

COROLLARY 2. *The Smith normal form S of a D-optimal design of order* $2v = 4t + 2$ *where* $4t + 1$ *is square free, t even, has the form*

$$\left(1,(2)^{\zeta},(4)^{\mu},(2t)^{4t-\zeta-\mu},2t(4t+1)\right). \tag{16}$$

LEMMA 4. *The Smith normal form of the first half of the D-optimal design given in* (2) *is given by*

$$\operatorname{diag}(XX^T + YY^T) = \left(2, \{2(v-1)\}^{v-2}, 2(v-1)(2v-1)\right),$$

and

$$\operatorname{diag}(XX^T + YY^T)^{-1} = \frac{1}{2(v-1)(2v-1)}\left(1, (2v-1)^{v-2}, (v-1)(2v-1)\right). \qquad \blacksquare$$

The results, calculated by computer using Matlab and Mathematica, for $2v < 100$ are given in Table 1, where the matrices X and Y are circulant, i.e., the corresponding D-optimal design is of circulant type, except for the case $2v = 18$, where we have two nonequivalent D-optimal designs that are not of circulant type.

4. SOME DIAGONALIZING CALCULATIONS

Suppose P and Q are integer matrices (or matrices over the appropriate Euclidean domain) with determinant 1 such that $PXQ = S$, the Smith normal form of X. We write the D-optimal design in the form (2) above.

We note that, since M given in (2) is a D-optimal design,

$$XY = YX \quad \text{and} \quad XY^T = Y^TX,$$

hence, pre- and postmultiplying by Y^{-1}, X^{-1}, and $(Y^T)^{-1}$ and transposing, we see that

$$Y^{-1}X = XY^{-1}, \qquad X^{-1}Y = YX^{-1},$$

$$X^T(Y^T)^{-1} = (Y^T)^{-1}X^T, \quad \text{and} \quad X^TY = YX^T.$$

Write $Z = XX^T + YY^T$.

TABLE 1
THE SMITH NORMAL FORM OF D-OPTIMAL DESIGNS OF SIZE < 100

$2v$	t	$[\log_2(2v-1)]+1$	Smith normal form	Comment
6	1	3	$\{1,(2)^4,10\}$	Unique [6].
10	2	4	$\{1,(2)^5,(4)^2,12,12\}$	Unique [6].
14	3	4	$\{1,(2)^7,(6)^5,78\}$	Unique [6].
18	4	5	$\{1,(2)^7,(4)^4,(8)^5,136\}$	Cohn [2] class 2.
18	4	5	$\{1,(2)^8,(4)^2,(8)^6,136\}$	Cohn [2] class 1.
18	4	5	$\{1,(2)^9,(8)^7,136\}$	Cohn [2] class 3.
22				Does not exist.
26	6	5	$\{1,(2)^{13},(12)^{11},300\}$	The first two equivalence classes from [6].[a]
26	6	5	$\{1,(2)^{13},(12)^{10},60,60\}$	The third equivalence class from [6]
30	7	5	$\{1,(2)^{15},(14)^{13},406\}$	$4t+1$ square free.[a]
34				Does not exist.
38	9	6	$\{1,(2)^{19},(18)^{17},666\}$	$4t+1$ square free.[a]
42	10	6	$\{1,(2)^{21},(20)^{19},820\}$	$4t+1$ square free.[a]
46	11	6	$\{1,(2)^{23},(22)^{20},66,330\}$	
50	12	6	$\{1,(2)^{25},(24)^{23},168,168\}$	
54	13	6	$\{1,(2)^{27},(26)^{25},1378\}$	$4t+1$ square free.[a]
58				Does not exist.
62	15	6	$\{1,(2)^{31},(30)^{29},1830\}$	$4t+1$ square free.[a]
66	16	7	$\{1,(2)^{33},(32)^{31},2080\}$	$4t+1$ square free.[a]
70				Does not exist.
74	18	7	$\{1,(2)^{37},(36)^{35},2628\}$	$4t+1$ square free.[a]
78				Does not exist.
82	20	7	$\{1,(2)^{41},(36)^{38},360,360\}$	
86	21	7	$\{1,(2)^{43},(42)^{41},3570\}$	$4t+1$ square free.[a]
90	22	7	$\{1,(2)^{45},(44)^{43},3916\}$	$4t+1$ square free.[a]
94				Does not exist.
98	24	7	$\{1,(2)^{49},(48)^{47},4656\}$	$4t+1$ square free.[a]

[a] The SNF is $(1,2,\ldots(2t+1 \text{ times})\ldots,2,2t,\ldots(2t-1 \text{ times})\ldots,2t,2t(4t+1))$.

Now consider

$$\begin{pmatrix} PX^TY^{-1}P^{-1} & -I \\ I & PX(Y^T)^{-1}P^{-1} \end{pmatrix}\begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix}\begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix}\begin{pmatrix} Q & 0 \\ 0 & Q \end{pmatrix}$$

$$= \begin{pmatrix} PX^TY^{-1} & -P \\ P & PX(Y^T)^{-1} \end{pmatrix}\begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix}\begin{pmatrix} Q & 0 \\ 0 & Q \end{pmatrix}$$

$$= \begin{pmatrix} PX^TY^{-1}X + PY^T & PX^T - PX^T \\ 0 & PY + PX(Y^T)^{-1}X^T \end{pmatrix} \begin{pmatrix} Q & 0 \\ 0 & Q \end{pmatrix}$$

$$= \begin{pmatrix} P(X^TX + Y^TY)Y^{-1}Q & 0 \\ 0 & P(YY^T + XX^T)(Y^T)^{-1}Q \end{pmatrix}.$$

This simplifies to

$$\frac{1}{2(v-1)(2v-1)}$$

$$\begin{pmatrix} P((2v-1)I - J)Y^{-1}Q & 0 \\ 0 & P((2v-1)I - J)(Y^T)^{-1}Q \end{pmatrix}.$$

This will have Smith normal form of type

$$\begin{pmatrix} \mathcal{Q} & 0 \\ 0 & \mathcal{Q} \end{pmatrix}.$$

If D in (2) is permuted to give

$$E = \begin{pmatrix} Y & X \\ -X & Y \end{pmatrix}$$

which clearly has the same Smith normal form, as only elementary operations have been performed, then E will have the Smith normal form

$$\begin{pmatrix} \mathcal{Q}_1 & 0 \\ 0 & \mathcal{Q}_1 \end{pmatrix}.$$

We note

$$\begin{pmatrix} X & Y \\ -Y^T & X^T \end{pmatrix}^{-1}$$

$$= \begin{pmatrix} \left(X + Y(X^T)^{-1}Y^T\right)^{-1} & -(Y^T + X^TY^{-1}X)^{-1} \\ (X^T)^{-1}Y^T\left(X + Y(X^T)^{-1}Y^T\right)^{-1} & Y^{-1}X(Y^T + X^TY^{-1}X)^{-1} \end{pmatrix},$$

$$= \begin{pmatrix} X^TZ^{-1} & -YZ^{-1} \\ Y^TZ^{-1} & XZ^{-1} \end{pmatrix},$$

so

$$D^{-1} = D^T\begin{pmatrix} Z^{-1} & 0 \\ 0 & Z^{-1} \end{pmatrix}.$$

It may be possible using these results to obtain formulae connecting the Smith normal forms of D and D^{-1}.

We now consider the Smith normal form of the matrix

$$B = \begin{pmatrix} X & X \\ -X & X \end{pmatrix}.$$

We say that if $S = PXQ$ is the SNF of X, then B is **Z**-equivalent to

$$C = \begin{pmatrix} S & 0 \\ 0 & 2S \end{pmatrix}.$$

However, if the elements of S are $\lambda_1, \dots, \lambda_n$ and the elements of C are $\lambda_1, \dots, \lambda_n$, $\lambda_{n+1} = 2\lambda_1, \dots, \lambda_{n+i} = 2\lambda_i, \dots, \lambda_{2n} = 2\lambda_n$, then C may not be an SNF, as we cannot be certain that $\lambda_j \mid \lambda_{j+1}$ for all $j = 1, \dots, 2n - 1$.

Suppose $\lambda_k \nmid \lambda_{k+1}$. Then proceed, as in [7, pp. 40–43], to consider

$$\begin{pmatrix} \lambda_k & 0 \\ 0 & \lambda_{k+1} \end{pmatrix} \sim \begin{pmatrix} \lambda_k & 0 \\ \lambda_{k+1} & \lambda_{k+1} \end{pmatrix}.$$

LEMMA 5. *If* $\lambda_{k+1} > \lambda_k$ *then*

$$\begin{pmatrix} \lambda_{k+1} & 0 \\ 0 & \lambda_k \end{pmatrix} \sim \begin{pmatrix} \lambda_k & 0 \\ 0 & \lambda_{k+1} \end{pmatrix}.$$

LEMMA 6. *If* $g = \gcd(\lambda_k, \lambda_{k+1})$ *and* $\lambda_k \nmid \lambda_{k+1}$, $\lambda_k < \lambda_{k+1}$, *then*

$$C = (c_{ij}) = \begin{pmatrix} \lambda_k & 0 \\ 0 & \lambda_{k+1} \end{pmatrix} \sim \begin{pmatrix} \lambda_k/g & 0 \\ 0 & g\lambda_{k+1} \end{pmatrix},$$

where $\sim$ *denotes* **Z***-equivalence or equivalence over the Euclidean domain using elementary operations.*

Proof. Proceed via the following steps:

(i) add column 2 to column 1;

(ii) subtract $l_i = [c_{21}/c_{11}]$ (the integer part of c_{21}/c_{11}) copies of row 1 from row 2;

(iii) subtract $l_{i+1} = [c_{11}/(c_{21} - l_i c_{11})]$ copies of row 2 from row 1, and increase i by two;

(iv) repeat steps (ii) and (iii) until the gcd (or λ_k/g) occurs in either c_{11} or c_{21}, and 0 in the other position.

So we have, since the determinant remains unchanged

$$\begin{pmatrix} g & 0 \\ 0 & \lambda_k \lambda_{k+1}/g \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \lambda_k/g & 0 \\ 0 & g\lambda_{k+1} \end{pmatrix}. \qquad \blacksquare$$

LEMMA 7. *Suppose the D-optimal design has the form*

$$B = \begin{pmatrix} A & A \\ A & -A \end{pmatrix}$$

where A has SNF

$$\big(1, \underbrace{2, \dots, 2}_{2t}, \underbrace{2t, \dots, 2t}_{2t-1}, 2t(4t+1)\big).$$

Then B has SNF

$$\big(1, \underbrace{2, \dots, 2}_{4t+1}, \underbrace{4t, \dots, 4t}_{4t-2}, 4t(4t+1), 4t(4t+1)\big).$$

Proof. From the above we have that $\operatorname{diag}(B) = \operatorname{diag}(A) \oplus 2\operatorname{diag}(A)$, giving

$$\operatorname{diag}(B) \sim \Big(1, \underbrace{2,\dots,2}_{2t}, \underbrace{2t,\dots,2t}_{2t-1}, 2t(4t+1), 2, \underbrace{4,\dots,4}_{2t}, \underbrace{4t,\dots,4t}_{2t-1}, 4t(4t+1)\Big).$$

Without loss of generality we rewrite this in ascending order as

$$\operatorname{diag}(B) \sim \Big(1, \underbrace{2,\dots,2}_{2t+1}, \underbrace{4,\dots,4}_{2t}, \underbrace{2t,\dots,2t}_{2t-1}, \underbrace{4t,\dots,4t}_{2t-1}, 2t(4t+1), 4t(4t+1)\Big).$$

We note that $4t$ does not divide $2t(4t+1)$ and 4 does not divide $2t$. Hence, proceeding as in Lemmas 5 and 6, we replace them by $2t$ and $4t(4t+1)$ and by 2 and $4t$, respectively. We repeat this operation until no 4's remain and then reorder the entries, obtaining the SNF of the enunciation. ■

EXAMPLE 1. For orders 5 and 13 use the following sequences, where — represents -1, for the circulant matrices A in the previous lemma:

$$(-\ 1\ 1\ 1\ 1) \quad \text{and} \quad (1\ 1\ 1\ 1\ 1\ -\ 1\ -\ -\ 1\ 1\ 1\ -).$$

Now the SNF of the circulant matrix with first row (— 1 1 1 1) is $(1,2,2,2,6)$. So $\operatorname{diag}(B)$ is $(1,2,2,2,6,2,4,4,4,12)$, and proceeding as in the previous lemma we find $\operatorname{diag}(B) = (1,2,2,2,2,4,4,4,6,12)$, and the SNF is

$$(1,2,2,2,2,2,4,4,12,12).$$

Since the SNF of the circulant matrix with first row

$$(1\ 1\ 1\ 1\ 1\ -\ 1\ -\ -\ 1\ 1\ 1\ -)$$

is $(1,2,2,2,2,2,2,6,6,6,6,6,30)$ or $(1,(2)^6,(6)^5,30)$, we have

$$\operatorname{diag}(B) = \Big(1, \underbrace{2,\dots,2}_{6}, \underbrace{6,\dots,6}_{5}, 30, 2, \underbrace{4,\dots,4}_{6}, \underbrace{12,\dots,12}_{5}, 60\Big),$$

and so

$$\operatorname{diag}(B) = \Big(1, \underbrace{2,\ldots,2}_{7}, \underbrace{4,\ldots,4}_{6}, \underbrace{6,\ldots,6}_{5}, \underbrace{12,\ldots,12}_{5}, 30, 60\Big).$$

Thus, using the lemma, we obtain

$$\operatorname{diag}(B) = \Big(1, \underbrace{2,\ldots,2}_{12}, 4, \underbrace{12,\ldots,12}_{9}, 6, 60, 60\Big),$$

and thus the SNF of B is

$$\Big(1, \underbrace{2,\ldots,2}_{13}, \underbrace{12,\ldots,12}_{10}, 60, 60\Big).$$

REMARK 3. We note when $4t + 1$ is not square free, the Smith normal form S of a D-optimal design of order $2v$ has the form

$$\big(1, (2)^{2t+1}, (2t)^{2t-2}, x, y\big)$$

with $xy = (2v - 1)(v - 1)^2$. For $t = 2$ and 6 we found, by computer, that $x = y = (v - 1)\sqrt{2v - 1} = t(t + 4)$.

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