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 Smith normal form 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.

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1 Introduction

The general question which gave rise to the present paper is the question of isomorphism of D-optimal designs. Theoretically it is enough to check $(n!)^2$ 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 (written $B \sim A$) if $B = PAQ$ for some 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, p41] and Marcus and Minc [8, p44].

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*

$$D = \mathrm{diag}(a_1,\ a_2,\ \cdots\ ,\ a_r,\ 0,\ \cdots\ ,\ 0),$$

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

$$a_1 a_2 \cdots a_i.$$

If $A \sim E$ *where*

$$E = \mathrm{diag}(a_1,\ a_2,\ \cdots\ ,\ a_i) \oplus\ F$$

then a_{i+1} *is the greatest common divisor of the non-zero 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 $2v \equiv\ 2\ mod\ 4$ and X, Y are $v \times v$ commuting 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 1s, 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 *or 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

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

we have $PMQ = N$. □

Now form the two sets $A = \{a_1, a_2, \ldots, a_r\}$ and $B = \{b_1, b_2, \ldots, b_s\}$ where a_i, b_j denote the positions of -1s in the first row of X, Y respectively.
If the matrices X, Y are circulant, then they satisfy (2) 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 $s \geq r \geq 0$ 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 $0 \leq \ a,\ b \ \leq v - 1$.

Now simple row and column operations can be used to show

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

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

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

We assert

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

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

$$\left(B^{T^{-1}}\right) AA^T = I, \qquad \text{and } \left(A^T B^{-1}\right) A = I. \tag{6}$$

Hence

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

and

$$A^T A = aI \ + \ \frac{b}{a + bv} A^T J A.$$

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

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

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

$$D^T C^{-1} D = I,$$

and

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

Lemma 2 *Suppose*

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

and $X^T J = XJ = xJ$, $Y^T J = YJ = yJ$. *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 $XX^T J \; + \; YY^T J = (x^2 \; + \; y^2) J_v = (a \; + \; bv) J_v$. 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

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

□

Remark 1 We recall here that

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

so for X, Y from a D-optimal design

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

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 the previous lemma 2 to obtain

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

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

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

This gives the required result. □

3 The Number of Small Invariants

If 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 two. We write $[x]$ for the largest integer not exceeding x. We use a result of Wallis quoted in [12, p411]

Theorem 3 (W.D.Wallis) *Suppose E is a $v \times v$ matrix with non-zero determinant whose entries are all 0 and 1 the identity elements of the Euclidean domain,* **Z**. *Then the number of invariants of E under* **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 through any column 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' theorem and has at least $[log_2\ (2v-1)] + 1$ equal elements (here 2) in its normalization over the Euclidean domain **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,

$$D = \mathrm{diag}(\lambda_1,\ \lambda_2,\ \ldots\ ,\ \lambda_{2v}),$$

such that $S \sim D$ and $\lambda_i \mid \lambda_{i+1}$ where the λ_i are non negative 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 $\lambda_1 = 1, \lambda_2 = 2, \ldots, \lambda_{[log_2\ (2v-1)]+2} = 2, \ldots, \lambda_{2v} = 2t^a(4t+1)$ for some a.

Notation 1 In order to simplify writing we will hence forth use the notation $(x)^t$ to denote t copies of x or $x,\ x, \cdots,\ x$ (t times). So that

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

will be denoted

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

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 5 elements in the Smith normal form which are 2. This leads us to the possibilities

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

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 non-equivalent D-optimal designs one of which is of circulant type, see also Cohn [2], so the possibilities $\zeta = 5$ or 6 are not realized.

If we use the following matrices in (2)

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

where $-$ represents -1, then the SNF of the corresponding D-optimal design is

$$(1,\ (2)^7,\ (4)^4,\ (8)^5, 136).$$

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 is

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

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, we obtain the SNF

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

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

$$S = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{2v})$$

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

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

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

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

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

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

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

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

and

$$\mathrm{diag}(XX^T + YY^T)^{-1}$$
$$= \frac{1}{2(v-1)(2v-1)}(1,\ (2v-1)^{v-2},\ (v-1)(2v-1)).$$

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.

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 post multiplying by Y^{-1}, X^{-1} and $(Y^T)^{-1}$ and transposing we see

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

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

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, E will have the Smith normal form

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

□

We note

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

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

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

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 $\mathbf{Z}$-equivalent to

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

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

Suppose $\lambda_k \not| \lambda_{k+1}$ then we 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 $\lambda_k \not| \lambda_{k+1}$, $\lambda_k < \lambda_{k+1}$ 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 two to column one;

(ii) subtract $\ell_i = \lceil \frac{c_{21}}{c_{11}} \rceil$ (the integer part of $\frac{c_{21}}{c_{11}}$) copies of row one from row two;

(iii) subtract $\ell_{i+1} = \lceil \frac{c_{11}}{c_{21} - \ell_i c_{11}} \rceil$ copies of row two from row one, 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:

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

□

Lemma 7 *Suppose the D-optimal design has the form* $B = \begin{pmatrix} A & A \\ A & -A \end{pmatrix}$ *where A has SNF*

$$(1, \underbrace{2, \cdots, 2}_{2t}, \underbrace{2t, \cdots, 2t}_{2t-1}, 2t(4t+1))$$

Then B has SNF

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

Proof. From above we have that $\mathrm{diag}(B) = \mathrm{diag}(A) \bigoplus 2{\cdot}\mathrm{diag}(A)$. Giving

$$\mathrm{diag(B)} \simeq (1, \underbrace{2, \cdots, 2}_{2t}, \underbrace{2t, \cdots, 2t}_{2t-1}, 2t(4t+1), 2, \underbrace{4, \cdots, 4}_{2t}, \underbrace{4t, \cdots, 4t}_{2t-1}, 4t(4t+1)).$$

Without loss of generality we rewrite this in ascending order as

$$\mathrm{diag(B)} \simeq (1, \underbrace{2, \cdots, 2}_{2t+1}, \underbrace{4, \cdots, 4}_{2t}, \underbrace{2t, \ldots, 2t}_{2t-1}, \underbrace{4t, \ldots, 4t}_{2t-1}, 2t(4t+1), 4t(4t+1)).$$

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 2 and $4t$ respectively. We repeat this operation until no fours 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 diag(B) is $(1, 2, 2, 2, 6, 2, 4, 4, 4, 12)$ and proceeding as in the previous lemma we find 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

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

and so

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

Thus, using the lemma we obtain

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

and thus the SNF of B is

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

□

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

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

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

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

Table 1: The Smith normal form of D-optimal designs of Size < 100.
$*$ The SNF is $(1,2,\cdots(2t+1 \text{ times})\cdots,2,2t,\cdots(2t-1 \text{ times})\cdots,2t,2t(4t+1))$

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