



An Overview of Two-level Supersaturated Designs with Cyclic Structure

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Abstract

An overview is given of the link between the k -circulant method of construction of two-level supersaturated designs and construction methods based on cyclic incomplete block designs. It is shown that this link enables a simple formula for the Es^2 -efficiency of all such designs to be derived. Generators are given for Es^2 -optimal and near-optimal designs that extend the range of previously known designs or that have a smaller number of highly correlated column pairs.

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1. Introduction

The goal of a screening experiment is to identify the few most “active” factors from a very large number of potentially important factors. Supersaturated designs have been advocated for screening when relatively few observations can be taken and when it can be assumed that the factor main effects will be much larger than the interactions. Some supersaturated designs allow interactions to be investigated but, usually, main effect models are fitted.

Various methods of analysis of supersaturated designs have been investigated in the literature. Frequentist methods include forward selection and stepwise regression (Westfall, Young and Lin, 1998; Abraham, Chipman and Vijayan, 1999; Kelly and Voelkel, (2000), penalized least squares methods (Lin, 1995; Li and Lin, 2002), the Dantzig selector (Phoa,

Pan and Xu, 2007). Bayesian methods that can be used for analysing supersaturated designs have been investigated by Chipman, Hamada and Wu (1997); Beattie, Fong and Lin, (2002) Meyer and Wilkinson, (1998), among others.

In trying to extract information about a large number of factor main effects from very few observations, it is inevitable that the chance of mis-identifying the most important effects can be fairly high. This is due to the fact that main effect estimates are correlated and sometimes more than one model fits the data equally well. To minimize mistakes, it is advisable to use designs with main effect contrast correlations as small as possible. Chen and Lin (1998) and Liu, Ruan and Dean (2006) suggest that a maximum correlation of 0.333 is desirable, but this cannot always be achieved for very large numbers of factors. However, provided that there are very few active factors (factor sparsity, see Box and Meyer, 1986) and provided that important effects are very large, it appears possible to identify most of the active factors, in general.

Supersaturated designs were introduced by Satterthwaite (1959) in terms of random balance designs. The first systematic study of the construction of efficient supersaturated designs was given by Booth and Cox (1962) who defined several criteria, including minimization of Es^2 (or $\text{ave}(s^2)$) and minimization of maximum column correlation, for evaluating and comparing designs. In recent years, the construction and analysis of supersaturated designs has been an especially active area of research. Construction methods based on Hadamard matrices have been investigated, for example, by Lin (1993), Wu (1993) Tang and Wu (1997), Cheng (1997), Butler, Mead, Eskridge and Gilmour (2001); methods based on balanced incomplete block designs have been discussed by Nguyen (1996), Cheng (1997), Bulutoglu and Cheng (2004); computer algorithmic methods have been employed by Lin (1995), Nguyen (1996), Li and Wu, (1997), and Bulutoglu and Cheng (2004); cyclic methods of construction have been explored, for example, by Liu and Zhang (2000), Eskridge, Gilmour, Mead, Butler and Travnicsek (2004), Liu and Dean (2004), and Georgiou (2008). All of the designs listed in the above papers are optimal or highly efficient under the Es^2 criterion. Cheng (1997), Butler, Mead, Eskridge and Gilmour (2001), and Bulutoglu and Cheng (2004) give fairly complete solutions to a wide range of Es^2 -optimal supersaturated designs with number of runs n a multiple of 4 and also $n = 10, 14, 18$ for a wide range of numbers of factors m .

In this paper, we concentrate on the link between cyclic methods of construction of n -run supersaturated designs with $m = k(n - 1)$ two-level factors (for any specified integer k). The method described by Nguyen (1996) for construction of Es^2 -optimal supersaturated designs was to adjoin the incidence matrices of pairs of cyclic balanced incomplete block designs (BIBD). An extension of this method was discussed by Eskridge, Gilmour, Mead, Bultler and Travnicsek (2004), where the incidence matrices of regular graph designs as well as balanced incomplete block designs were used. Liu and Zhang (2000) developed an algorithm for constructing Es^2 -optimal supersaturated designs from cyclic BIBDs. A related method based on cyclic generators was given by Liu and Dean (2004). The link between these construction methods is explored in Section 3 and is exploited in Section 4 to give a simple formula for the Es^2 -efficiency of all such designs. Cyclic generators are given for Es^2 -optimal and near-optimal designs that extend the range of previously known designs, or that have a smaller number of highly correlated pairs of columns.

Since this paper concentrates on cyclic generation of supersaturated designs, it does not cover all the known Es^2 -optimal designs. In particular Es^2 -optimal designs based on non-

2 cyclic Hadamard matrices and incomplete block designs are not covered. Various non-cyclic
 solutions for Es^2 -optimal supersaturated designs for ranges of n and m have been provided
 by Butler, Mead, Eskridge and Gilmour (2001), Bulutoglu and Cheng (2004), Ryan and
 4 Bulutoglu (2007) and Das, Dey, Chan and Chatterjee (2008).

2. Bounds for Es^2 -efficiency

6 We represent a supersaturated design d with two-level factors by a “design matrix” or
 “treatment matrix”, T , whose rows represent the n treatment combinations to be observed
 8 and whose columns designate the m factors to be examined. The (i, f) th element of T
 determines the level at which factor f is to be observed in the i th observation or “run”. We
 10 code the high and low levels of each factor as $+1$ and -1 in T , and abbreviate these to
 “ $+$ ” and “ $-$ ” where convenient. For mean-orthogonal two-level designs, where the levels
 12 of each factor are observed the same number of times, the columns of T coincide with main
 effect contrasts. We will use the standard main effects model

14
$$Y = X\phi + \varepsilon$$

where $X = [\mathbf{1}_n \ T]$ and $\mathbf{1}_n$ denotes the n -dimensional column vector with all entries equal
 16 to 1; ϕ is a vector containing the mean and main effect parameters and ε is a vector of n
 independent and identically distributed normal random variables with mean zero and variance
 18 σ^2 . The information matrix for estimating ϕ is

$$\begin{bmatrix} n & 0 \\ 0 & T'T \end{bmatrix}.$$

20 Let s_{ij} be the element in the i th row and j th column of $T'T$ ($i, j = 1, \dots, m$). Then,
 $s_{ij} = t_i't_j$, where t_i and t_j are, respectively, the columns i and j of T . If $s_{ij} = 0$, the i th and j th
 22 main effect contrasts are orthogonal and can be estimated independently. If n is even, but
 not a multiple of 4, then s_{ij} cannot equal 0 and the main effect contrasts for factors i and j
 24 will be said to be nearly orthogonal if s_{ij} is close to 0 (that is, $s_{ij} = \pm 2$ when $n \equiv 2(\text{mod}4)$).
 When $s_{ij} = \pm n$ then the main effects of factors i and j are completely aliased, and such
 26 designs are usually avoided.

Booth and Cox (1962) proposed as a criterion for comparing designs the minimization of
 28 the average correlation between the main effect contrasts, called $ave(s^2)$, or Es^2 , where

$$Es^2 = \sum_{1 \leq i < j \leq m} s_{ij}^2 / \binom{m}{2}. \tag{2.1}$$

30 A supersaturated design is said to be Es^2 -optimal if no other design of the same size has
 higher Es^2 -efficiency, defined as LB/Es^2 , where LB is an appropriate lower bound for Es^2
 32 as discussed below. Although minimizing Es^2 (which is a function of the entries of $T'T$)
 is not identical to the criterion of minimizing the average correlation between the contrast
 34 estimators (which is a function of the entries of $[X'X]^{-1}$), it does lead to highly efficient
 designs under this latter criterion provided that the designs are mean-orthogonal.

36 Lower bounds for Es^2 for supersaturated designs with n runs and $m = k(n - 1)$ factors

have been derived for $n \equiv 0 \pmod{4}$ by Nguyen (1996) and Tang and Wu (1997), and bounds for other values of n and m have been given by Cheng (1997), Butler, Mead, Estridge and Gilmour (2001), and Das, Dey, Chan and Chatterjee (2008). Using the results of these papers for the designs discussed here, with $m = k(n-1)$ factors ($k > 1$), we have the following lower bounds for Es^2 :

(i) Nguyen (1996), Tang and Wu (1997), Cheng (1997).

If $n \equiv 0 \pmod{4}$ with any $k > 1$ or if $n \equiv 2 \pmod{4}$ with k even, then

$$Es^2 \geq LB = \frac{m-n+1}{(m-1)(n-1)}n^2. \quad (2.2)$$

(ii) Das et al. (2008).

If $n \equiv 2 \pmod{4}$ with k odd, then

$$Es^2 \geq \max\{LB, 4\}, \quad \text{where } LB = \frac{n^2(m-n+1)}{(m-1)(n-1)} + \frac{2n^2-4n+x}{m(m-1)} \quad (2.3)$$

and $x = 32$ if $\left\{ \frac{m-1-2i}{4} + \left\lceil \frac{m+(1+2i)(n-1)}{4(n-1)} \right\rceil \right\} \equiv (1-i) \pmod{2}$ for $i = 0$ or 1 , and $[\cdot]$ denotes integer part. Otherwise, $x = 0$. It can be shown that, for $k \geq 3$, $LB > 4$ so that the bound is given by (2.3).

3. Cyclic construction methods

3.1. Cyclic generators

The cyclic construction method used by Plackett and Burman (1946) for orthogonal saturated designs was generalized by Liu and Dean (2004) to obtain a class of supersaturated designs called *k-circulant designs*. A *k-circulant design* with $n = 2t$ runs (for t an integer) and $m = k(n-1)$ factors each having two levels is constructed by cycling elements of a generator $G = (g_1, \dots, g_m)$ containing kt elements equal to -1 and $k(t-1)$ elements equal to $+1$, where the cycling is done k elements at a time. A row of $+1$'s is added to the resulting $(n-1) \times m$ array D to give the supersaturated design matrix $T = [D', \mathbf{1}_{k(n-1)}]'$. The generators listed by Liu and Dean (2004) give rise to designs that are mean-orthogonal and which are either Es^2 -optimal or have at least 96.4% efficiency. The following three results summarize the links between *k-circulant designs*, the concatenation of k individual saturated cyclic (1-circulant) designs and the designs of Nguyen (1996), Eskridge, Gilmour, Mead, Butler and Travnicsek (2004), and Bulutoglu and Cheng (2004) formed from the incidence matrices of cyclic incomplete block designs. These links are illustrated in Example 3.1.

Result 3.1 (Liu and Dean, 2004, Section 3). *Any k-circulant mean-orthogonal supersaturated design $T = [D', \mathbf{1}]'$ with $n = 2t$ runs, $m = k(n-1)$ factors and generator $G = (g_1, g_2, \dots, g_m)$ is equivalent to the concatenation of k individual 1-circulant designs, T_1, T_2, \dots, T_k , each having $(n-1)$ factors, where the i th design $T_i = [D'_i, \mathbf{1}_{n-1}]'$ is obtained by cycling the elements of the generator $G_i = (g_i, g_{i+k}, g_{i+2k}, \dots, g_{i+(n-2)k})$ and adding a row of 1 's, ($i = 1, \dots, k$).*

2 Result 3.1, together with expression (2) of Eskridge, Gilmour, Mead, Butler and Travnicsek
 (2001) leads to the following result.

4 **Result 3.2.** Any k -circulant supersaturated design matrix $T = [D', \mathbf{1}_{k(n-1)}]'$ with $n = 2t$
 runs and $m = k(n - 1)$ factors and generator $G = (g_1, g_2, \dots, g_m)$ can be obtained from the
 6 incidence matrix, $N = [N_1, \dots, N_k]$ of an incomplete block design consisting of k cyclic sub-
 designs with $n - 1$ blocks each, where the i th subdesign ($1 \leq i \leq k$) has circulant incidence
 matrix N_i with first row

8
$$2^{-1} (1 + g_i, 1 + g_{i+k}, 1 + g_{i+2k}, \dots, 1 + g_{i+(n-2)k}) .$$

Then $D = 2N - \mathbf{1}_{n-1} \mathbf{1}'_m$.

10 The third result links Es^2 -optimality of certain k -circulant designs and the existence of bal-
 anced incomplete block designs.

12 **Result 3.3** (Cheng, 1997, Section 2). The incomplete block design in Result 3.2 with in-
 cidence matrix N is a balanced incomplete block design if and only if the corresponding
 14 k -circulant design T is Es^2 -optimal attaining bound (2.2).

Example 3.1. Consider the 3-circulant Es^2 -optimal supersaturated design with $n = 12 = 2t$
 16 ($t = 6$) experimental runs and $m = 33 = (2t - 1)k$ factors listed in Table 4 of Liu and Dean
 (2004). The listed generator has $kt = 18$ elements equal to -1 and $k(t - 1) = 15$ elements
 18 equal to 1 , as follows

$$G = (- - - - - - - - - - + + + - - - + + + + - + - + - - + + + + +) .$$

20 Cycling $k = 3$ elements at a time gives an Es^2 -optimal 3-circulant supersaturated design
 with maximum column correlation $r_{max} = (\max |s_{ij}|) / n = 0.67$ and $Es^2 = 9$. If the columns
 22 of the design are rearranged into the following order:

$$1, 4, 7, \dots, 31; 2, 5, \dots, 32; 3, 6, \dots, 33;$$

24 the design can be seen to be the concatenation of $k = 3$ separate cyclic (1-circulant) designs
 with respective generators

26
$$G_1 = (- - - - + - + - + + +)$$

$$G_2 = (- - - - + - + + - + +)$$

 28
$$G_3 = (- - - + - + + - - + +)$$

where G_i consists of elements $i, i + 3, i + 6, \dots, i + 30$ of G . The generators can further be
 30 rewritten by noting the positions which hold $+1$, that is the positions in the first rows of the
 cyclic subarrays that hold $+1$:

32
$$G_1^{(R)} = (5, 7, 9, 10, 11); \quad G_2^{(R)} = (5, 7, 8, 10, 11); \quad G_3^{(R)} = (4, 6, 7, 10, 11) .$$

34 Arrays that are formed by cycling the rows may also be obtained by cycling the columns, so
 we may rewrite the i th generator in terms of the $(t - 1)$ positions $p_{i1}, \dots, p_{i,t-1}$ of the first
 column of array i which contain $+1$. Then, $p_{ij} = (n + 1) - a_{ij}$, where a_{ij} is the j th column

entry in $G_i^{(R)}$. Thus, with $n = 12$, the three generators become

$$G_1^{(C)} = (8, 6, 4, 3, 2); \quad G_2^{(C)} = (8, 6, 5, 3, 2); \quad G_3^{(C)} = (9, 7, 6, 3, 2).$$

In this form the generators can be regarded as the initial blocks of cyclic subdesigns with $v = 11$ treatments (coded $1, 2, \dots, 11$) and $b = 11$ blocks of size 5. This is the notation used by Liu and Zhang (2000), Butler, Mead, Eskridge and Gilmour (2001), and Eskridge, Gilmour, Mead, Butler and Travnicek (2004), after subtracting 1 from each entry. It can be verified that the three subdesigns, taken together, form a balanced incomplete block design with 33 blocks of size 5.

3.2. The autocorrelation function

Liu and Dean (2004, Theorem 3.2) showed that the elements s_{ij} of $T'T$ can be written in terms of the elements of the generators of the k -circulant design T . In Lemma 3.1, we express this result in terms of the periodic autocorrelation functions, defined below, which are used in Section 4 for the construction of Es^2 -optimal and near optimal designs.

Let A be a (finite) sequence of ℓ real numbers $\{a_0, a_1, \dots, a_{\ell-1}\}$. The *periodic autocorrelation function* $P_A(x)$ is defined by

$$P_A(x) = \sum_{q=0}^{\ell-1} a_q a_{q+x}, \quad x = 0, 1, \dots, [\ell/2] \quad (3.1)$$

$$P_A(x) = P_A(\ell - x)$$

where $q + x$ is reduced modulo ℓ and $[z]$ is the integer part of z .

Lemma 3.1. *Let T be a design matrix of the form $T = [D', \mathbf{1}]'$, where D is a 1-circulant matrix with generator $G = (g_1, g_2, \dots, g_{n-1})$. Then, the (i, j) th element s_{ij} of the matrix $T'T$ can be expressed in terms of the generator elements as*

$$s_{ij} = 1 + \sum_{q=0}^{n-2} g_{q+i} g_{q+j} = 1 + \sum_{q=0}^{n-2} g_q g_{q+|i-j|} = 1 + P_G(|i-j|), \quad i, j = 1, 2, \dots, n-1,$$

where g_0 is defined to be g_{n-1} . Also,

$$s_{q+i, q+j} = s_{ij}; \quad i, j = 1, 2, \dots, (n-1); \quad q = 0, 1, \dots, (n-2),$$

where, if $q + x > n - 1$ then it is replaced by $q + x - (n - 1)$.

In Theorem 3.1, we generate a k -circulant supersaturated design by concatenating k 1-circulant designs and show how the value of s_{ij} can be calculated by using the generators of the k individual 1-circulant design matrices.

Theorem 3.1. *Suppose that D_z is a 1-circulant matrix with first row $G_z = (g_1^{(z)}, g_2^{(z)}, \dots, g_{n-1}^{(z)})$, $g_j^{(z)} \in \{1, -1\}$, $z = 1, 2, \dots, k$, $j = 1, 2, \dots, n-1$ and $n = 2t$, $t > 0$. Denote by T , the k -*

circulant mean-orthogonal supersaturated design defined by

$$T = \begin{bmatrix} D & & & \\ & \mathbf{1}'_{k(n-1)} & & \\ & & D_1 & D_2 & \cdots & D_k \\ & & \mathbf{1}'_{n-1} & \mathbf{1}'_{n-1} & \cdots & \mathbf{1}'_{n-1} \end{bmatrix}. \quad (3.2)$$

The (i, j) th element $1 \leq i, j \leq k(n-1)$ of $T'T$ can be expressed in terms of the generator elements as

$$s_{ij} = 1 + \sum_{u=0}^{n-2} g_{u+a}^{(z)} g_{u+b}^{(w)},$$

where z, w are the unique integers such that $1 \leq z, w \leq k$ and $(z-1)(n-1) < i \leq z(n-1)$, $(w-1)(n-1) < j \leq w(n-1)$, and where $a = i - (z-1)(n-1)$ and $b = j - (w-1)(n-1)$.

Proof. The proof follows from Lemma 3.1. □

Since any p -circulant supersaturated design is equivalent to concatenating p 1-circulant designs, Theorem 3.1 can be extended by replacing any subset(s) of p 1-circulant matrices D_i by a corresponding p -circulant matrix. The following Theorem 3.2 expresses the periodic autocorrelation function of a k -circulant supersaturated design in terms of the s_{ij} 's (off-diagonal elements of $T'T$).

Theorem 3.2. Let T be an $n \times m$ k -circulant mean-orthogonal supersaturated design with generator $G = \{g_1, g_2, \dots, g_k, g_{k+1}, \dots, g_{2k}, \dots, g_{m-k+1}, \dots, g_m\}$ and $m = k(n-1)$, $n = 2t$, $t > 0$. Then

$$P_G(x) = \sum_{j=1}^k s_{j, j+x} - k, \quad x = 0, 1, \dots, [m/2]. \quad (3.3)$$

Proof. Define $g_0 = g_m$, then

$$\begin{aligned} P_G(x) &= \sum_{i=1}^m g_i g_{i+x} \\ &= \sum_{q=0}^{n-2} g_{qk+1} g_{qk+1+x} + \sum_{q=0}^{n-2} g_{qk+2} g_{qk+2+x} + \cdots + \sum_{q=0}^{n-2} g_{qk+k} g_{qk+k+x} \\ &= \sum_{j=1}^k \left(\sum_{q=0}^{n-2} g_{qk+j} g_{qk+j+x} + 1 \right) - k \\ &= \sum_{j=1}^k s_{j, j+x} - k, \end{aligned}$$

where the last line follows from the fact that $s_{qk+j, qk+j+x} = s_{j, j+x}$, for all $q = 0, 1, \dots, n-2$, and where $k(n-1)$ is subtracted from any subscript greater than $k(n-1)$. □

In Theorem 3.3, we show how the elements of $T'T$ for a mean-orthogonal supersaturated design T are linked to the elements of the concurrence matrix of the dual of the corresponding incomplete block design. Then for the special case of k -circulant mean-orthogonal supersaturated designs, Theorem 3.4 shows the link between the elements of $T'T$ and the

elements of the concurrence matrix of the corresponding incomplete block design. In the theorem, the notation $J_{a,b}$ denotes an $a \times b$ matrix of unit elements. If $a = b$, we write J_a .

Theorem 3.3. Let N be the incidence matrix of the incomplete block design d corresponding to supersaturated design $T = [D', \mathbf{1}_{k(n-1)}]'$ so that $N = [D + J_{(n-1),k(n-1)}]/2$. Let μ_{pq} be the (p, q) th element of the concurrence matrix of the dual of d . Then

$$s_{pq} = 4\mu_{pq} - (n - 4). \quad (3.4)$$

Proof. If N is the incidence matrix of d , then N' is the incidence matrix and $N'N$ is the concurrence matrix of the dual of d (see Street and Street, 1987, Section 2.2). Further

$$\begin{aligned} 4N'N &= D'D + D'J_{(n-1),k(n-1)} + J_{k(n-1),(n-1)}D + J_{k(n-1),(n-1)}J_{(n-1),k(n-1)} \\ &= D'D - J_{k(n-1)} - J_{k(n-1)} + (n-1)J_{k(n-1)} \\ &= D'D + (n-3)J_{k(n-1)}. \end{aligned}$$

Since s_{pq} is the (p, q) th element of $T'T = D'D + J_{k(n-1)}$, it follows that

$$4\mu_{pq} = (s_{pq} - 1) + (n - 3),$$

and the result follows.

Theorem 3.4. Let λ_{pq} be the (p, q) th element of the concurrence matrix NN' of incomplete block design d with incidence matrix $N = [N_1, N_2, \dots, N_k]$, where $N_i = [D_i + J_{n-1}]/2$, corresponding to k -circulant supersaturated design T as given in (3.2). Then

$$4\lambda_{p,q} = \left[\sum_{z=1}^k s_{n-p,n-q}^{(z)} \right] + k(n-4),$$

where $s_{n-p,n-q}^{(z)}$ is element $[(n-p), (n-q)]$ of $(D'_z D_z + J_{n-1})$, $z = 1, \dots, k$.

Proof. Let T be as given in (3.2) and let $N = [D + J_{n-1,k(n-1)}]/2$ be the incidence matrix of the corresponding incomplete block design. Then,

$$\begin{aligned} 4NN' &= [D + J_{n-1,k(n-1)}][D' + J_{k(n-1),n-1}] \\ &= DD' + J_{n-1,k(n-1)}D' + DJ_{k(n-1),n-1} + k(n-1)J_{n-1} \\ &= DD' - kJ_{n-1} - kJ_{n-1} + k(n-1)J_{n-1} \\ &= DD' + k(n-3)J_{n-1}. \end{aligned}$$

Let $r_i^{(z)}$ be the reverse of row i of D_z . Then, due to the cyclic construction of D_z , column $n-i$ of D_z is $c_{n-i}^{(z)} = r_i^{(z)}$. Also, element (p, q) of $D_z D'_z$ is $r_p^{(z)'} r_q^{(z)} = c_{n-p}^{(z)'} c_{n-q}^{(z)}$. Writing $d = [D_1, \dots, D_k]$,

$$4NN' = \sum_{i=1}^k D_i D'_i + k(n-3)J_{n-1}.$$

Then since λ_{pq} is the (p, q) th element of NN' , we have

$$\begin{aligned}
 4\lambda_{pq} - k(n-3) &= \sum_{z=1}^k r_p^{(z)'} r_q^{(z)} \\
 &= \sum_{z=1}^k c_{n-p}^{(z)'} c_{n-q}^{(z)} \\
 &= \sum_{z=1}^k \left(s_{n-p, n-q}^{(z)} - 1 \right)
 \end{aligned}$$

and the result follows. □

4. Compatibility of circulant designs

In order to achieve Es^2 -optimal supersaturated designs by concatenating cyclic saturated designs, we look at the properties of the designs in terms of their autocorrelation functions as follows. Sequences $A_i, i = 1, 2, \dots, k$, of identical length ℓ are called *compatible* if the sum of their periodic autocorrelations is a constant, say γ , except for the 0-th term. That is,

$$\sum_{i=1}^k P_{A_i}(x) = \gamma, \quad \text{for all } x = 1, 2, \dots, [\ell/2]. \tag{4.1}$$

We say that such sequences have *constant periodic autocorrelation sum*. If A_1, A_2, \dots, A_k are compatible so that (4.1) holds, and if D_i is a circulant matrix with first row given by the elements of A_i , then

$$\sum_{i=1}^k D_i D_i' = (k\ell - \gamma)I_\ell + \gamma J_\ell, \tag{4.2}$$

where I_ℓ is the identity matrix of order ℓ and J_ℓ is a square matrix of order ℓ with all its entries equal to one. Where there is no confusion, we will use the same symbols to represent sequences and their corresponding circulant matrices.

The following Theorem shows the link between the compatibility of sequences of length $\ell = n - 1$ and designs that attain bound (2.2).

Theorem 4.1. *Let T be as described in Theorem 3.2. The following are equivalent:*

- (a) *The design T is an Es^2 -optimal k -circulant mean-orthogonal supersaturated design with $n = 2t$ runs and $m = (2t - 1)k$ factors, satisfying bound (2.2).*
- (b) $\sum_{i=1}^k P_{G_i}(q) = \gamma$, where $\gamma = -k$, for all $q = 1, 2, \dots, t - 1$.

Proof. The proof follows from Result 3.1 together with Theorem 2 in Georgiou [12]. □

We note that Theorem 4.1 provides an alternative proof of Result 3.3 (originally proved by Cheng, 1997, Section 2) since, from Result 3.2 $N = [N_1, \dots, N_k]$ and $N_i = [D_i + J_{n-1}]/2$, so

2

$$\begin{aligned}
 NN' &= \sum_{i=1}^k N_i N_i' \\
 &= \sum_{i=1}^k D_i D_i' + \sum_{i=1}^k D_i J_{n-1} + \sum_{i=1}^k J_{n-1} D_i' + k(n-1)J_{n-1} \\
 &= \frac{kn}{4} I_{n-1} + \frac{k(n-4)}{4} J_{n-1}
 \end{aligned}$$

6 which is the concurrence matrix for a BIBD with parameter $\lambda = k(n-4)/4$. Thus, the
 8 balanced incomplete block design of Example 3.1 has $\lambda = 3(12-4)/4 = 6$. Theorem 4.2
 gives a formula for Es^2 -efficiency of a k -circulant design when the corresponding periodic
 autocorrelation sequences are not compatible.

10 **Theorem 4.2.** Let T be a mean-orthogonal supersaturated design as described in Theo-
 12 rem 3.2, with the property that $\sum_{i=1}^k P_{G_i}(q) \neq \gamma$ for at least one value of $q = 1, 2, \dots, t-1$,
 then the value of Es^2 for T is

$$Es^2 = \frac{nm(m-n) + (n-1)(\sum_{j=1}^{n-2} \gamma_j^2 + 2k^2)}{m(m-1)},$$

14 where $\gamma_j = \sum_{z=1}^k P_{G_z}(j)$ and $m = k(n-1)$.

16 *Proof.* By definition, since T is a k -circulant mean-orthogonal supersaturated design, the
 row sum of each of its first $n-1$ rows is equal to $-k$ (see Section 3.1). Then from (3.2),

$$TT' = \begin{bmatrix} \sum_{z=1}^k D_z D_z' & -k\mathbf{1}_{(n-1)} \\ -k\mathbf{1}_{(n-1)} & k(n-1) \end{bmatrix}$$

18 where $[D_z', \mathbf{1}]'$ is a 1-circulant design with first row $G_z = (g_1^{(z)}, g_2^{(z)}, \dots, g_{n-1}^{(z)})$, $z = 1, 2, \dots, k$.
 Consider the (u, v) th element, $d_{u,v}^{(z)}$, of $D_z D_z'$ and let $x = |u-v|$. Then $d_{u,v}^{(z)} = \sum_{j=1}^{n-1} g_j^{(z)} g_{j+x}^{(z)}$.
 20 So, the (u, v) th element of $\sum_{i=1}^k D_z D_z'$ is

$$\sum_{z=1}^k D_z D_z' = \sum_{z=1}^k \sum_{i=0}^{n-2} g_{i+1}^{(z)} g_{i+1+x}^{(z)} = \sum_{z=1}^k P_{G_z}(x) = \gamma_x.$$

22 Note that $\gamma_0 = k(n-1) = m$, then

$$TT' = \begin{bmatrix} m & \gamma_1 & \gamma_2 & \cdots & \cdots & \gamma_{n-2} & -k \\ \gamma_1 & m & \gamma_1 & \ddots & & \vdots & \vdots \\ \gamma_2 & \gamma_1 & m & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \gamma_1 & \gamma_2 & -k \\ \vdots & & \ddots & \gamma_1 & m & \gamma_1 & -k \\ \gamma_{n-2} & \cdots & \cdots & \gamma_2 & \gamma_1 & m & -k \\ -k & -k & \cdots & \cdots & -k & -k & m \end{bmatrix}$$

Since, from (3.1), $\gamma_x = \gamma_{(n-1)-x}$, each of the first $n - 1$ diagonal elements of $(TT')(TT')$ is $m^2 + k^2 + \sum_{i=1}^{n-2} \gamma_i^2$. The n th diagonal element is $k^2(n - 1) + m^2$. Now, by (2.1), Es^2 may be written

$$\begin{aligned}
 Es^2 &= \sum_{i \neq j=1}^m s_{ij}^2 / m(m - 1) = \sum_{i,j=1}^m (s_{ij}^2 - mn^2) / m(m - 1) \\
 &= (\text{trace}(T'TT'T) - mn^2) / m(m - 1) \\
 &= (\text{trace}(TT'TT') - mn^2) / m(m - 1) \\
 &= \frac{nm^2 + (n - 1) \sum_{i=1}^{n-2} \gamma_i^2 + 2(n - 1)k^2 - mn^2}{m(m - 1)} \\
 &= \frac{nm(m - n) + (n - 1)(\sum_{i=1}^{n-2} \gamma_i^2 + 2k^2)}{m(m - 1)}
 \end{aligned}$$

In the following example, we illustrate the construction of Es^2 -optimal and near-optimal k -circulant supersaturated designs using the information from the autocorrelation function.

Example 4.1. Consider the construction of $E(s^2)$ -optimal and near-optimal 10-run supersaturated designs using Theorems 3.1 and 4.1 with $n = 2t = 10$ and $m = 18, 27, 36, 45$ factors. There are in total $9^{-1} \binom{9}{5} = 14$ distinct generators of length 9, where “distinct” means that the generated designs have no duplicated columns. Table 4.1 displays the 14 generators together with their periodic autocorrelation functions $P_{G_i}(q)$ for $q = 1, 2, 3$, and 4.

Consider the generators G_2, G_3, G_4, G_9 and G_{11} and their respective 1-circulant 10×9 design matrices T_2, T_3, T_4, T_9 and T_{11} . For example, G_4 will produce

$$T_4 = \begin{pmatrix}
 +++----+- \\
 -++++---+ \\
 ---++++--- \\
 +----++++ \\
 -+----++++ \\
 --+---++++ \\
 ---+---++++ \\
 +----++++ \\
 ++----++++ \\
 +++----++++ \\
 ++++++++
 \end{pmatrix} \quad \text{with } P_{G_4}(1) = 1, P_{G_4}(2) = -3, P_{G_4}(3) = -3, P_{G_4}(4) = 1.$$

The 10-run design with $m = 18$ factors, $[T_2, T_{11}]$, is $E(s^2)$ -optimal since $\sum_{i=1}^{k-2} P_{G_i}(q) = -k$ for all $q = 1, 2, 3, 4$. Similarly for $m = 36$, the design $[T_2, T_3, T_9, T_{11}]$ has $\sum P_G(q) = -4$ for $q = 1, 2, 3, 4$. There are no 10-run $E(s^2)$ -optimal designs for $m = 27$ or $m = 45$ using cyclic generators. Out of the $\binom{14}{3} = 364$ possible designs, there are 69 which have $E(s^2) = 8.10$. Using equation (2.3) we obtain the lower bound of 7.92 which implies that all these designs are 97.7% efficient. One such design is $[T_2, T_3, T_{11}]$. The two designs $[T_2, T_3, T_4, T_9, T_{11}]$ and $[T_1, T_3, T_{10}, T_{12}, T_{14}]$ with $m = 45$ factors are near Es^2 -optimal designs with $E(s^2) = 9.23$. Comparing this value to the lower bound we obtain 99.3% efficiency. It is interesting to note very different autocorrelation function values in Table 4.1 for T_i 's which comprise these two designs.

Table 4.1. Cyclic generators and their periodic autocorrelation functions

i	G_i	q			
		1	2	3	4
1	++++-----	5	1	-3	-7
2	+++-+-----	1	1	-3	-3
3	+++--+----	1	-3	-3	1
4	+++----+---	1	-3	-3	1
5	+++-----+-	1	1	-3	-3
6	++-++-----	1	-3	1	-3
7	++-+-+-----	-3	1	-3	1
8	++-+--+----	-3	-3	5	-3
9	++-+-----+-	-3	1	1	-3
10	++--++-----	1	-7	-3	5
11	++--+-+---	-3	-3	1	1
12	++--+-+---	-3	-3	5	-3
13	++--+-+---	-3	1	-3	1
14	+--+--+-----	-7	5	-3	1

Table 4.2. Equivalent generators for the designs with $n = 10$ and $m = 9i, i \leq 7$

Eskridge, Gilmour, Mead, Butler and Travnicek(2004)	From Table 4.1
(0124)	G_5
(0125) (0137)	$G_4 G_9$
(0134) (0135)	$G_6 G_{13}$
(0124) (0146)	$G_5 G_{11}$

Bulutoglu and Cheng (2004) gave the complete set of solutions for 10-run supersaturated designs attaining bound (2.2) and they showed that they exist only for $m = 18t$ factors with $t = 1, \dots, 6$. Eskridge, Gilmour, Mead, Butler and Travnicek (2004) provided seven generators for cyclic incomplete block designs that produce Es^2 optimal (for k even) or near optimal (for k odd) supersaturated designs with $n = 10$ runs and $m = 9i, i \leq 7$. Table 4.2 shows the seven generators provided by Eskridge, Gilmour, Mead, Butler and Travnicek (2004) and their equivalents from Table 4.1.

In Table 4.3, we present new Es^2 -optimal supersaturated designs with n runs ($10 \leq n \leq 26$) and $m = k(n - 1)$ factors for and their properties. We enumerate the elements of the cyclic generator and we present them in column 'Generators' using the incomplete block design notation. The second column of Table 4.3, labelled f_h shows the frequency with which each value of $s_{ij}^2 = h$ occurs in $T'T$ for every integer h for which the frequency is non-zero. The third column gives the maximum value r_{max} of s_{ij}^2/n . Table 4.4 lists further new supersaturated designs with k odd and which are at least 98.5% efficient; that is, whose Es^2 values are at least 0.985 of the corresponding lower bounds. The value of Es^2 , the lower bound (2.3), and the efficiency LB/Es^2 is given for each design in columns 5–7 of the table.

Table 4.3. Generators and properties for new Es^2 -optimal supersaturated designs with n runs and m factors

n	m	f_h	r_{max}	Generators
10	90	3240 ₂ , 765 ₆	0.6	$G_2 - G_9, G_{11}, G_{13}$.
10	108	4640 ₂ , 1134 ₆	0.6	$G_1 - G_5, G_7 - G_{12}, G_{14}$.
10	126	6300 ₂ , 1575 ₆	0.6	$G_1 - G_{14}$.
12	77	1144 ₀ , 1683 ₄ , 99 ₈	0.667	(0,1,4,7,9); (1,5,6,8,10); (0,2,3,7,10); (0,3,7,8,9); (0,1,3,5,6); (3,5,6,7,8); (0,1,6,7,8).
12	88	1452 ₀ , 2244 ₄ , 132 ₈	0.667	(0,1,6,7,9); (1,5,7,8,9); (0,2,3,6,10); (0,3,5,6,7); (0,3,5,8,9); (0,1,2,4,10); (0,2,4,6,7); (0,5,6,9,10).
12	99	1947 ₀ , 2684 ₄ , 220 ₈	0.667	(0,1,5,6,7); (1,5,6,8,10); (0,2,3,6,8); (0,3,4,6,7); (0,1,2,8,10); (0,1,2,4,5); (0,2,5,9,10); (0,2,5,6,9); (0,2,3,5,6).
12	110	2431 ₀ , 3267 ₄ , 297 ₈	0.667	(0,1,2,4,9); (1,4,6,7,8); (0,1,4,7,10); (0,2,6,7,9); (0,1,2,3,7); (0,1,2,7,8); (0,1,2,4,5); (0,2,5,7,10); (0,2,5,6,9); (0,2,3,5,6).
14	130	6032 ₂ , 2262 ₆ , 91 ₁₀	0.714	(0,1,2,4,6,8); (2,4,5,6,10,11); (0,3,5,6,9,12); (0,3,5,7,10,11); (0,1,5,7,8,12); (0,1,2,4,5,9); (1,2,4,5,6,11); (0,2,3,5,6,7); (0,2,3,5,8,11); (0,7,8,10,11,12);
16	45	360 ₀ , 600 ₄ , 30 ₈	0.5	(0,1,2,3,7,8,13); (0,1,5,7,9,10,13); (0,3,4,6,7,8,10).
16	60	510 ₀ , 1200 ₄ , 60 ₈	0.5	(0,1,2,5,7,11,13); (0,1,3,5,8,11,12); (0,1,2,4,5,7,14); (3,4,5,9,10,12,13).
16	75	870 ₀ , 1740 ₄ , 165 ₈	0.5	(0,1,2,6,8,11,12); (0,1,3,5,9,10,12); (0,4,6,7,11,12,14); (1,7,8,9,11,12,14); (0,1,2,3,4,6,9).
16	90	1350 ₀ , 2340 ₄ , 315 ₈	0.5	(0,5,7,8,10,12,13); (1,3,5,6,9,12,14); (0,1,2,5,6,9,12); (0,5,6,9,12,13,14); (1,3,7,8,12,13,14); (0,1,2,6,12,13,14).
16	105	1860 ₀ , 3120 ₄ , 480 ₈	0.5	(0,1,2,5,7,9,10); (5,6,9,10,12,13,14); (0,2,7,9,11,13,14); (3,6,8,9,11,13,14); (5,7,8,11,12,13,14); (3,7,8,10,12,13,14); (2,7,8,10,11,13,14).
16	120	2400 ₀ , 4080 ₄ , 660 ₈	0.5	(0,1,2,5,7,8,11); (5,6,8,9,12,13,14); (0,2,7,10,11,12,14); (3,6,8,11,12,13,14); (0,1,2,4,6,8,13); (0,2,5,6,8,11,13); (0,2,3,6,12,13,14); (2,3,5,6,7,12,13).
16	135	3420 ₀ , 4620 ₄ , 1005 ₈	0.5	(0,1,2,4,6,9,13); (0,2,5,6,10,12,13); (0,2,3,6,7,9,10); (2,3,5,6,10,11,12); (0,1,2,4,5,6,12); (3,4,5,6,7,10,13); (0,1,3,5,6,7,10); (0,3,4,5,9,11,13); (0,1,3,4,5,10,13).
18	68	1530 ₂ , 768 ₆	0.333	(0,1,5,6,12,13,14,15); (2,7,8,9,10,12,14,16); (0,1,5,8,10,11,14,16); (2,6,8,11,12,13,15,16).
18	102	3349 ₂ , 1734 ₆ , 68 ₁₀	0.556	(0,2,3,4,6,7,9,16); (0,3,6,8,9,10,15,16); (0,2,3,6,7,11,12,16); (0,1,3,5,6,7,12,15); (0,1,2,3,5,9,11,15); (0,2,6,9,10,11,12,15).
20	76	855 ₀ , 1710 ₄ , 285 ₈	0.4	(0,1,2,5,6,8,13,15,18); (4,5,7,8,10,12,14,16,17); (0,1,2,5,6,11,13,16,17); (4,5,8,12,13,14,15,16,18).
20	95	1254 ₀ , 2698 ₄ , 513 ₈	0.4	(0,1,3,5,6,7,9,10,17); (3,5,6,10,11,12,13,16,18); (0,5,6,10,14,15,16,17,18); (0,1,2,5,6,9,11,14,17); (4,5,7,8,11,12,14,16,18).

(Contd.)

n	m	f_h	r_{max}	Generators
20	114	2109 ₀ , 3401 ₄ , 931 ₈	0.4	(0,1,3,5,8,14,16,17,18); (2,4,5,7,9,13,14,15,17); (0,2,4,7,9,10,13,14,18); (0,1,3,5,6,7,10,13,14); (3,5,6,9,10,11,12,13,18); (0,5,6,9,13,14,16,17,18).
20	133	2964 ₀ , 4427 ₄ , 1387 ₈	0.4	(0,1,5,7,8,13,15,16,18); (0,3,5,9,11,15,16,17,18); (0,2,3,10,11,12,13,17,18); (4,6,7,8,10,11,13,14,16); (0,1,4,5,7,9,12,14,16); (3,4,7,9,10,13,15,16,18); (0,1,6,10,11,14,15,16,18).
22	84	2058 ₂ , 1407 ₆ , 21 ₁₀	0.454	(0,1,6,8,9,12,14,15,18,19); (1,4,8,12,13,14,15,16,17,18); (0,2,5,7,9,10,11,13,18,19); (2,4,7,11,12,13,14,17,18,19).
22	126	4683 ₂ , 2898 ₆ , 294 ₁₀	0.454	(0,1,3,4,6,7,10,12,16,20); (0,3,4,5,6,8,10,18,19,20); (0,3,7,9,10,11,12,13,19,20); (0,2,7,10,12,14,15,17,19,20); (1,5,6,9,10,12,14,15,19,20); (0,3,6,7,10,12,13,14,18,19).
24	69	621 ₀ , 1472 ₄ , 253 ₈	0.333	(0,7,8,11,12,16,17,18,19,21,22); (1,5,6,8,11,12,14,17,20,21,22); (0,7,9,10,12,14,15,16,18,20,22).
24	92	943 ₀ , 2668 ₄ , 575 ₈	0.333	(0,3,6,7,10,14,16,17,18,19,21); (2,5,8,10,12,13,14,19,20,21,22); (0,7,8,9,10,12,13,14,15,18,19); (1,5,6,9,11,12,14,18,19,20,22).
24	115	2346 ₀ , 2852 ₄ , 1357 ₈	0.333	(0,3,6,7,12,17,18,19,20,21,22); (2,5,8,9,11,12,13,14,15,20,22); (0,1,6,7,9,14,15,17,19,20,22); (0,1,3,4,5,9,10,12,14,16,19); (3,5,6,9,10,14,16,18,20,21,22).
24	138	3082 ₀ , 4393 ₄ , 1955 ₈ , 23 ₁₂	0.5	(0,1,3,7,8,9,12,17,19,20,22); (2,3,4,5,9,11,14,15,18,20,21); (0,4,11,12,13,14,15,16,19,20,21); (0,3,6,7,8,10,11,13,15,16,20); (0,2,6,8,10,11,14,15,19,20,21); (1,5,6,7,8,10,11,13,19,21,22).
24	161	4278 ₀ , 5865 ₄ , 2622 ₈ , 115 ₁₂	0.5	(0,2,3,5,6,7,10,11,15,21,22); (2,4,5,7,10,12,13,14,15,16,21); (2,3,4,9,10,14,15,16,17,18,20); (4,5,9,10,12,14,16,17,18,19,21); (0,3,6,7,8,10,11,13,17,20,22); (0,2,6,8,10,11,13,14,16,17,21); (1,5,6,7,8,10,11,14,16,20,21).
26	50	850 ₂ , 375 ₆	0.231	(0,2,6,7,9,12,14,17,18,21,23,24); (0,8,10,12,13,16,17,18,21,22,23,24).
26	100	2650 ₂ , 2175 ₆ , 125 ₁₀	0.385	(0,1,3,10,11,13,15,16,18,19,23,24); (1,3,4,5,7,9,10,11,15,17,18,21); (0,3,4,5,6,10,13,19,20,22,23,24); (2,3,6,7,9,12,14,16,18,19,20,23).

Table 4.4. Generators and properties for new near-optimal supersaturated designs with n runs and $m = k(n - 1)$ factors, with k odd.

n	m	f_h	r_{max}	Es^2	LB	Eff	Generators
10	81	2628 ₂ , 612 ₆	0.6	10.04	10.02	99.8%	$G_2 - G_9, G_{11}$.
10	99	3906 ₂ , 945 ₆	0.6	10.23	10.22	99.9%	$G_1 - G_3, G_5, G_7 - G_{13}$.
10	117	5436 ₂ , 1350 ₆	0.6	10.37	10.36	99.9%	$G_1, G_3 - G_{14}$.
14	39	585 ₂ , 156 ₆	0.429	10.74	10.56	98.4%	(0,5,6,8,9,11); (2,6,7,8,11,12);(5,6,7,9,11,12).
14	65	1534 ₂ , 546 ₆	0.429	12.4	12.35	99.5%	(0,2,3,6,11,12); (0,1,4,6,9,12); (0,2,4,6,9,10); (0,1,2,7,11,12); (0,2,4,6,7,12);
14	91	2925 ₂ , 1170 ₆	0.429	13.14	13.11	99.8%	(0,3,5,6,9,12); (1,4,6,9,10,11); (0,4,6,7,11,12); (0,1,4,10,11,12); (1,3,4,5,7,9); (0,3,5,7,10,11); (0,1,2,4,5,9),
18	51	901 ₂ , 374 ₆	0.333	13.39	13.19	98.5%	(0,3,6,8,9,12,13,15); (2,3,4,9,10,11,13,14); (2,5,6,7,9,10,11,13).
18	85	2295 ₂ , 1258 ₆ , 17 ₁₀	0.556	15.73	15.51	98.6%	(0,2,3,6,10,12,14,15); (5,6,9,10,13,14,15,16); (1,5,6,8,12,13,14,16); (3,8,10,11,12,13,14,15); (1,2,4,9,10,13,15,16).
18	119	4641 ₂ , 2193 ₆ , 187 ₁₀	0.556	16.55	16.52	99.8%	(1,6,7,8,10,11,15,17); (3,4,5,6,7,8,12,17); (2,3,5,8,10,13,14,16); (2,4,6,10,13,14,15,16); (1,2,3,5,11,13,14,15); (2,3,7,9,10,12,14,16); (1,2,4,6,7,13,14,17).
22	63	1218 ₂ , 735 ₆	0.273	16.04	15.85	98.8%	(0,3,4,6,7,9,10,16,18,20); (3,6,9,10,11,12,14,18,19,20); (1,5,10,11,12,13,15,17,18,20).
26	75	1750 ₂ , 900 ₆ , 125 ₁₀	0.385	18.70	18.50	98.9%	(3,6,7,8,12,14,15,17,19,20,21,23); (4,6,7,8,10,11,12,14,16,19,20,21); (0,1,4,7,10,12,14,15,19,20,21,22).

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