

# Construction of orthogonal and nearly orthogonal designs for computer experiments

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## SUMMARY

This paper presents new infinite families of orthogonal designs for computer experiments. In cases where orthogonal designs cannot exist, we construct alternative, nearly orthogonal designs. Our designs can accommodate many factors and a large set of levels. No iterative computer search is required. To build up the desired orthogonal designs we develop and use new infinite classes of periodic Golay pairs.

*Some key words:* Column-orthogonal design; Design of experiment; Golay sequence; Orthogonal design; Periodic Golay pair; U-type design.

## 1. INTRODUCTION

Computer experiments have become very common (e.g., Fang et al., 2006; Sacks et al., 1989). Latin hypercube designs, which have  $n$  equally spaced levels on  $n$  runs, form a major class of designs for computer experiments and have been widely studied (Georgiou, 2009; Lin et al., 2009; Sun et al., 2009; Yang & Liu, 2012; Georgiou & Efthimiou, 2014). Bingham et al. (2009) relaxed the condition that the number of levels for each factor must be identical to the run size, and constructed an extended and useful class of orthogonal and nearly orthogonal designs for computer experiments. Lin et al. (2010) proposed a method for constructing new designs for computer experiments by using the Kronecker product on small designs with specific properties. Under some circumstances these designs are orthogonal designs.

An orthogonal design, denoted by  $\text{OD}(n; q^m)$ , is an  $n \times m$  matrix with entries from a set of  $q$  levels such that the  $m$  columns are pairwise orthogonal. The columns and rows can be identified with factors and experimental runs, respectively. Orthogonal designs have been referred to in the literature also as column-orthogonal designs (e.g., Sun et al., 2011). If the columns are only approximately orthogonal, then the design is called nearly orthogonal and denoted by  $\text{NOD}(n; q^m)$ . We consider orthogonal and nearly orthogonal designs such that the  $q$  levels are symmetrically placed about 0 and for every nonzero  $l$ , the levels  $+l$  and  $-l$  appear equally often in each column. As a consequence, these designs are mean orthogonal. Indeed, quite a few of the designs obtained here are of the U-type in the sense of having all  $q$  levels equally replicated in every column. Clearly, if the levels are equally spaced and  $q = n$ , then an  $\text{OD}(n; q^m)$  as considered here reduces to an orthogonal Latin hypercube.

The main result of this paper is the construction of new orthogonal and nearly orthogonal designs that can be used for computer experiments or for screening. These constructions rely heavily on circulant matrices, Golay sequences, and new classes of periodic Golay pairs, which are also developed in this paper. Our results fill gaps in the list of known periodic Golay pairs, orthogonal and nearly orthogonal designs. The methodology and new results equip practitioners with directly applicable tools for experimentation.

## 2. NEW RESULTS ON PERIODIC GOLAY PAIRS

Circulant matrices will be extensively used for the proposed constructions. A matrix is said to be circulant if each row vector is rotated one element to the right relative to the preceding row vector. Circulant matrices with an opposite direction of shift are called back-circulant. We will use  $B = \text{circ}(A)$  to denote that the circulant matrix  $B$  is generated by the row vector  $A$ . More details on circulant and back-circulant matrices can be found in [Geramita & Seberry \(1979, pp. 81–82\)](#).

Let  $A = \{A_j : A_j = (a_{j,0}, \dots, a_{j,n-1}), j = 1, \dots, \ell\}$ , be a set of  $\ell$  row vectors of length  $n$ . The periodic autocorrelation function  $P_A(s)$  and the non-periodic autocorrelation function  $N_A(s)$  are defined, reducing  $i + s$  modulo  $n$ , as

$$P_A(s) = \sum_{j=1}^{\ell} \sum_{i=0}^{n-1} a_{j,i} a_{j,i+s}, \quad N_A(s) = \sum_{j=1}^{\ell} \sum_{i=0}^{n-s-1} a_{j,i} a_{j,i+s} \quad (s = 0, \dots, n-1).$$

The set of row vectors  $A$  is said to have zero periodic autocorrelation function if  $P_A(s) = 0$  and zero non-periodic autocorrelation function if  $N_A(s) = 0$  ( $s = 1, \dots, n-1$ ). We again refer to [Geramita & Seberry \(1979, p. 130\)](#), for more details.

Throughout this paper we use  $\bar{a}$  to denote  $-a$ . Two sequences of variables are directed if the sequences have zero periodic autocorrelation function without relying on the commutativity of the variables. For example  $(a, b)$  and  $(a, \bar{b})$  are two directed sequences while  $(a, b)$  and  $(b, \bar{a})$  are not. Let  $A_j$  ( $j = 1, \dots, m$ ) be  $m$  sequences of length  $n$ . These sequences are of type  $(u_1, \dots, u_t)$  if the sequences are composed of  $t$  variables, say  $x_i$  ( $i = 1, \dots, t$ ) with  $x_i$  and  $-x_i$  occurring a total of  $u_i$  times ( $i = 1, \dots, t$ ). A set  $\{A_1, \dots, A_{2k}\}$  of square real matrices of order  $n$  is additive if  $\sum_{i=1}^{2k} A_i A_i^T = f I_n$  for some real number  $f$  and it is amicable if  $\sum_{i=1}^k (A_{2i-1} A_{2i}^T - A_{2i} A_{2i-1}^T) = 0$  ([Kharaghani, 2000](#)). Two square matrices are disjoint if their elementwise product is the zero matrix; see [Geramita & Seberry \(1979, p. 2\)](#).

Golay sequences, also known as Golay pairs, are two row vectors  $(A_1, A_2)$  of length  $n$ , with elements from the set  $\{1, -1\}$ , that have zero non-periodic autocorrelation function. These sequences are known to exist for lengths  $g = 2^a 10^b 26^c$ , where  $a, b, c$  are nonnegative integers. More details can be found in [Borwein & Ferguson \(2003\)](#). Periodic Golay pairs (e.g., [Bomer & Antweiler, 1990](#)) are the natural generalization of Golay sequences with zero periodic autocorrelation function. Any positive integer  $g$  for which Golay sequences exist is called a Golay number. Similarly, any positive integer  $p$  for which a periodic Golay pair exists is called a periodic Golay number. It is obvious that any Golay number is also a periodic Golay number but the converse is not generally true. Both periodic Golay pairs and Golay sequences can be used to generate orthogonal block-circulant matrices even though the latter can provide some useful multiplication methods and give more general results. The existence of periodic Golay pairs is important especially when Golay sequences do not exist, cannot be constructed or are unknown.

Periodic Golay pairs of length  $n$  are also hard to construct. Periodic Golay pairs that are not Golay sequences are known only for lengths  $n = 34, 50, 58, 74, 82, 122, 136, 164, 202, 226$  and all of them have been constructed by intensive computer search; see a 2013 unpublished technical report by D. Z. Djokovic and I. S. Kotsireas (arXiv: 1310.5773). With the use of Lemma 1 and Theorem 1 we construct new periodic Golay pairs, of an infinite variety of different lengths, without any computer search.

**LEMMA 1.** *There exist directed sequences with zero periodic autocorrelation function of lengths  $p$  and type  $(p, p)$ , for  $p \in P = \{34, 50, 58, 74, 82, 122, 136, 202, 226\}$ .*

[illegible]

*Example 1.* Suppose we wish to construct a periodic Golay pair  $(T_1, T_2)$  of length 68. We have  $68 = 2 \times 34$ , so we have to use the directed sequences  $D_1, D_2$  of length 34 and type  $(34, 34)$  given in Table 1 with the Golay sequences  $A = (+, +)$  and  $B = (+, -)$ , where  $+$  stands for  $+1$  and  $-$  stands for  $-1$ . The resulting periodic Golay pair is

$$T_1 = (+ + + + + - - - - - + - - + + - + + - + - + + - + - \\ + + + - + + + - + + - + - + + + - - + - - + + + - + - ++),$$
$$T_2 = (+ - - - - + - + - - + + - + - - - - + + - - + - + + - + - \\ - - - - + + + + - - + + - + + - + + + - + - + - + + - + -).$$

COROLLARY 1. *Periodic Golay pairs can be constructed for all lengths  $t = 2^{a_1} 10^{a_2} 26^{a_3} p^{a_4}$ , where  $a_1, a_2, a_3$  are nonnegative integers,  $p \in \{34, 50, 58, 74, 82, 122, 202, 226\}$  and  $a_4 = 0, 1$ .*

### 3. CONSTRUCTION OF ORTHOGONAL DESIGNS

Let  $A_i$  ( $i = 1, \dots, 8$ ) be circulant matrices of order  $n$  and  $R_n$  the back-diagonal identity matrix of order  $n$ . The following constructions are known:

$$C_2 = \begin{pmatrix} A_1 & A_2 R_n \\ -A_2 R_n & A_1 \end{pmatrix}, \quad C_4 = \begin{pmatrix} A_1 & A_2 R_n & A_3 R_n & A_4 R_n \\ -A_2 R_n & A_1 & A_4^T R_n & -A_3^T R_n \\ -A_3 R_n & -A_4^T R_n & A_1 & A_2^T R_n \\ -A_4 R_n & A_3^T R_n & -A_2^T R_n & A_1 \end{pmatrix},$$

$$C_8 = \begin{pmatrix} A_1 & A_2 & A_4 R_n & A_3 R_n & A_6 R_n & A_5 R_n & A_8 R_n & A_7 R_n \\ -A_2 & A_1 & A_3 R_n & -A_4 R_n & A_5 R_n & -A_6 R_n & A_7 R_n & -A_8 R_n \\ -A_4 R_n & -A_3 R_n & A_1 & A_2 & -A_8^T R_n & A_7^T R_n & A_6^T R_n & -A_5^T R_n \\ -A_3 R_n & A_4 R_n & -A_2 & A_1 & A_7^T R_n & A_8^T R_n & -A_5^T R_n & -A_6^T R_n \\ -A_6 R_n & -A_5 R_n & A_8^T R_n & -A_7^T R_n & A_1 & A_2 & -A_4^T R_n & A_3^T R_n \\ -A_5 R_n & A_6 R_n & -A_7^T R_n & -A_8^T R_n & -A_2 & A_1 & A_3^T R_n & A_4^T R_n \\ -A_8 R_n & -A_7 R_n & -A_6^T R_n & A_5^T R_n & A_4^T R_n & -A_3^T R_n & A_1 & A_2 \\ -A_7 R_n & A_8 R_n & A_5^T R_n & A_6^T R_n & -A_3^T R_n & -A_4^T R_n & -A_2 & A_1 \end{pmatrix}.$$

Arrays  $C_2$  and  $C_4$  are orthogonal when the circulant matrices used are additive (Geramita & Seberry, 1979, pp. 97–9). Array  $C_8$  is orthogonal when the circulant matrices used are simultaneously additive and amicable (Kharaghani, 2000).

From periodic Golay pairs  $T_1, T_2$  of length  $t$  and their corresponding circulant matrices  $Z_1 = \text{circ}(T_1)$ ,  $Z_2 = \text{circ}(T_2)$  we can define

$$X = (Z_1 + Z_2)/2, \quad W = (Z_1 - Z_2)/2. \quad (1)$$

LEMMA 2. *The matrices  $X$  and  $W$  in (1) are circulant, disjoint, additive, amicable matrices of order  $t$ , with entries from  $\{0, 1, -1\}$  and  $X \pm W$  is a  $\pm 1$  matrix.*

*Proof.* Follows by simple calculations.  $\square$

Let  $(T_1, T_2)$  be the periodic Golay pair of length  $t = 2^{a_1} 10^{a_2} 26^{a_3} p^{a_4}$ , where  $a_1, a_2, a_3$  are nonnegative integers,  $p \in \{34, 50, 58, 74, 82, 122, 202, 226\}$  and  $a_4 = 0$  or 1. Using matrices  $X$  and  $W$  from (1), consider the constructions

$$A_i = (2i - 1)X + (2i + 1)W, \quad A_{i+1} = (2i + 1)X - (2i - 1)W, \quad (i = 1, 3, 5, 7), \quad (2)$$

$$A_{2i-1} = (2i - 1)X + 2iW, \quad A_{2i} = 2iX - (2i - 1)W, \quad (i = 1, 2, 3, 4), \quad (3)$$

$$A_i = (2i + 1)X + (2i + 3)W, \quad A_{i+1} = (2i + 3)X - (2i + 1)W, \quad (i = 1, 3, 5, 7), \quad (4)$$

$$A_{2i-1} = 2iX + (2i + 1)W, \quad A_{2i} = (2i + 1)X - 2iW, \quad (i = 1, 2, 3, 4), \quad (5)$$

$$A_i = (2i + 3)X + (2i + 5)W, \quad A_{i+1} = (2i + 5)X - (2i + 3)W, \quad (i = 1, 3, 5, 7), \quad (6)$$

$$A_{2i-1} = (2i + 1)X + 2(i + 1)W, \quad A_{2i} = 2(i + 1)X - (2i + 1)W, \quad (i = 1, 2, 3, 4). \quad (7)$$

THEOREM 2. *Let  $t = 2^{a_1} 10^{a_2} 26^{a_3} p^{a_4}$ , where  $a_1, a_2, a_3$  are nonnegative integers,  $p \in \{34, 50, 58, 74, 82, 122, 202, 226\}$  and  $a_4 = 0$  or 1. The following orthogonal designs for computer experiments exist: (i)  $\text{OD}(2^{b+1}t; q_1^\ell)$  and (ii)  $\text{OD}(2^{b+1}t + s; q_2^\ell)$ ,  $q_1 = 2^{b+1}$ ,  $q_2 = 2^{b+1} + 1$ ,  $\ell \leq 2^b t$ , for  $b = 1, 2, 3$  and for any positive integer  $s$ .*

*Proof.* To prove the existence of orthogonal designs (i) and (ii) of the theorem we use the constructions given in (2) and (3) respectively. From Lemma 2 we have that the matrices  $\{A_i\}_{i=1}^8$  are circulant,

Table 2. Some orthogonal designs  $\text{OD}(n; q^m)$  constructed from two circulant matrices. All designs for  $q = 4, 8, 16$  or  $q = n$  are additionally of U-type. Designs marked with an asterisk are constructed using periodic Golay pairs that are developed as in § 2

$q = 4$		$q = 5$		$q = 8$		$q = 9$		$q = 16$		$q = 17$	
$n$	$m$	$n$	$m$	$n$	$m$	$n$	$m$	$n$	$m$	$n$	$m$
4	2	5	2	8	4	9	4	16	8	17	8
8	4	9	4	16	8	17	8	32	16	33	16
16	8	17	8	32	16	33	16	64	32	65	32
32	16	33	16	64	32	65	32	128	64	129	64
40	20	41	20	80	40	81	40	160	80	161	80
64	32	65	32	128	64	129	64	256	128	257	128
80	40	81	40	160	80	161	80	320	160	321	160
104	52	105	52	208	104	209	104	416	208	417	208
128	64	129	64	256	128	257	128	512	256	513	256
136	68*	137	68*	272	136*	273	136*	544	272*	545	272*
160	80	161	80	320	160	321	160	640	320	641	320
200	100*	201	100*	400	200*	401	200*	800	400*	801	400*
208	104	209	104	416	208	417	208	832	416	833	416
232	116*	233	116*	464	232*	465	232*	928	464*	929	464*
256	128	257	128	512	256	513	256	1024	512	1025	512
272	136*	273	136*	544	272*	545	272*	1088	544*	1089	544*
296	148*	297	148*	592	296*	593	296*	1184	592*	1185	592*
320	160	321	160	640	320	641	320	1280	640	1281	640
328	164*	329	164*	656	328*	657	328*	1312	656*	1313	656*
400	200	401	200	800	400	801	400	1600	800	1601	800
416	208	417	208	832	416	833	416	1664	832	1665	832
464	232*	465	232*	928	464*	929	464*	1856	928*	1857	928*
488	244*	489	244*	976	488*	977	488*	1952	976*	1953	976*
512	256	513	256	1024	512	1025	512	2048	1024	2049	1024
544	272*	545	272*	1088	544*	1089	544*	2176	1088*	2177	1088*

additive and amicable. For  $b = 1, 2, 3$  and a fixed  $1 \leq \ell \leq 2^b t$ , the desired orthogonal design is obtained by randomly selecting any  $\ell$  columns from the matrix  $(C_{2^b}^T, -C_{2^b}^T)^T$  or  $(C_{2^b}^T, 0_{2^b t \times s}, -C_{2^b}^T)^T$  for (i) or (ii) respectively, where  $C_{2^b}$  is the square matrix of order  $2^b t$  obtained using  $\{A_1, \dots, A_{2^b}\}$ .  $\square$

To illustrate the construction described in Theorem 2, we provide a detailed example. Even though the desired design in this example is quite large, it is quite easy to construct and to present due to its block-circulant structure.

*Example 2.* Suppose we wish to construct an  $\text{OD}(272; 4^\ell)$ ,  $\ell = 1, \dots, 136$ . From Theorem 1, we construct the periodic Golay pair  $(T_1, T_2)$  of length  $t = 68$  as is illustrated in Example 1. Define the disjoint circulant matrices  $X$  and  $W$  as in Lemma 2. So,

$$X = \text{circ}(+000000 - 00 - - - +0 - 000 - -0 + 000000 + 0 - + - 000 - 0 + + + + - \\ -0 + 00 - + + 0 + 0000 - +0 + + - + - +0),$$

$$W = \text{circ}(0 + + + + + -0 - -0000 - 0 - + + 00 + 0 - + + - + -0 + 000 + + + 0 - \\ 000000 + 0 - +000 + 0 - - + -00 + 000000+).$$

We have  $b = 1$ , so by construction (2) we have

$$A_1 = \text{circ}(1333333\bar{1}\bar{3}\bar{3}\bar{1}\bar{1}\bar{1}\bar{1}\bar{3}\bar{1}\bar{3}\bar{3}\bar{3}\bar{1}\bar{3}\bar{1}\bar{1}\bar{3}\bar{3}\bar{3}\bar{1}\bar{3}\bar{1}\bar{1}\bar{1}\bar{3}\bar{3}\bar{1}\bar{1}\bar{1}\bar{1}\bar{3}\bar{3}\bar{1}\bar{1}\bar{1}\bar{3}\bar{3}\bar{3}\bar{1}\bar{1}\bar{3}\bar{1}\bar{1}\bar{1}\bar{1}\bar{3}),$$

$$A_2 = \text{circ}(3\bar{1}\bar{1}\bar{1}\bar{1}\bar{1}\bar{3}\bar{1}\bar{1}\bar{3}\bar{3}\bar{3}\bar{1}\bar{3}\bar{1}\bar{1}\bar{3}\bar{3}\bar{1}\bar{3}\bar{1}\bar{1}\bar{1}\bar{1}\bar{3}\bar{3}\bar{3}\bar{1}\bar{1}\bar{3}\bar{1}\bar{3}\bar{3}\bar{3}\bar{3}\bar{1}\bar{3}\bar{1}\bar{1}\bar{3}\bar{3}\bar{3}\bar{3}\bar{3}\bar{1}).$$

It is easy to verify that matrices  $A_1$  and  $A_2$  are circulant, additive and amicable. The desired  $\text{OD}(272, 4^\ell)$  is obtained by randomly selecting any  $\ell$  columns from the matrix  $(C_{136}^T, -C_{136}^T)^T$ , where  $C_{136}$  is the square matrix of order 136, obtained using the matrices  $A_1$  and  $A_2$  in structure  $C_2$ .

The orthogonal design presented in Example 2 is constructed by two circulant matrices. The parameters of some further orthogonal designs are given in Table 2.

The following corollaries are straightforward applications of Theorem 2 but they provide new infinite classes of orthogonal designs.

**COROLLARY 2.** *If  $t$  is a Golay or a periodic Golay number then the following orthogonal designs for computer experiments exist:  $\text{OD}(4t; 4^{2t})$ ,  $\text{OD}(4t + 1; 5^{2t})$ ,  $\text{OD}(8t; 8^{4t})$ ,  $\text{OD}(8t + 1; 9^{4t})$ ,  $\text{OD}(16t; 16^{8t})$  and  $\text{OD}(16t + 1; 17^{8t})$ .*

**COROLLARY 3.** *Let  $t = 2^{a_1} 10^{a_2} 26^{a_3} p^{a_4}$ , where  $a_1, a_2, a_3$  are nonnegative integers,  $p \in \{34, 50, 58, 74, 82, 122, 202, 226\}$  and  $a_4 = 0$  or 1. The following orthogonal designs for computer experiments exist: (i)  $\text{OD}(2^{b+1}t; q_1^\ell)$  and (ii)  $\text{OD}(2^{b+1}t + s; q_2^\ell)$ ,  $\ell \leq 2^b t$ , for  $b = 1, 2, 3$ , for any positive integer  $s$ ,  $q_1 = 2, \dots, 2^{b+1}$ , and  $q_2 = 3, \dots, 2^{b+1} + 1$ .*

*Proof.* The results follow from Theorem 2 by equating and/or killing levels, as needed, before foldover. Here equating means setting the largest level equal to the previous level, with repetition if necessary, and killing means setting the largest level equal to zero, with repetition if necessary.  $\square$

The proposed method can also be expanded and used for the construction of nearly orthogonal designs, as in Bingham et al. (2009). In such cases, the correlation of the derived designs is pre-calculated by the periodic function of the used row vectors and the design structure.

**THEOREM 3.** *Let  $t = 2^{a_1} 10^{a_2} 26^{a_3} p^{a_4}$ , where  $a_1, a_2, a_3$  are nonnegative integers,  $p \in \{34, 50, 58, 74, 82, 122, 202, 226\}$  and  $a_4 = 0$  or 1. The following nearly orthogonal designs for computer experiments exist: (i)  $\text{NOD}(2(2^b t + 1); [\{2(2^{b+1} + 1)\}^\ell])$ , (ii)  $\text{NOD}(2^{b+1}t + s + 2; (2^{b+1} + 3)^\ell)$ , (iii)  $\text{NOD}(2^2(2^{b-1}t + 1); [\{2^2(2^{b-1} + 1)\}^\ell])$  and (iv)  $\text{NOD}(2^{b+1}t + s + 4; (2^{b+1} + 5)^\ell)$ ,  $\ell \leq 2^b t$ , for  $b = 1, 2, 3$  and for any positive integer  $s$ .*

*Proof.* To prove the existence of the nearly orthogonal designs described in (i), (ii), (iii) and (iv), we use the construction given in (4), (5), (6), and (7) respectively. From Lemma 2 we have that matrices  $\{A_i\}_{i=1}^8$  are circulant, additive and amicable. For  $b = 1, 2, 3$  and a fixed  $1 \leq \ell \leq 2^b t$ , the desired nearly orthogonal design (i), (ii), (iii), or (iv) is obtained by randomly selecting any  $\ell$  columns from the matrix  $(C_{2^b}^T, 1^T, -1^T, -C_{2^b}^T)^T$ ,  $(C_{2^b}^T, 1^T, 0_{2^b t \times s}^T, -1^T, -C_{2^b}^T)^T$ ,  $(C_{2^b}^T, 3^T, 1^T, -1^T, -3^T, -C_{2^b}^T)^T$ , or  $(C_{2^b}^T, 2^T, 1^T, 0_{2^b t \times s}^T, -1^T, -2^T, -C_{2^b}^T)^T$ , respectively, where  $C_{2^b}$  is the square matrix of order  $2^b t$  obtained using  $\{A_1, \dots, A_{2^b}\}$ .  $\square$

A design is called  $\ell$ -orthogonal if the sum of the elementwise products of any  $\ell$  columns is zero. Obviously, an  $\ell$ -orthogonal design is mean orthogonal when  $\ell = 1$  and its main effects are pairwise orthogonal when  $\ell = 2$ . From the foldover structure of the designs we have the following lemma.

**LEMMA 3.** *All the designs constructed by Theorems 2 and 3 are  $2\ell + 1$  orthogonal,  $\ell$  any nonnegative integer.*

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