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Title: Selection Between Variance-Optimal and Bias-Optimal Designs when Some Two-Factor Interactions are Important

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Abstract

Fractional factorial designs are useful for collecting data in many fields of studies because they allow us to study the effects of many factors on the response. As the primary interest of most experiments is for screening important factors, interactions are generally assumed to be negligible. When some two-factor interactions are important, variance-optimal designs and bias-optimal designs are available. In this study, we compare these two types of designs by using a mean squared error criterion that takes effect sparsity into consideration. We obtain a closed-form expression of this mean squared error criterion for the two types of designs. Under different levels of sparsity, results are obtained for designs of 10, 12, 14, 20, 26, 28 runs, which will help practitioners to choose between the two types of designs.

Keywords: Effect sparsity; foldover design; mean squared error criterion; orthogonal array

D d ca

To my dearest and the loveliest lady, my grandma, Peiyin Lin.

Ac d

Praise to my God, the Almighty, who is my strength and my shield! Thank You for Your unconditional love that I could be able to do everything in You. I would also like to express my deepest appreciation to my supervisor, Dr. Boxin Tang, for his constant support over the past few years during my undergraduate and master's study at SFU. I am thankful for his guidance and effort in helping me through my graduate and my project. A special gratitude to Guanzhou Chen, who provided me with his kind help when I encountered with difficulties on my project. Further, an enormous 'Thank You' to the wonderful instructors I have worked with closely, Dr. Lloyd Elliott and Ian Bercovitz, for their encouragements and patience in guiding me at each step of work. I especially want to thank Dr. Rachel Altman for spending time not only helping me with my schoolwork, but also providing me with helpful suggestions in my life. Also, I sincerely thank Sadika Jungic for encouraging me to ask for every opportunity that help achieve my goal, and thanks to Charlene Bradbury for her generous help. Thank you to all the faculty members and staffs in our department that made my time at SFU so comfortable as home. From outside the department, a thank you to Dr. Wan-Cheng Tan for her guidance in maturing my writing skill and improving my professions at work. Last but not least, the biggest thank you for the love and support from my family, my church family and friends, and my best friend and partner, Shanzhao.

Tab C

C a 1

I d c

Factorial designs are useful for examining which factors have primary effects on a response variable in a factor-screening experiment (Cheng, 2016). In general, a two-level factorial design consists of two or more factors, where each factor has two levels represented by ± 1. Each combination of levels of the factors is called a treatment or a run, and the change caused by a treatment or a run to the response is called an effect. A full factorial design consists of all possible combinations of the factors, and it requires a run size to be a power of two when there are two levels per factor. We use m to denote the number of factors in a two-level factorial design. Given that m factors are to be studied, at least 2^m runs are needed in order to estimate all $2^m - 1$ effects. However, higher-order interaction effects are generally not expected to be important in a screening experiment. Fractional factorial designs are more popular because they allow us to study the effects of multiple factors using only a fraction of runs from a full factorial design. One consequence of using a fractional factorial design is that some effects may not be distinguishable from other effects, and this is known as aliasing or confounding. There are two common ways to construct fractional factorial designs, which give rise to regular and nonregular designs.

A regular design is generally referred to as a $^{m-}$

2m 2m

the two remaining factors, we use generators D=AB and E=AC, meaning that the column for factor D is obtained by multiplying the elements in the columns of A and B, and the column for factor E is obtained by multiplying columns A and C. The effects in a $^{m-p}$ fractional factorial design are either orthogonal or fully aliased.

Nonregular designs such as Plackett-Burman designs (Plackett & Burman, 1946) are orthogonal arrays, which can be obtained by selecting columns from a Hadamard matrix. A Hadamard matrix is a square matrix of entries ± 1 with orthogonal columns. For example, to create an orthogonal array for five factors and eight runs, we select any five columns from an $\times$ Hadamard matrix with an exception of a column of all $+1$'s. The main difference between a regular design and a nonregular design is that, for a nonregular design, two effects can be partially aliased. The run sizes of nonregular designs are more flexible than regular designs, and they only need to be multiples of four.

We consider the problem of estimating main effects, but allow possible existence of two-factor interactions (2fis). In this case, orthogonal arrays and nearly orthogonal arrays are variance-optimal but not bias-optimal. On the other hand, non-orthogonal foldover designs as considered by Margolin (1969) and further studied by Miller and Sitter (2005) are bias-optimal but not variance-optimal. The thrust of this project is to evaluate and compare these two types of designs using a mean squared error criterion that takes effect sparsity into consideration.

We now give an overview. In Chapter 2, we introduce linear models, discuss orthogonal

C a 2

M d y

Section 2.1 introduces two linear models that are used in our study. In Section 2.2, we provide construction details and properties of variance-optimal designs, orthogonal arrays and related designs. We discuss bias-optimal designs, those given by foldover designs in Section 2.3. Lastly, an MSE criterion with consideration of sparsity for comparing the two types of designs is presented in Section 2.4.

2.1 T L a M d

Consider a fractional factorial design involving $m \geqslant$

$$
\begin{aligned}
E(\beta^{(1)}) &= (X_1^T X_1)^{-1} X_1^T E(Y) \\
&= (X_1^T X_1)^{-1} X_1^T X_1 \beta^{(1)} \\
&= \beta^{(1)}
\end{aligned}
$$

$\beta^{(1)} = (X_1^T X_1)^{-1} X_1^T Y$ now has an expectation

$$
\begin{aligned}
E(\beta^{(1)}) &= (X_1^T X_1)^{-1} X_1^T E(Y) \\
&= (X_1^T X_1)^{-1} X_1^T (X_1 \beta^{(1)} + X \ \beta^{(\ )}) \\
&= (X_1^T X_1)^{-1} X_1^T X_1 \beta^{(1)} + (X_1^T X_1)^{-1} X_1^T X \ \beta^{(\ )} \\
&= \beta^{(1)} + (X_1^T X_1 \ _1 E \ _1 \ ^T \quad X \quad t \quad f
\end{aligned}
$$

an $OA(\ ,\ ,$ [illegible]$)$:

A	B	C	D
1	1	1	1
1	1	-1	-1
1	-1	1	-1
1	-1	-1	1
-1	1	1	-1
-1	1	-1	1
-1	-1	1	1
-1	-1	-1	-1

In this example, the eight triplets, $(1, 1, 1)$, $(1, 1, -1)$, $(1, -1, 1)$, $(1, -1, -1)$, $(-1, 1, 1)$, $(-1, 1, -1)$, $(-1, -1, 1)$, $(-1, -1, -1)$ appear exactly once in any three columns. Furthermore, each column in this array is orthogonal to another column and is also orthogonal to the products of any two columns. This implies that we can obtain unbiased estimates for the main eects even when some 2fis are important. In general, OAs of strength three allow main eects to be estimated with minimum variance and without bias. A disadvantage of OAs of strength three is that the run size needs to be a multiple of eight. For run sizes of 12, 20 and 28 in our study, no OAs of strength three can exist. In this situation, we consider using OAs of strength two, which still optimize the variance, but the estimate of $\beta^{(1)}$ is no longer unbiased if not all 2fis are negligible. OAs of strength two are optimal for estimating the main eects, but they require run sizes to be multiples of four. If a design of run size n when n is even but not a multiple of four is desired, we can obtain an optimal design by adding two specific runs to an OA. The resulting nearly orthogonal array (NOA) is still optimal. This result, avaiable in Dey and Mukerjee (1999), is given below.

Lemma 1. [illegible] ℓ_1 [illegible] $(1, \ldots, 1)$ [illegible] ℓ [illegible] $(1, \ldots, 1, -1, \ldots, -1)$ [illegible]

The first run ℓ_1 is a vector containing m $+1$'s. The second run ℓ is a vector of m_1 $+1$'s and m -1's, where m_1 is the largest integer that is smaller than or equal to $m/2$, and

m is the smallest integer that is greater than or equal to $m/2$. For example, in order to construct a 10-run NOA with 5 factors, we first obtain an $OA(\ , \ \ , \ )$ matrix by selecting five columns from an $\ \times\ $ Hadamard matrix, as displayed below:

A	B	C	D	E
1	1	1	1	1
-1	1	-1	1	$-$

C a 3

R

Section 3.1 presents the results of our study. We compare the MSEs of variance-optimal

Table 3.1: Comparison of variance, bias and MSE for OA/NOA and BFD when all 2fis are important

			OA/NOA			BFD		
n	m	$C = \frac{\tau}{\sigma}$	Variance	Bias	MSE	Variance	Bias	MSE
10	5	0.025	0.536	0.004	0.539	0.556	0	0.556
		0.05	0.536	0.014	0.55	0.556	0	0.556
		0.1	0.536	0.057	0.592	0.556	0	0.556
		0.25	0.536	0.353	0.88[(0.014)-23457933.55259999 (0.353 0 1 17 (0.556)]TJ2.5			

20	10	0.025	0.5	0.013	0.513	0.556	0	0.556
		0.05	0.5	0.053	0.553	0.556	0	0.556
		0.1	0.5	0.211	0.711	0.556	0	0.556
		0.25	0.5	1.32	1.82	0.556	0	0.556
		0.5	0.5	5.28	5.78	0.556	0	0.556
		1	0.5	21.12	21.62	0.556	0	0.556
		2	0.5	84.48	84.98	0.556	0	0.556
26	13	0.025	0.513	0.023	0.536	0.52	0	0.52
		0.05	0.513	0.091	0.604	0.52	0	0.52
		0.1	0.513	0.362	0.875	0.52	0	0.52
		0.25	0.513	2.265	2.778	0.52	0	0.52
		0.5	0.513	9.058	9.571	0.52	0	0.52
		1	0.513	36.232	36.745	0.52	0	0.52
		2	0.513	144.928	145.441	0.52	0	0.52
28	14	0.025	0.5	0.028	0.528	0.538	0	0.538
		0.05	0.5	0.111	0.611	0.538	0	0.538
		0.1	0.5	0.443	0.943	0.538	0	0.538
		0.25	0.5	2.77	3.27	0.538	0	0.538
		0.5	0.5	11.082	11.582	0.538	0	0.538
		1	0.5	44.327	44.827	0.538	0	0.538
		2	0.5	177.306	177.806	0.538	0	0.538

From Table 3.1, we observe that the MSEs for variance-optimal designs are small at lower values of C. This makes sense when we look back at equation (2.4), where the variance of estimated main effects remains unchanged for both variance-optimal and bias-optimal designs as τ changes, but the bias varies with τ for variance-optimal designs. Thus, when τ

is small, the bias (and correspondingly the MSE) for variance-optimal designs is also small. We see that before C reaches a boundary point, the MSE of a variance-optimal design is smaller than the MSE of a bias-optimal design, and this suggests that designs such as OAs and NOAs are better than BFDs at lower values of C. For example, between the two designs of 14 runs, when $C < 0.$, the NOA gives lower Δ values than the BFD, and this indicates that practitioners should consider using the NOA as it performs better than the BFD.

But, when sparsity is considered, for instance, suppose 0% of 2fis are nonnegligible, that is when $\pi = 1/$, the bias of the NOA with seven factors needs to be multiplied by π based on Equation (2.4), which gives a smaller value of Δ than the one with a full set of important 2fis. Table 3.2 provides the C^* values for different designs and different levels of sparsity when $C = \frac{\tau}{\sigma} < C^*$, variance-optimal designs are better than bias-optimal designs. Taking $n = 14$ as an example, C^* values are 0.157, 0.222, and 0.314 for $\pi = 1, 1/$ and $1/4$,

Figure 3.1: Comparisons of Δ values of variance-optimal design (red line) and bias-optimal design (blue line) for n = 14 when π = 1, 1/2, 1/4, 1/8, 1/16, 1/32

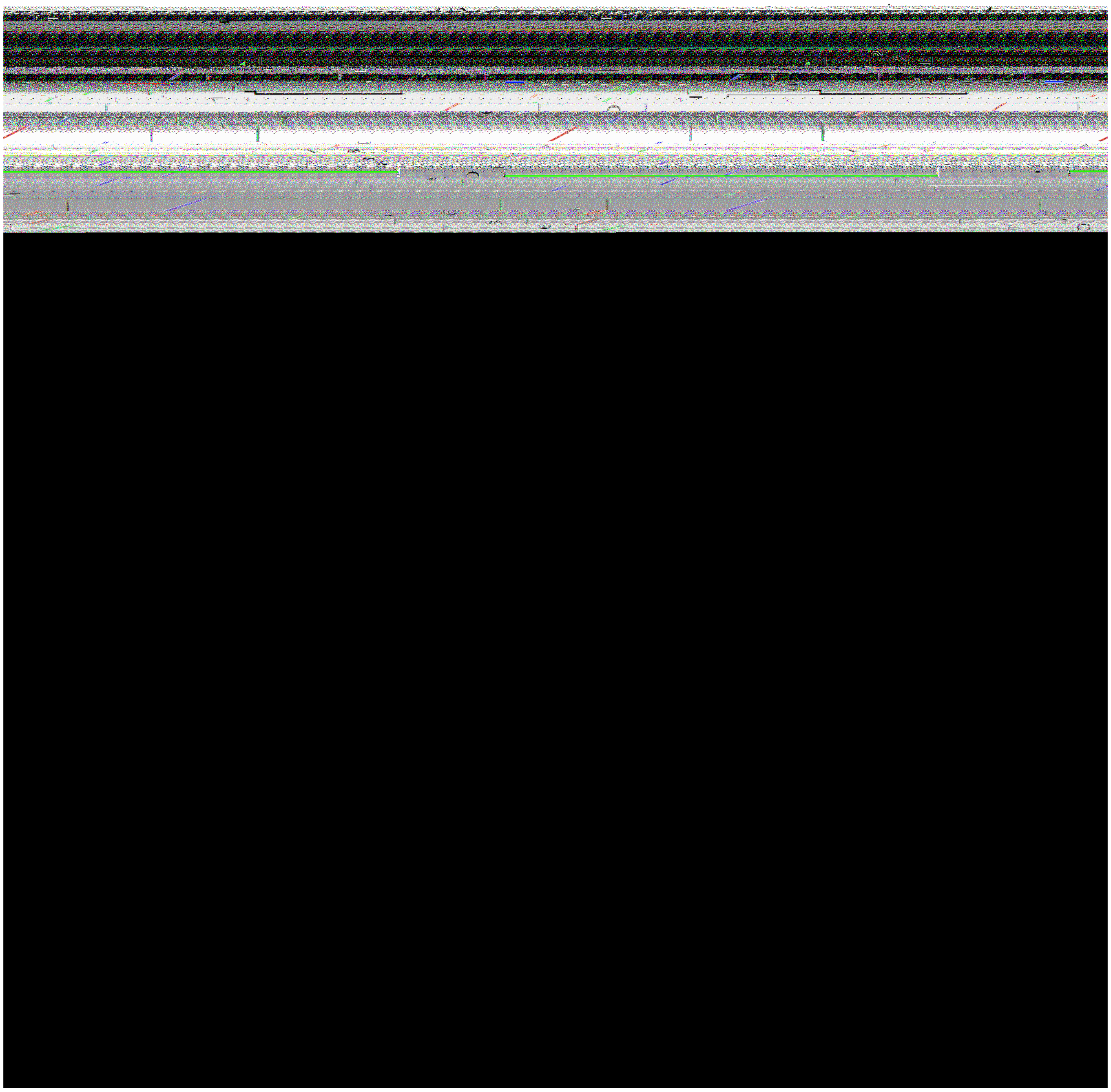
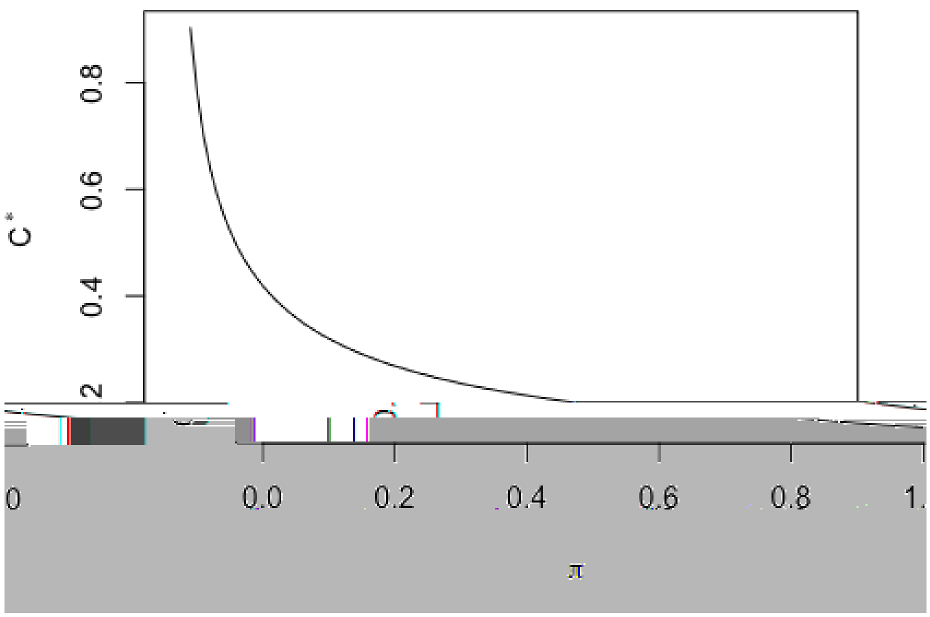


Figure 3.2: Change of C^* values at different π for designs of 14 runs



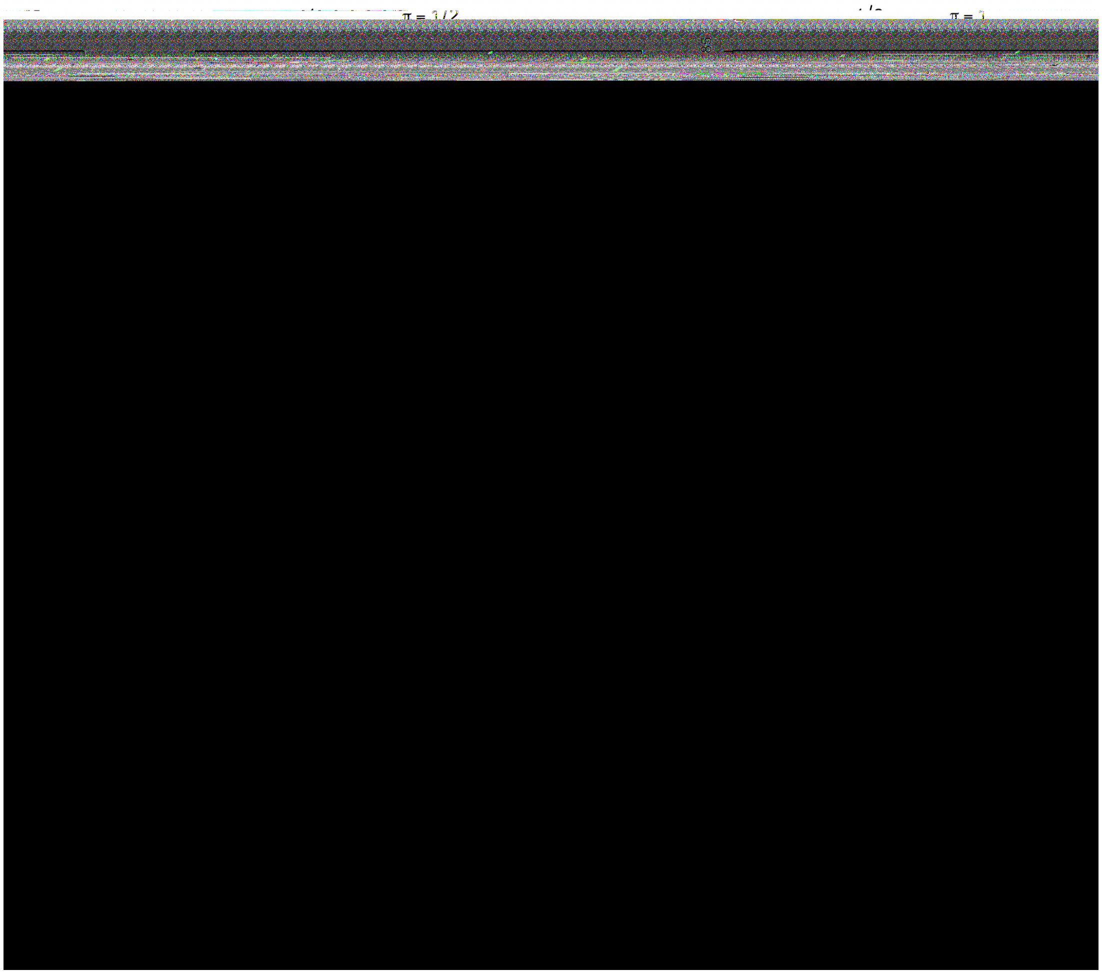
3.2 A A a D

rounded up to three decimal places. For example, when all 2fis are significant, that is when $\pi = 1$, as long as $0.0 \quad < C = \frac{\tau}{\sigma} < 0. \ 1$, the alternative design is the best among the three designs. Figure 3.3 displays a more detailed comparison of the Δ values of the three types of designs: alternative design (green line), variance-optimal design (red line), bias-optimal design (blue line) for diﬀerent C values for diﬀerent given π values. As clearly shown in Figure 3.3, the variance-optimal design is the best if $C < C_1$; the alternative design is the best if $C_1 < C < C$; and the bias-optimal design is the best if $C > C$.

Table 3.3: Range of C Values for Alternative Design to be the Optimal Design with 14 Runs

	$\pi = \mathbf{1}$	$\pi = \mathbf{1/2}$	$\pi = \mathbf{1/4}$	$\pi = \mathbf{1/8}$	$\pi = \mathbf{1/16}$	$\pi = \mathbf{1/32}$
1	0.065	0.091	0.129	0.182	0.257	0.363
2	0.219	0.309	0.437	0.618	0.873	1.235

Figure 3.3: Comparisons of Δ values of alternative design (green line), variance-optimal design (red line) and bias-optimal design (blue line) for n =14 when π = 1, 1/2, 1/4, 1/8, 1/16, 1/32



R c

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A d A

Va a c - a D

For n=10,

A	B	C	D	E
1	1	1	1	1
−1	1	−1	1	−1
1	−1	−1	1	1
−1	−1	1	1	−1
1	1	1	−1	−1
−1	1	−1	−1	1
1	−1	−1	−1	−1
−1	−1	1	−1	1
1	1	1	1	1
1	1	−1	−1	−1

For n=12,

A	B	C	D	E	F								
1	−1	−1	−1	1	−1								
1	1	−1	1	1	1								
1	1	1	−1	−1		1	1	1	1(1) 1	1 001 11	1	1	1
				1	1	1	1	1					
		1	1	1	1	1							
1	1	1	1	1									

For n=14,

A	B	C	D	E	F	G
−1	−1	1	−1	1	1	−1
−1	−1	−1	1	−1	1	1
1	−1	−1	−1	1	−1	1
−1	−1	−1	−1	−1	−1	−1
1	1	−1	−1	−1	1	−1
1	1	1	−1	−1	−1	1
1	1	−1	1	1	1	−1
−1	1	−1	1	1	−1	1
1	−1	1	1	−1	1	1
1	−1	1	1	1	−1	−1
−1	1	1	−1	1	1	1
−1	1	1	1	−1	−1	−1
1	1	1	1	1	1	1
1	1	1	−1	−1	−1	−1

For n=20,

A	B	C	D	E	F	G	H	I	J
1	1	−1	−1	1	1	1	1	−1	1
1	1	−1	1	−1	1	−1	−1	−1	−1
−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
1	−1	1	1	−1	−1	1	1	1	1
1	1	1	−1	1	−1	1	−1	−1	−1
−1	1	−1	1	−1	−1	−1	−1	1	1
1	1	−1	1	1	−1	−1	1	1	1
1	−1	−1	1	1	1	1	−1	1	−1
−1	−1	−1	1	1	−1	1	1	−1	−1
−1	1	1	1	1	−1	1	−1	1	−1
−1	1	1	−1	1	1	−1	−1	1	1
−1	−1	1	1	−1	1	1	−1	−1	1
1	1	1	1	−1	1	−1	1	−1	−1
1	−1	1	−1	−1	−1	−1	1	1	−1
−1	1	−1	−1	−1	−1	1	1	−1	1
1	−1	−1	−1	−1	1	1	−1	1	1
−1	−1	1	1	1	1	−1	1	−1	1
−1	−1	−1	−1	1	1	−1	1	1	−1
1	−1	1	−1	1	−1	−1	−1	−1	1
−1	1	1	−1	−1	1	1	1	1	−1

For n=26,

$$A \quad B \quad C \quad D \quad E \quad F \quad G \quad H \quad I \quad J \quad K \quad L \quad M$$

For n=28,

A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1
1	−1	−1	−1	−1	1	1	−1	−1	1	1	−1	−1	1
1	−1	1	1	1	1	−1	−1	−1	−1	1	−1	−1	−1
1	−1	−1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
−1	−1	1	1	−1	−1	1	−1	−1	−1	1	1	1	1
1	−1	−1	1	−1	−1	−1	−1	1	1	1	−1	1	1
1	1	1	−1	−1	−1	1	1	−1	1	−1	−1	1	−1
−1	1	−1	−1	1	−1	1	−1	−1	−1	1	1	−1	1
1	−1	1	1	1	−1	1	−1	1	−1	−1	−1	1	−1
−1	1	1	1	1	1	−1	−1	−1	1	−1	−1	−1	1
1	1	1	−1	−1	−1	−1	1	1	−1	1	−1	−1	1
1	−1	1	−1	1	1	−1	1	1	−1	1	1	1	1
1	1	−1	1	1	−1	−1	1	1	1	1	1	−1	−1
−1	1	−1	−1	−1	1	−1	−1	1	1	1	−1	1	−1
−1	1	−1	1	−1	−1	−1	1	−1	−1	1	1	1	−1
−1	−1	−1	−1	1	1	1	1	1	−1	1	−1	1	−1
−1	−1	1	−1	1	−1	−1	−1	1	1	−1	1	1	1
−1	1	1	1	−1	1	−1	1	1	−1	−1	−1	−1	1
1	1	−1	1	−1	1	1	−1	1	1	−1	1	1	1
−1	−1	1	−1	−1	1	−1	1	−1	1	−1	1	1	−1
1	1	−1	1	1	1	−1	−1	−1	−1	−1	1	1	−1
−1	1	1	−1	1	1	1	−1	1	1	1	1	−1	−1
−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1
1	−1	1	1	−1	1	1	1	−1	1	1	1	−1	−1
−1	−1	−1	1	−1	1	1	1	1	−1	−1	1	−1	1
−1	−1	−1	1	1	−1	1	1	1	1	−1	−1	−1	−1
−1	1	1	1	1	−1	1	1	−1	1	1	−1	1	1
1	1	1	−1	−1	−1	1	−1	1	−1	−1	1	−1	−1

A d B

B a - a D

For n=10,

A	B	C	D	E
1	1	1	−1	1
1	1	−1	1	1
1	−1	1	1	1
−1	1	1	1	1
−1	−1	−1	−1	1

For n=14,

A	B	C	D	E	F	G
1	−1	−1	−1	−1	−1	−1
−1	1	−1	−1	−1	−1	−1
−1	−1	1	−1	−1	−1	−1
−1	−1	−1	1	−1	−1	−1
−1	−1	−1	−1	1	−1	−1
−1	−1	−1	−1	−1	1	−1
−1	−1	−1	−1	−1	−1	1
−1	1	1	1	1	1	1
1	−1	1	1	1	1	1
1	1	−1	1	1	1	1
1	1	1	−1	1	1	1
1	1	1	1	−1	1	1
1	1	1	11	−		

1 1 −1 −1 −1111 0 1 11 1 1 1

−1 1 −1 −1 −1

1 1 −1 −1 − −1

1 1 −1 −1 −1 −1 1 −1 −

−1 −1 −1 1 −1 −1 −1 −1 1 −

−1 −1 −1 −1 1 −1 −1 −1 −1 1 11 11

− 1 − 1 1 − 4 1− − 1 −1 −1 −1 −1

For n=26,

A	B	C	D	E	F	G	H	I	J	K	L	M
1	1	−1	1	−1	−1	−1	−1	−1	1	−1	−1	−1
−1	1	1	−1	1	−1	−1	−1	−1	−1	1	−1	−1
−1	−1	1	1	−1	1	−1	−1	−1	−1	−1	1	−1
−1	−1	−1	1	1	−1	1	−1	−1	−1	−1	−1	1
1	−1	−1	−1	1	1	−1	1	−1	−1	−1	−1	−1
−1	1	−1	−1	−1	1	1	−1	1	−1	−1	−1	−1
−1	−1	1	−1	−1	−1	1	1	−1	1	−1	−1	−1
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−1	−1	−1	−1	−1	1	−1	−1	−1	1	1	−1	1
1	−1	−1	−1	−1	−1	1	−1	−1	−1	1	1	−1
−1	1	−1	−1	−1	−1	−1	1	−1	−1	−1	1	1
1	−1	1	−1	−1	−1	−1	−1	1	−1	−1	−1	1
−1	−1	1	−1	1	1	1	1	1	−1	1	1	1
1	−1	−1	1	−1	1	1	1	1	1	−1	1	1
1	1	−1	−1	1	−1	1	1	1	1	1	−1	1
1	1	1	−1	−1	1	−1	1	1	1	1	1	−1
−1	1	1	1	−1	−1	1	−1	1	1	1	1	1
1	−1	1	1	1	−1	−1	1	−1	1	1	1	1
1	1	−1	1	1	1	−1	−1	1	−1	1	1	1
1	1	1	−1	1	1	1	−1	−1	1	−1	1	1
1	1	1	1	−1	1	1	1	−1	−1	1	−1	1
1	1	1	1	1	−1	1	1	1	−1	−1	1	−1
−1	1	1	1	1	1	−1	1	1	1	−1	−1	1
1	−1	1	1	1	1	1	−1	1	1	1	−1	−1
−1	1	−1	1	1	1	1	1	−1	1	1	1	−1

For n=28,

A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	−1	−1	−1	−1	−1	−1	1	1	−1	1	−1	−1	−1
−1	1	−1	−1	−1	−1	−1	1	−1	1	−1	−1	−1	1
−1	−1	1	−1	−1	−1	−1	−1	1	−1	−1	−1	1	1
−1	−1	−1	1	−1	−1	−1	1	−1	−1	−1	1	1	−1
−1	−1	−1	−1	1	−1	−1	−1	−1	−1	1	1	−1	1
−1	−1	−1	−1	−1	1	−1	−1	−1	1	1	−1	1	−1
−1	−1	−1	−1	−1	−1	1	−1	1	1	−1	1	−1	−1
−1	−1	1	−1	1	1	1	1	−1	−1	−1	−1	−1	−1
−1	1	−1	1	1	1	−1	−1	1	−1	−1	−1	−1	−1
1	−1	1	1	1	−1	−1	−1	−1	1	−1	−1	−1	−1
−1	1	1	1	−1	−1	1	−1	−1	−1	1	−1	−1	−1
1	1	1	−1	−1	1	−1	−1	−1	−1	−1	1	−1	−1
1	1	−1	−1	1	−1	1	−1	−1	−1	−1	−1	1	−1
1	−1	−1	1	−1	1	1	−1	−1	−1	−1	−1	−1	1
−1	1	1	1	1	1	1	−1	−1	1	−1	1	1	1
1	−1	1	1	1	1	1	−1	1	−1	1	1	1	−1
1	1	−1	1	1	1	1	1	−1	1	1	1	−1	−1
1	1	1	−1	1	1	1	−1	1	1	1	−1	−1	1
1	1	1	1	−1	1	1	1	1	1	−1	−1	1	−1
1	1	1	1	1	−1	1	1	1	−1	−1	1	−1	1
1	1	1	1	1	1	−1	1	−1	−1	1	−1	1	1
1	1	−1	1	−1	−1	−1	−1	1	1	1	1	1	1
1	−1	1	−1	−1	−1	1	1	−1	1	1	1	1	1
−1	1	−1	−1	−1	1	1	1	1	−1	1	1	1	1
1	−1	−1	−1	1	1	−1	1	1	1	−1	1	1	1
−1	−1	−1	1	1	−1	1	1	1	1	1	−1	1	1
−1	−1	1	1	−1	1	−1	1	1	1	1	1	−1	1
−1	1	1	−1	1	−1	−1	1	1	1	1	1	1	−1