Construction of large two-level nonregular designs of strength three

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Outline

1. Introduction

2. Evaluation of designs

3. Construction method

4. Results and discussion



Applications of large two-level orthogonal designs

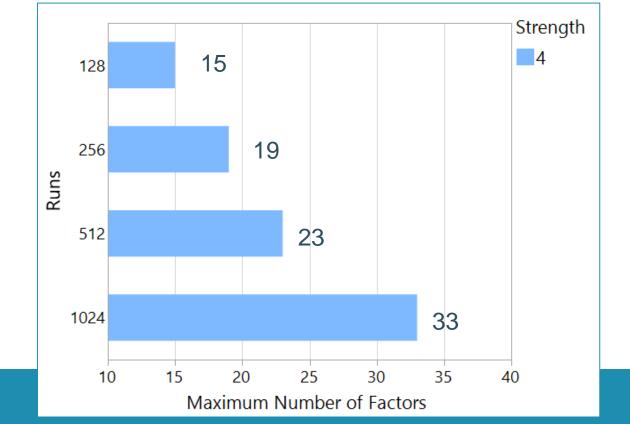
- Simulation of a software development process: 128 runs & 30 factors (Houston et al. 2001).
- Simulation of a combat aircraft: 1024 runs & 40 factors (Lefebvre et al. 2010).
- Investigate the regulation of specific cells: 128 runs & 13 factors (Barminko et al. 2014).
- Develop treatments to inhibit Tuberculosis: 128 runs & 14 factors (Silva et al. 2016).

Goal: Study the main effects and two-factor interactions of the factors.

Literature review

Strength-4 orthogonal designs. Properties:

 All main effects and all two-factor interactions are orthogonal to each other.

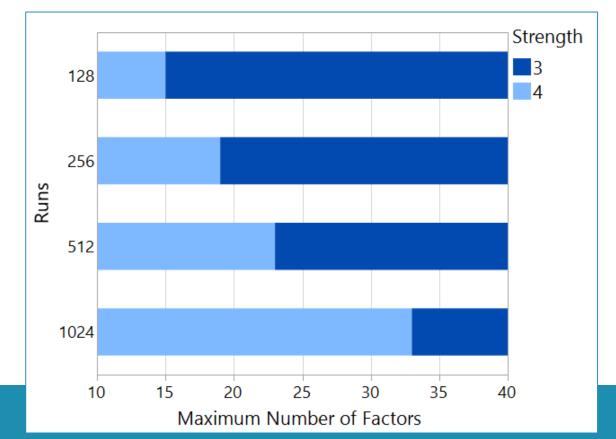


See Hedayat et al. (1999), Mee (2004), Sanchez & Sanchez (2005), Xu (2009) and Schoen et al. (2010).

Literature review

Strength-3 orthogonal designs. Properties:

- 1. Main effects are orthogonal to the two-factor interactions.
- 2. Pairs of two-factor interactions can be correlated.

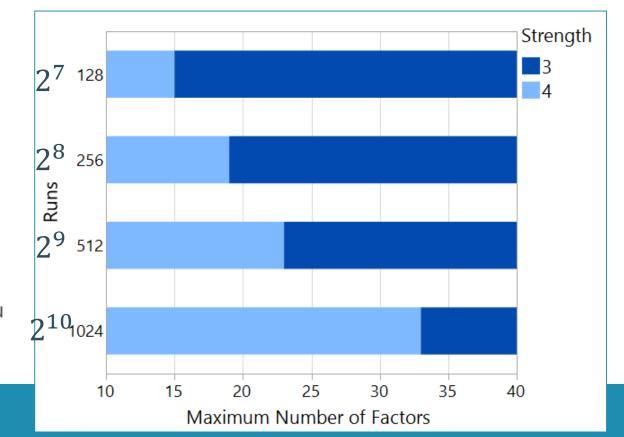


See Block & Mee (2005), Xu & Wong (2007), Xu (2009), Ryan & Bulutoglu (2010).

Literature review

Strength-3 orthogonal designs. Properties:

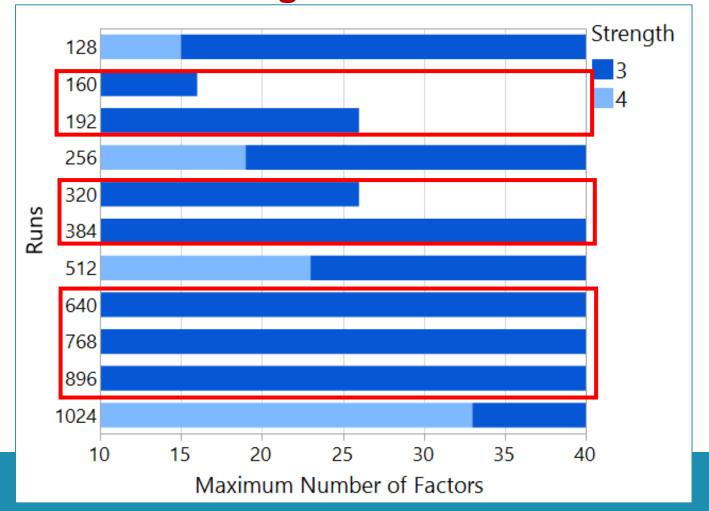
- 1. Main effects are orthogonal to the two-factor interactions.
- 2. Pairs of two-factor interactions can be correlated.



See Block & Mee (2005), Xu & Wong (2007), Xu (2009), Ryan & Bulutoglu (2010).

This talk

Alternative strength-3 orthogonal designs which fill the gaps between the available designs.



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Evaluating two-level strength-3 designs

Example I: Compare experimental designs with 32 runs and 10 factors.

Regular resolution-IV design

Nonregular strength-3 design

1	2	3	4	5	6	7	8	9	10
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	1	1	1	1
-1	-1	-1	-1	1	1	-1	-1	1	1
-1	-1	-1	-1	1	1	1	1	-1	-1
-1	-1	1	1	-1	-1	-1	-1	-1	-1
-1	-1	1	1	-1	1	-1	1	1	1
-1	-1	1	1	1	-1	1	1	-1	1
-1	-1	1	1	1	1	1	-1	1	-1
-1	1	-1	1	-1	-1	1	-1	1	1
-1	1	-1	1	-1	1	1	1	-1	-1
-1	1	-1	1	1	-1	-1	1	1	-1
-1	1	-1	1	1	1	-1	-1	-1	1
-1	1	1	-1	-1	1	-1	1	1	-1
-1	1	1	-1	-1	1	1	-1	-1	1
-1	1	1	-1	1	-1	-1	1	-1	1
-1	1	1	-1	1	-1	1	-1	1	-1
1	-1	-1	1	-1	1	-1	1	-1	1
1	-1	-1	1	-1	1	1	-1	1	-1
1	-1	-1	1	1	-1	-1	1	1	-1
1	-1	-1	1	1	-1	1	-1	-1	1
1	-1	1	-1	-1	-1	1	1	1	-1
1	-1	1	-1	-1	1	1	-1	-1	1
1	-1	1	-1	1	-1	-1	-1	1	1
1	-1	1	-1	1	1	-1	1	-1	-1
1	1	-1	-1	-1	-1	-1	1	-1	1
1	1	-1	-1	-1	1	-1	-1	1	-1
1	1	-1	-1	1	-1	1	-1	-1	-1
1	1	-1	-1	1	1	1	1	1	1
1	1	1	1	-1	-1	-1	-1	1	1
1	1	1	1	-1	-1	1	1	-1	-1
1	1	1	1	1	1	-1	-1	-1	-1

Wu & Hamada (2009)

Schoen & Mee (2010)

How can we measure the correlation between pairs of two-factor interactions in strength-3 designs?

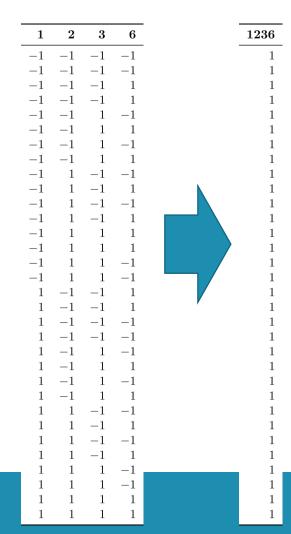
Compute the J_4 -characteristics (Deng & Tang, 1999) for all subsets of 4 factors.

Regular design

1	2	3	4	5	6	7	8	9	10
-1	-1	-1	-1	-1	-1	-1	-1	1	1
-1	-1	-1	-1	1	-1	-1	1	-1	-1
-1	-1	-1	1	-1	-1	1	-1	-1	-1
-1	-1	-1	1	1	-1	1	1	1	1
-1	-1	1	-1	-1	1	-1	-1	-1	-1
-1	-1	1	-1	1	1	-1	1	1	1
-1	-1	1	1	-1	1	1	-1	1	1
-1	-1	1	1	1	1	1	1	-1	-1
-1	1	-1	-1	-1	1	1	1	1	-1
-1	1	-1	-1	1	1	1	-1	-1	1
-1	1	-1	1	-1	1	-1	1	-1	1
-1	1	-1	1	1	1	-1	-1	1	-1
-1	1	1	-1	-1	-1	1	1	-1	1
-1	1	1	-1	1	-1	1	-1	1	-1
-1	1	1	1	-1	-1	-1	1	1	-1
-1	1	1	1	1	-1	-1	-1	-1	1
1	-1	-1	-1	-1	1	1	1	-1	1
1	-1	-1	-1	1	1	1	-1	1	-1
1	-1	-1	1	-1	1	-1	1	1	-1
1	-1	-1	1	1	1	-1	-1	-1	1
1	-1	1	-1	-1	-1	1	1	1	-1
1	-1	1	-1	1	-1	1	-1	-1	1
1	-1	1	1	-1	-1	-1	1	-1	1
1	-1	1	1	1	-1	-1	-1	1	-1
1	1	-1	-1	-1	-1	-1	-1	-1	-1
1	1	-1	-1	1	-1	$^{-1}$	1	1	1
1	1	-1	1	-1	-1	1	-1	1	1
1	1	-1	1	1	-1	1	1	-1	-1
1	1	1	-1	-1	1	-1	-1	1	1
1	1	1	-1	1	1	-1	1	-1	-1
1	1	1	1	-1	1	1	-1	-1	-1
1	1	1	1	1	1	1	1	1	1

How can we measure the correlation between pairs of two-factor interactions in strength-3 designs?

Compute the J_4 -characteristics (Deng & Tang, 1999) for all subsets of 4 factors.



Sum of all elements in the column:

$$j_4(\{1,2,3,6\}) = 32.$$

$$\frac{J_4(\{1,2,3,6\})}{|j_4(\{1,2,3,6\})|} = \frac{32}{32} = 1$$

3 pairs of interactions which are fully correlated: 12 & 36, 13 & 26, 16 & 23.



For regular designs, all J_4 -characteristics are either 0 or 1.

For nonregular designs, the J_4 -characteristics can have values of 0, 0.5 or 1 (Deng & Tang, 1999).

Two criteria to compare the correlation between pairs of two-factor interactions in regular and nonregular designs:

- The F_4 vector. Alternative summaries of all the J_4 -
- The B_4 value. characteristics.

The F_4 vector

The F_4 vector has entries equal to the frequencies for the possible values of the J_4 -characteristics (Deng & Tang, 1999).

Example I (cont.): 32-run 10-factor designs.

Regular design

$$F_4(1, 0.5) = (10, 0)$$

30 pairs of 2FIs

Nonregular design

$$F_4(1, 0.5) = (1, 62)$$

189 pairs of 2FIs

Sequentially minimizing F_4 is equivalent to minimizing: (1) the maximum absolute correlation between pairs of two-factor interactions; and, (2) the total number of pairs involved.

The B_4 value

The B_4 value is the sum of squared J_4 -characteristics (Tang & Deng, 1999).

Example I (cont.): 32-run 10-factor designs.

Regular design

$$B_4 = 10(1)^2 + 0(0.5)^2 = 10$$

Nonregular design

$$B_4 = 1(1)^2 + 62(0.5)^2 = 16.5$$

Minimizing B_4 is equivalent to minimizing the sum of squared correlations between pairs of two-factor interactions.

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Construction by example

Example II: Construct a two-level design with 96 runs and 14 factors.

Step 1: Consider the 32-run 14-factor, MA regular design, call it 2¹⁴⁻⁹.

Step 2: Construct the concatenated design *D*.

Step 3: Consider column permutations and fold-overs of columns in the copies of 2^{14-9} to sequentially minimize F_4 or minimize the B_4 value of D.

$$D = \begin{pmatrix} 2^{14-9} \\ 2^{14-9} \\ 2^{14-9} \end{pmatrix}$$

See also Addelman (1961), Pajak & Addelman (1975), Mee (2004).



Construction by example

Example II: Construct a two-level design with 96 runs and 14 factors.

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$$D = \begin{pmatrix} 2^{14-9} \\ 2^{14-9} \\ 2^{14-9} \end{pmatrix}$$

Evaluating all possible concatenated designs would require $2 \times 14! \times 2^{14} = 2.8 \times 10^{15}$ evaluations.

Factor column permutations

Generated factors

Basic factors

		Oic	, 10			Ochlerated						14000				
	1	2	9	4	F	23	124	134	234	125	135	235	145	245		
_	1	2	3	4	5	6	7	8	9	10	11	12	13	14		
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
	-1	-1	-1	-1	1	-1	-1	-1	-1	1	1	1	1	1		
	-1	-1	-1	1	-1	-1	1	1	1	-1	-1	-1	1	1		
	-1	-1	-1	1	1	-1	1	1	1	1	1	1	-1	-1		
	-1	-1	1	-1	-1	1	-1	1	1	-1	1	1	-1	-1		
	-1	-1	1	-1	1	1	-1	1	1	1	-1	-1	1	1		
	-1	-1	1	1	-1	1	1	-1	-1	-1	1	1	1	1		
4.4.0	-1	-1	1	1	1	1	1	-1	-1	1	-1	-1	-1	-1		
$2^{14-9} =$	-1	1	-1	-1	-1	1	1	-1	1	1	-1	1	-1	1		
Z^{-}	-1	1	-1	-1	1	1	1	-1	1	-1	1	-1	1	-1		
	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1	1	-1		
	-1	1	-1	1	1	1	-1	1	-1	-1	1	-1	-1	1		
	-1	1	1	-1	-1	-1	1	1	-1	1	1	-1	-1	1		
	-1	1	1	-1	1	-1	1	1	-1	-1	-1	1	1	-1		
	-1	1	1	1	-1	-1	-1	-1	1	1	1	-1	1	-1		
	-1	1	1	1	1	-1	-1	-1	1	-1	-1	1	-1	1		
	1	-1	-1	-1	-1	1	1	1	-1	1	1	-1	1	-1		
	1	-1	-1	-1	1	1	1	1	-1	-1	-1	1	-1	1		
	1	-1	-1	1	-1	1	-1	-1	1	1	1	-1	-1	1		
	1	-1	-1	1	1	1	-1	-1	1	-1	-1	1	1	-1		
	1	-1	1	-1	-1	-1	1	-1	1	1	-1	1	1	-1		
	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1	-1	1		
	1	-1	1	1	-1	-1	-1	1	-1	1	-1	1	-1	1		
	1	-1	1	1	1	-1	-1	1	-1	-1	1	-1	1	-1		
	1	1	-1	-1	-1	-1	-1	1	1	-1	1	1	1	1		
	1	1	-1	-1	1	-1	-1	1	1	1	-1	-1	-1	-1		
	1	1	-1	1	-1	-1	1	-1	-1	-1	1	1	-1	-1		
	1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	1	1		
	1	1	1	-1	-1	1	-1	-1	-1	-1	-1	-1	1	1		
	1	1	1	-1	1	1	-1	-1	-1	1	1	1	-1	-1		
	1	1	1	1	-1	1	1	1	1	-1	-1	-1	-1	-1		
	1	1	1	1	1	1	1	1	1	1	1	1	1	1		
_																

Permute the basic factors using linear permutations.

Factor column permutations

Generated factors

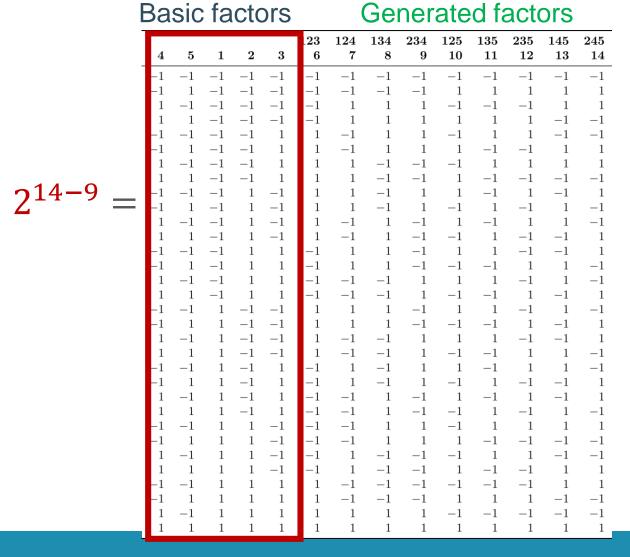
Basic factors

	Dasic factors				Generaled factors									
	5	1	2	3	4	.23 6	$124\\7$	$\frac{134}{8}$	$\begin{array}{c} 234 \\ 9 \end{array}$	$\frac{125}{10}$	$\frac{135}{11}$	$\begin{array}{c} 235 \\ 12 \end{array}$	$\frac{145}{13}$	$\frac{245}{14}$
_	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
	-1	$-1 \\ -1$	$-1 \\ -1$	$-1 \\ -1$	$-1 \\ 1$	$-1 \\ -1$	$-1 \\ 1$	$-1 \\ 1$	-1 1	$1 \\ -1$	$\begin{array}{c} 1 \\ -1 \end{array}$	$1 \\ -1$	1 1	1 1
	1	$-1 \\ -1$	$-1 \\ -1$	$-1 \\ -1$	1	$-1 \\ -1$	1	1	1	$\frac{-1}{1}$	1	-1	-1	-1
	-1	-1	-1	1	-1	1	-1	1	1	-1	1	1	-1	-1
	1	-1	-1	1	-1	1	-1	1	1	1	-1	-1	1	1
	-1	-1	-1	1	1	1	1	-1	-1	-1	1	1	1	1
4.4.0	1	$-1 \\ -1 \\ -1$	-1	1	1	1	1	-1	-1	1	-1	-1	-1	-1
$2^{14-9} =$	-1	-1	1	-1	-1	1	1	-1	1	1	-1	1	-1	1
<u>_</u>	1	-1	1	-1	-1	1	1	-1	1	-1	1	-1	1	-1
	-1	-1	1	-1	1	1	-1	1	-1	1	-1	1	1	-1
	1	-1	1	-1	1	1	-1	1	-1	-1	1	-1	-1	1
	-1	-1	1	1	-1	-1	1	1	-1	1	1	-1	-1	1
	1	-1	1	1	-1	-1	1	1	-1	-1	-1	1	1	-1
	1	$-1 \\ -1$	1 1	1 1	$\frac{1}{1}$	$-1 \\ -1$	$-1 \\ -1$	$-1 \\ -1$	$\frac{1}{1}$	$\begin{array}{c} 1 \\ -1 \end{array}$	$\begin{array}{c} 1 \\ -1 \end{array}$	$-1 \\ 1$	-1	-1 1
	-1	1	-1	-1	-1	1	1	1	-1	1	1	-1	$^{-1}$	-1
	1	1	-1	-1	-1	1	1	1	-1	-1	-1	1	-1	1
	-1	1	-1	-1	1	1	-1	-1	1	1	1	-1	-1	1
	1	1	-1	-1	1	1	-1	-1	1	-1	-1	1	1	-1
	-1	1	-1	1	-1	-1	1	-1	1	1	-1	1	1	-1
	1	1	-1	1	-1	-1	1	-1	1	-1	1	-1	-1	1
	-1	1	-1	1	1	-1	-1	1	-1	1	-1	1	-1	1
	1	1	-1	1	1	-1	-1	1	-1	-1	1	-1	1	-1
	-1	1	1	-1	-1	-1	-1	1	1	-1	1	1	1	1
	1	1	1	-1	-1	-1	-1	1	1	1	-1	-1	-1	-1
	-1	1	1	-1	1	-1	1	-1	-1	-1	1	1	-1	-1
	1	1	1	-1_{1}	1	-1	1	-1	-1	1	-1	-1	1	1
	- I 1	1 1	1 1	1 1	$-1 \\ -1$	1 1	$-1 \\ -1$	$-1 \\ -1$	-1 -1	-1 1	$-1 \\ 1$	$-1 \\ 1$	-1	$1 \\ -1$
	-1	1	1	1	$\frac{-1}{1}$	1	-1 1	-1 1	-1 1	-1	-1	-1	-1 -1	-1 -1
	1	1	1	1	1	1	1	1	1	1	1	1	1	1

Permute the basic factors using linear permutations.

Blue copy
$$2^{10-5}$$
Column New Position
$$\begin{array}{cccc}
1 & \rightarrow & 2 \\
2 & \rightarrow & 3 \\
3 & \rightarrow & 4 \\
4 & \rightarrow & 5 \\
5 & \rightarrow & 1
\end{array}$$

Factor column permutations



Permute the basic factors using linear permutations.

```
Red copy 2^{10-5}
Column New Position

\begin{array}{cccc}
1 & \rightarrow & 3 \\
2 & \rightarrow & 4 \\
3 & \rightarrow & 5 \\
4 & \rightarrow & 1 \\
5 & \rightarrow & 2
\end{array}
```

Theorem: Let 2^{m-p} be a regular design with a prime number of basic factors b = m - p. We can calculate the J_4 -characteristics of the concatenated design D from the ones of 2^{m-p} .

$$D = \begin{pmatrix} 2^{m-p} \\ 2^{m-p} \\ 2^{m-p} \end{pmatrix}$$
 Shift 1 position
 Shift 2 positions

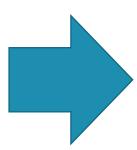
Theorem: Let 2^{m-p} be a regular design with a prime number of basic factors b = m - p. We can calculate the J_4 -characteristics of the concatenated design D from the ones of 2^{m-p} .

Let s be a 4-factor subset and $J_4(s; 2^{10-5}) = 1$.

• If $s = \{1, 2, 3, 6\}$ with a subset of basic factors,

$$\rightarrow J_4(\{1,2,3,6\};D) = J_4(\{2,3,4,6\};D) = J_4(\{3,4,5,6\};D) = 1/3.$$

For each s of this type in 2^{m-p}



d J_4 -characteristics equal to 1/d in D.

d = # concatenated copies of 2^{m-p} .

Theorem: Let 2^{m-p} be a regular design with a prime number of basic factors b = m - p. We can calculate the J_4 -characteristics of the concatenated design D from the ones of 2^{m-p} .

Let s be a 4-factor subset and $J_4(s; 2^{10-5}) = 1$.

- If $s = \{6, 7, 8, 9\}$ with only generated factors, $\rightarrow J_4(\{6, 7, 8, 9\}; D) = 1.$

If
$$J_4(s; 2^{14-9}) = 0 \rightarrow J_4(s; D) = 0$$
.

Example II (cont.):

32-run 14-factor design

Step 1:
$$2^{14-9}$$
 5 basic factors

$$F_4(1,0.5) = (77,0)$$

- 68 include basic factors
- 9 include only generated factors

96-run 14-factor design

Steps 2 & 3:
$$D = \begin{pmatrix} 2^{14-9} \\ 2^{14-9} \\ 2^{14-9} \end{pmatrix}$$
 Shift 1 position Shift 2 positions

$$F_4(1, 0.33) = (9, 204)$$

- 3 x 68 = 204 include basic factors
- 9 include only generated factors

How can we improve the 96-run concatenated design?



Step 3': Variable Neighborhood Search (VNS).

- Framework to develop effective algorithms.
- One move: Fold-over a column in a copy of 2^{14-9} .

$$F_4(1, 0.33) = (9, 204)$$

```
8 9 10 11 12 13 14
-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
```



Step 3': Variable Neighborhood Search (VNS).

- Framework to develop effective algorithms.
- One move: Fold-over a column in a copy of 2^{14-9} .

$$F_4(1,0.33) = (5,208)$$

Fold-over column 8 in blue copy

```
6 7 8 9 10 11 12 13 14
-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
```

Step 3': Variable Neighborhood Search (VNS).

- Framework to develop effective algorithms.
- One move: Fold-over a column in a copy of 2^{14-9} .

$$F_4(1,0.33) = (3,210)$$

Fold-over column 12 in blue copy

```
8 9 10 11 12 13 14
-1 -1 -1 -1 -1 -1 -1 -1 -1 -1
```

Step 3': Variable Neighborhood Search (VNS).

- Framework to develop effective algorithms.
- One move: Fold-over a column in a copy of 2^{14-9} .

$$F_4(1,0.33) = (1,212)$$

Fold-over column 9 in red copy

```
8 9 10 11 12 13 14
-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
-1 -1 -1 -1 -1 -1 -1
  1 -1 -1 -1 -1 -1
       -1 -1 -1 1 1 -1
```

Step 3': Variable Neighborhood Search (VNS).

- Framework to develop effective algorithms.
- One move: Fold-over a column in a copy of 2^{14-9} .

$$F_4(1,0.33) = (0,213)$$

Fold-over column 13 in red copy

```
-1 -1 -1 -1 -1 -1 -1 -1 -1 -1
```

Step 3': Variable Neighborhood Search (VNS).

- Framework to develop effective algorithms.
- One move: Fold-over a column in a copy of 2^{14-9} .

```
96-run 14-factor design

F_4(1, 0.33) = (0, 213)

B_4 = 23.67
```

```
8 9 10 11 12 13 14
-1 -1 -1 -1 -1 -1 -1 -1 -1 -1 -1
```

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Results

We used our method to construct large two-level designs from 32and 128-run resolution-IV MA designs.

	5 basic factors	7 basic factors
Number of concatenated copies	32-run MA design	128-run MA design
3	96	384
4	128	512
5	160	640
6	-	768
7	-	896

Up to 16 factors

Up to 40 factors

Good strength-3 designs in terms of the F_4 vector.



Results

Example III: Construct large two-level designs for 28 factors.

Design	Runs	Maximum absolute correlation between pairs of 2FIs	B_4
Regular	512	1	13
Ours	512	0.5	43
Ours	640	0.6	32.5
Ours	768	0.33	26.9
Ours	896	0.14	22
Strength 4	1,024	0	0



Discussion

- Our method can be used to construct large concatenated designs using 2^{m-p} regular designs with m-p not a prime number.
- We constructed two-level nonregular designs of strength 3 with 96, 128, 160, 192, 256, 320, 384, 512, 640, 768 and 896 runs, and up to 40 factors.
- An extra column can be added to block the designs.

Vazquez, A. R. and Xu, H. (2018) Construction of two-level nonregular designs of strength three with large run sizes. *Technometrics*. Published online.