Two-level orthogonal screening designs with 80, 96 and 112 runs: Construction and evaluation

Alan R. Vazquez
University of California, Los Angeles
alanrvazquez@stat.ucla.edu

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Outline

- 1. Tuberculosis inhibition experiment
- 2. Criteria to evaluate designs

3. Construction method

4. Results and discussion

Tuberculosis inhibition experiment

- Silva et al. (2016) conducted a study to develop a treatment that maximizes the percentage of inhibition of tuberculosis in infected human cells.
- The first stage of the study involved a screening experiment.
- 14 factors (drugs) at two levels (presence or absence).

Goal:

Identify the influential main effects and two-factor interactions of the factors.

For the experiment, the researchers chose an attractive two-level design with 14 factors and 128 runs.

It is a strength-4 orthogonal design (Hedayat et al. 1999) which allows to estimate all main effects and all two-factor interactions with full precision.

In the end, however, only 8 main effects and 6 two-factor interactions were active.

Research question:

Could we have identified the active effects with a smaller design?

Literature review

Strength-3 orthogonal designs. Properties:

- 1. Main effects are **not correlated** with each other **nor** with two-factor interactions.
- 2. Pairs of two-factor interactions can be correlated.
- 3. Exist for run sizes which are multiples of 8.

Example:

- Regular fractional factorial designs of resolution IV.
- Folded-over Plackett-Burman designs (nonregular).

Catalogs of strength-3 designs with 16, 24, 32, 40 and 48 runs and up to 24 factors are available (Schoen et al., 2010).

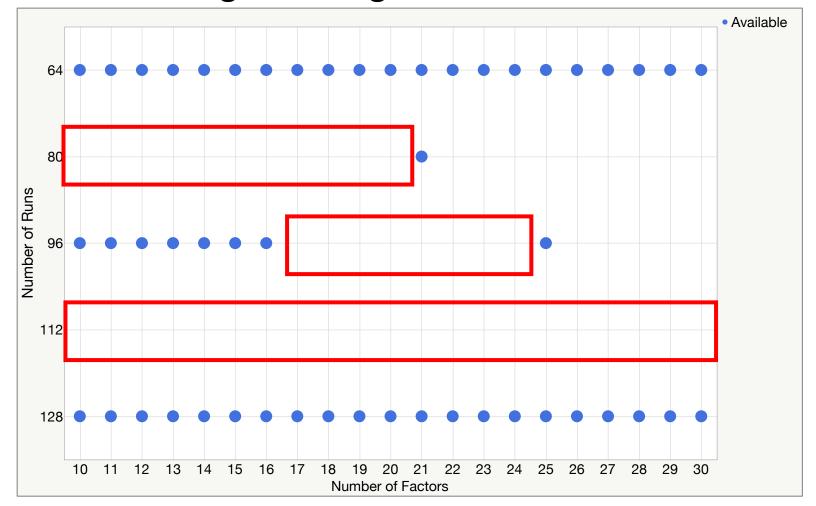
Available strength-3 designs with run sizes from 64 to 128

Chen et al. (1993); Xu & Wong (2007); Cheng et al. (2008); Vazquez & Xu (2019); Vazquez et al. (2019).

Cheng et al. (2008).

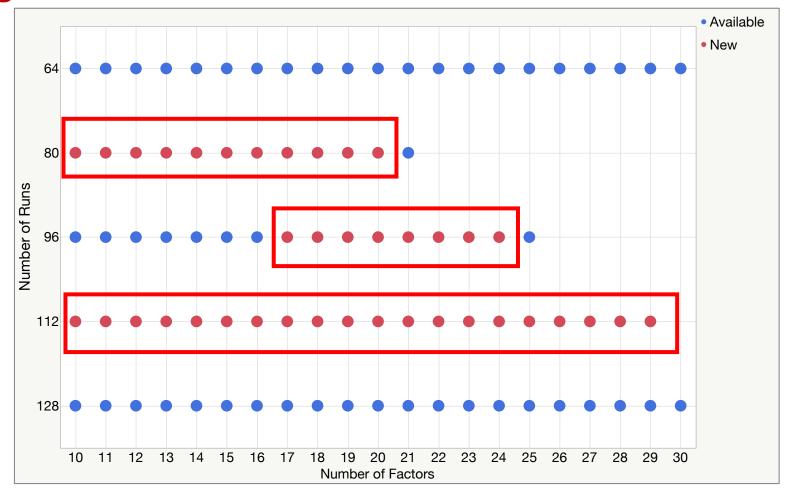
Cheng et al. (2008); Vazquez & Xu (2019).

Ryan & Bulutoglu (2010); Xu & Wong (2007); Vazquez & Xu (2019); Vazquez et al. (2019)



This talk

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



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Evaluating two-level strength-3 designs

Example: Compare designs with 32 runs and 10 factors.

Regular resolution-IV 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

Schoen & Mee (2010)

Nonregular strength-3 design

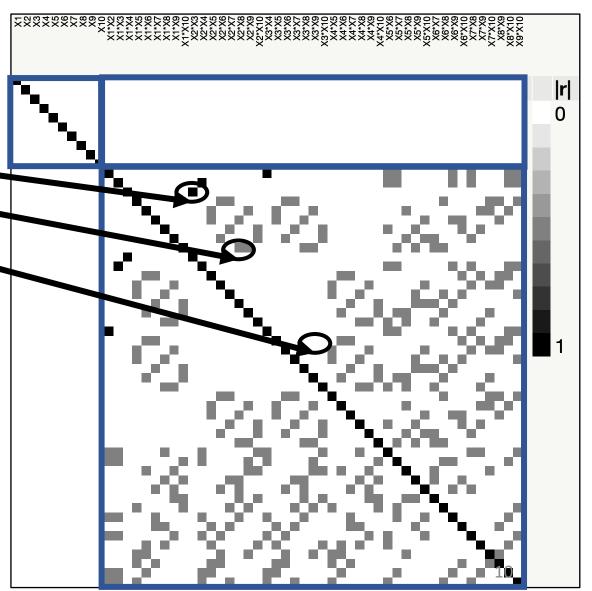
1	2	3	4	5	6	7	8	9	10
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
-1	-1	-1	-1	-1	-1	1	1	1	1
-1	-1	-1	-1	1	1	-1	-1	1	1
-1	-1	-1	-1	1	1	1	1	-1	-1
-1	-1	1	1	-1	-1	-1	-1	-1	-1
-1	-1	1	1	-1	1	-1	1	1	1
-1	-1	1	1	1	-1	1	1	-1	1
-1	-1	1	1	1	1	1	-1	1	-1
-1	1	-1	1	-1	-1	1	-1	1	1
-1	1	-1	1	-1	1	1	1	-1	-1
-1	1	-1	1	1	-1	-1	1	1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

Wu & Hamada (2009)

Color map on correlations

For 32-run designs, the absolute correlations can have values of 0, 0.5 or 1 (Deng & Tang, 1999).

Nonregular strength-3 design



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

Nonregular strength-3 design

Two statistical criteria:

- The F_4 vector
- The B_4 value

(Deng & Tang, 1999; Tang & Deng 1999)

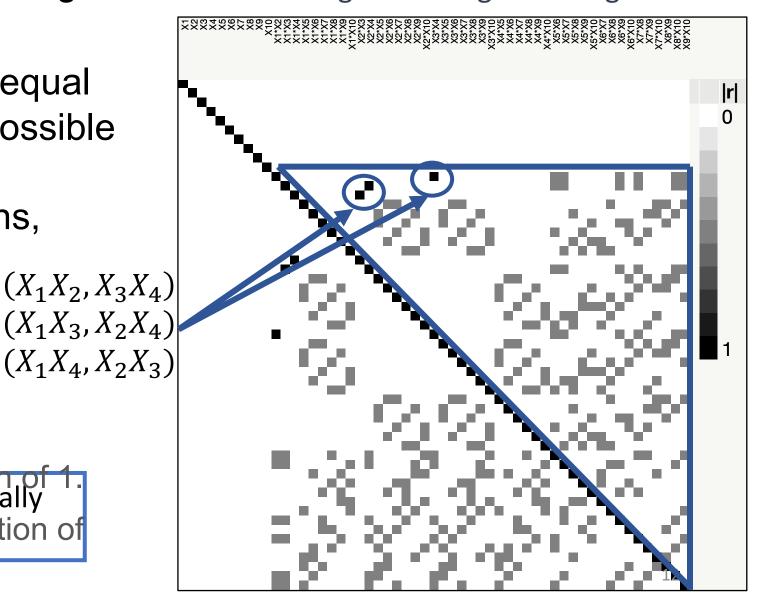
How can we summarize the correlation between pairs of two-factor interactions in strength-3 designs?

Nonregular strength-3 design

The F_4 vector has entries equal to the frequencies for the possible absolute correlation values between pairs of interactions, divided by three (X_1X_2, X_3X_4) (Deng & Tang, 1999). (X_1X_3, X_2X_4)

• $F_4(1, 0.5) = (1, 62)$

A good strength-3 design sequentially mirronizes the ith vectors. correlation of 0.5.



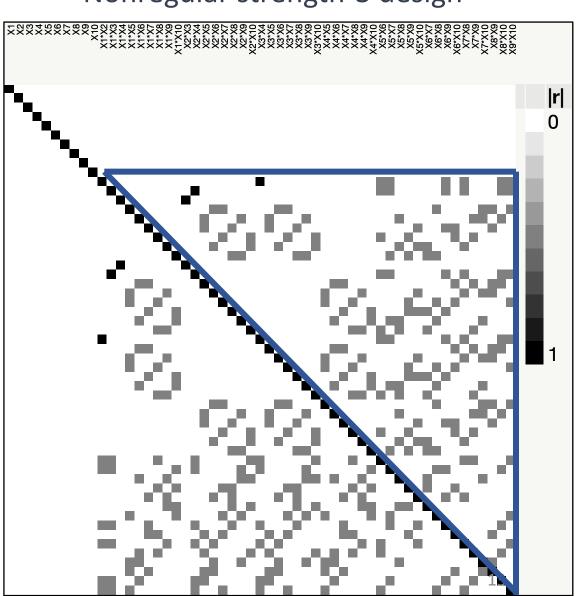
How can we summarize the correlation between pairs of two-factor interactions in strength-3 designs?

Nonregular strength-3 design

The B_4 value equals the sum of squared correlations between pairs of interactions divided by three (Tang & Deng, 1999).

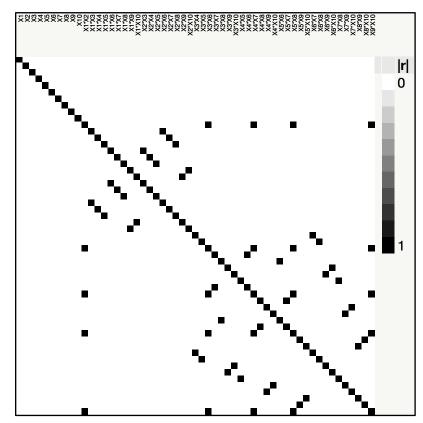
•
$$B_4 = 1(1)^2 + 62(0.5)^2 = 16.5$$

Ideally, the B_4 value of a strength-3 design is small.



Regular resolution-IV design

Example (cont.):

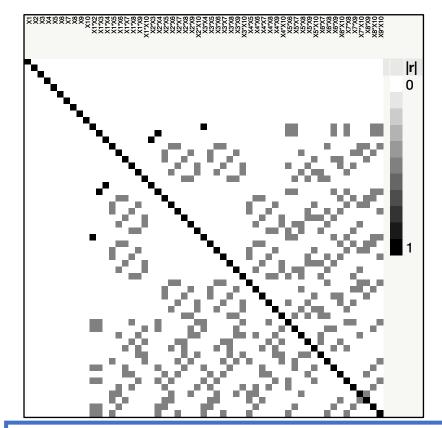


 $F_4(1,0.5) = (10,0)$

30 pairs with an abs. correlation of 1.

$$B_4 = 10$$

Nonregular strength-3 design



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

3 pairs with an abs correlation of 1.

$$B_4 = 16.5$$

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Goal: Construct a strength-3 design with 32 runs and 9 factors.

Step 1. Consider two good equallysized strength-3 designs with 16 runs and 8 factors. Call them D_u and D_l .

Minimum aberration 2_{IV}^{8-4} design

Goal: Construct a strength-3 design with 32 runs and 9 factors.

Step 1. Consider two good equallysized strength-3 designs with 16 runs and 8 factors. Call them D_{11} and D_{12} .

Step 2. Construct the 32-run 9-factor concatenated design *D*.

-1	4								
-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
1 1 -1 1 -1 -1 1 -1 1 1 1 -1 -1 -1 1 1 1 1 1 1 -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

 D_u

 D_{l}

17

Vazquez et al. (2019)

Step 3. Use the Column-Change Variable Neighborhood Search algorithm (Vazquez et al., 2019) to sequentially minimize the F_4 vector or minimize the B_4 value of D.

Two moves in D_l: (1) foldover columns
(2) swap columns

Example: $F_4(1, 0.5) = (14, 0)$

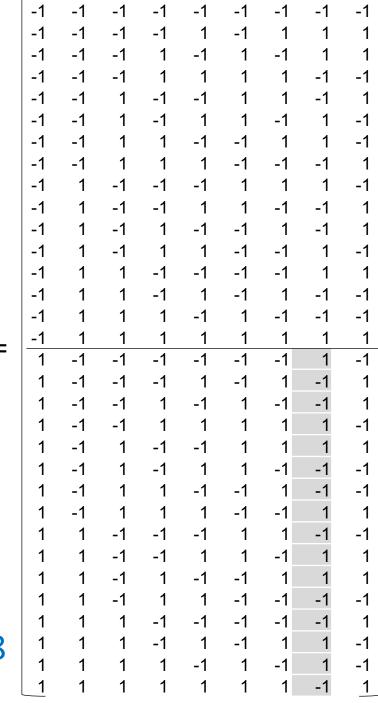
									_	
	-1	-1	-1	-1	-1	-1	-1	-1	-1	
	-1	-1	-1	-1	1	-1	1	1	1	
	-1	-1	-1	1	-1	1	-1	1	1	
	-1	-1	-1	1	1	1	1	-1	-1	
	-1	-1	1	-1	-1	1	1	-1	1	
	-1	-1	1	-1	1	1	-1	1	-1	
	-1	-1	1	1	-1	-1	1	1	-1	
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	-1	1	-1	-1	-1	1	1	1	-1	$\boldsymbol{\nu}_u$
	-1	1	-1	-1	1	1	-1	-1	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	
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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	ח
	1	1	-1	-1	-1	1	1	1	-1	D_l
	1	1	-1	-1	1	1	-1	-1	1	
	1	1	-1	1	-1	-1	1	-1	1	
	1	1	-1	1	1	-1	-1	1	-1	
	1		1	-1	-1	-1	-1	1	1	
	1	1	1	-1	1		1	-1	-1	
	1	1	1	1		1	-1	-1	-1	18
	1	1	1	1	1	1	1	1	1	10

Step 3. Use the Column-Change Variable Neighborhood Search algorithm (Vazquez et al., 2019) to sequentially minimize the F_4 vector or minimize the B_4 value of D.

• Two moves in D_l : (1) foldover columns (2) swap columns

Example: $F_4(1, 0.5) = (7, 0)$

Foldover column 8

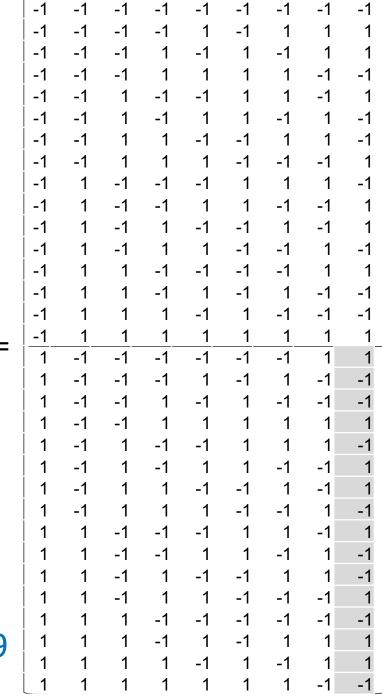


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• Two moves in D_l : (1) foldover columns (2) swap columns

Example: $F_4(1, 0.5) = (6, 0)$

Foldover column 9



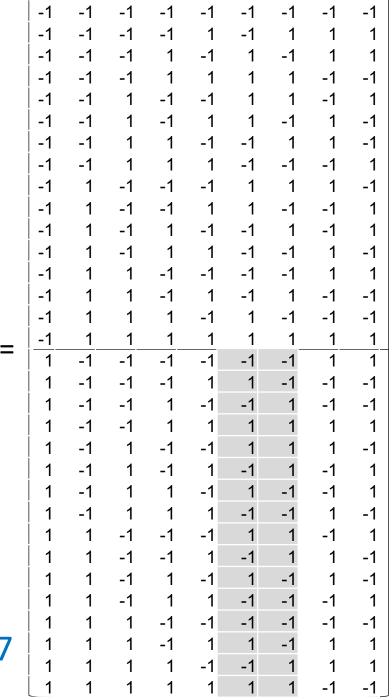
Step 3. Use the Column-Change Variable Neighborhood Search algorithm (Vazquez et al., 2019) to sequentially minimize the F_4 vector or minimize the B_4 value of D.

• Two moves in D_l : (1) foldover columns (2) swap columns

Example:

$$F_4(1,0.5) = (2,16)$$

Swap columns 6 and 7



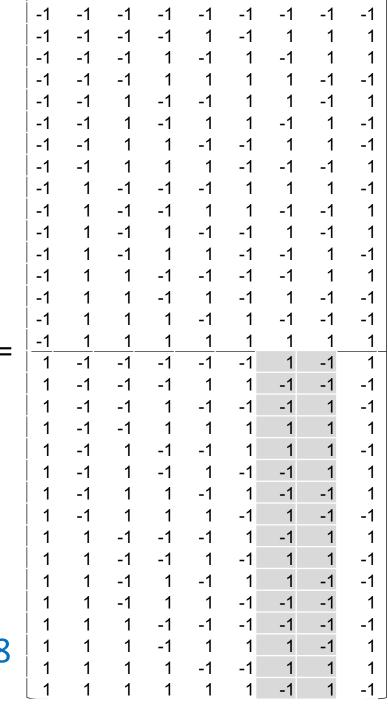
Step 3. Use the Column-Change Variable Neighborhood Search algorithm (Vazquez et al., 2019) to sequentially minimize the F_4 vector or minimize the B_4 value of D.

• Two moves in D_l : (1) foldover columns (2) swap columns

Example:

$$\overline{F_4(1,0.5)} = (0,24)$$

Swap columns 7 and 8



Step 3. Use the Column-Change Variable Neighborhood Search algorithm (Vazquez et al., 2019) to sequentially minimize the F_4 vector or minimize the B_4 value of D.

Two moves in D_l: (1) foldover columns
(2) swap columns

Example: $F_4(1, 0.5) = (0, 24)$

	-1	-1	-1	-1	-1	-1	-1	-1	-1
	-1	-1	-1	-1	1	-1	1	1	1
	-1	-1	-1	1	-1	1	-1	1	1
	-1	-1	-1	1	1	1	1	-1	-1
	-1	-1	1	-1	-1	1	1	-1	1
	-1	-1	1	-1	1	1	-1	1	-1
	-1	-1	1	1	-1	-1	1	1	-1
	-1	-1	1	1	1	-1	-1	-1	1
	-1	1	-1	-1	-1	1	1	1	-1
	-1	1	-1	-1	1	1	-1	-1	1
	-1	1	-1	1	-1	-1	1	-1	1
	-1	1	-1	1	1	-1	-1	1	-1
	-1	1	1	-1	-1	-1	-1	1	1
	-1	1	1	-1	1	-1	1	-1	-1
	-1	1	1	1	-1	1	-1	-1	-1
$D^* =$	-1	1	1	1	1	1	1	1	1
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	1	1	1	1
	1	-1	1	-1	-1	1	1	1	-1
	1	-1	1	-1	1	-1	-1	1	1
	1	-1	1	1	-1	1	-1	-1	1
	1	-1	1	1	1	-1	1	-1	-1
	1	1	-1	-1	-1	1	-1	1	1
	1	1	-1	-1	1	-1	1	1	-1
	1	1	-1	1	-1	1	1	-1	-1
	1	1	-1	1	1	-1	-1	-1	1
	1	1	1	-1	-1	-1	-1	-1	-1
	1	1	1	-1	1	1	1	-1	1
	1	1	1	1	-1	-1	1	1	1
	1	1	1	1	1	1	-1	1	-1

Outline

1. Tuberculosis inhibition experiment

2. Criteria to evaluate designs

3. Construction method

4. Results and discussion

Alternative 14-factor designs for the tuberculosis inhibition experiment

First entry of F_4 vector

Parent Designs $(D_u \text{ and } D_l)$	Run Size	Maximum Absolute Correlation Among Interactions	# Pairs of Interactions Involved	B_4 value
Good 40-run strength-3 designs (Schoen et al., 2010).	80	0.60	3	17.56
	δU	0.40	48	19.16
Good 48-run strength-3 designs (Schoen and Mee, 2012).	96	0.34	63	8.33
	90	0.34	24	10.06
56-run strength-3 designs obtained by dropping columns	112	0.43	3	11.00
from the folded-over 28-run Plackett-Burman design	112	0.29	129	11.86

Alternative 14-factor designs for the tuberculosis inhibition experiment

First entry of F_4 vector

Parent Designs	Run Size	Maximum Absolute Correlation Among Interactions	# Pairs of Interactions Involved	B_4 value					
Good 48-run strength-3 designs (Schoen and Mee, 2012).	96	0.34	63	8.33					
	90	0.34	24	10.06					
Benchmark strength-3 design									
Vazquez and Xu (2019)	96	0.34	639	23.67					

Simulation study

• Using simulations, we evaluate the performance of our 14-factor designs. We restrict our attention to those with best F_4 vector.

- We also consider two-level benchmark designs in the literature:
 - Strength-3 design with 64 runs (Xu & Wong, 2007)
 - Bayesian D-optimal designs with 64, 80, 96 and 112 runs (DuMouchel & Jones, 1994).
 - D-optimal design with 112 runs (Atkinson et al., 2007).
 - Strength-4 design with 128 runs (Silva et al., 2016).

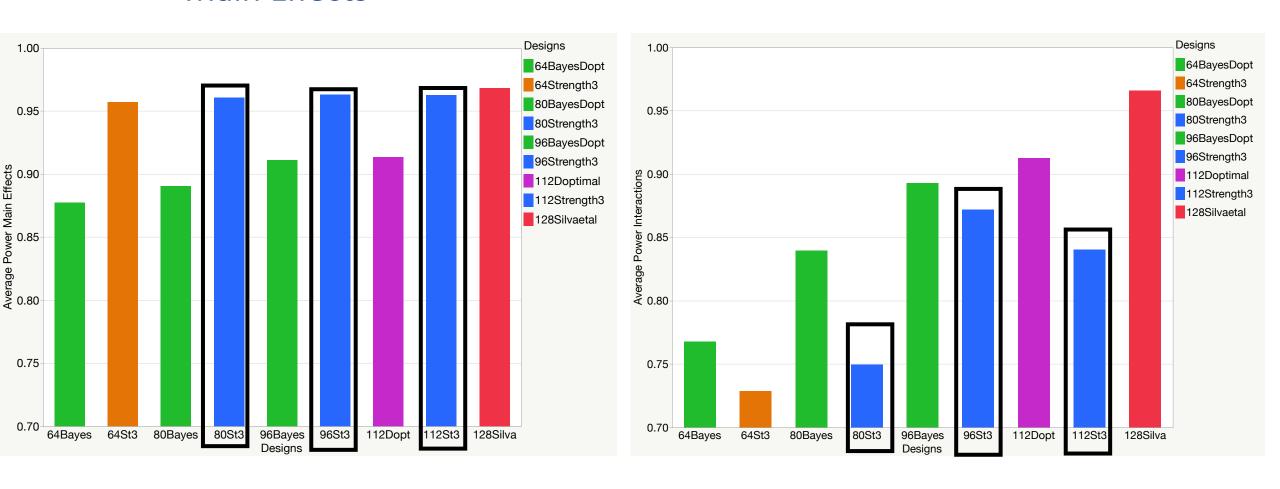
Simulation protocol

- 1. We randomly selected 8 main effects and 6 two-factor interactions (satisfying weak effect heredity) as active.
- 2. We obtained coefficients for the active effects by adding a 1 to an exponentially distributed random number. A '+' or '-' was randomly assigned.
- 3. The coefficients for the inactive effects were drawn from $N(0, 0.25^2)$.
- 4. We simulated response vectors with residuals following N(0,1).
- 5. We used the Dantzig selector (Candes & Tao, 2007) to identify the active effects.

1,000 simulations

Main Effects

Two-Factor Interactions



Power: Proportion of active effects that are successfully detected.

(Mee, Schoen & Edwards, 2017; Eendebak & Schoen, 2017; Vazquez & Xu, 2019)

Discussion

- For active effects larger than 2, our simulations show that all 80-, 96- and 112-run designs have powers close to 1.
- Using our methodology, we generated a new collection of attractive two-level strength-3 designs with 80, 96 and 112 runs and up to 29 factors.
- Constructing good two-level strength-3 designs with 72, 88, 104 and 120 runs is an interesting topic for future research.

Vazquez, A. R., Schoen, E. D., and Goos, P. (2021). Two-level orthogonal screening designs with 80, 96 and 112 runs, and up to 29 factors. *Journal of Quality Technology*. Published online.