Advances in Orthogonal Minimally Aliased Response Surface (OMARS) Designs

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Response surface designs

- Experimental plans used in product and process optimization.
- Involves the study of several quantitative factors
- The estimation of a complete second-order response surface is often the goal:
  - Main effects
  - Second-order effects (SOEs): interaction effects + quadratic effects
- Best-known designs are:
  - (Small) Central Composite Design
  - Box-Behnken design

3-level screening designs

- Experimental plans used in product and process optimization.
- Involves the study of several quantitative factors
- The estimation of a partial second-order response surface is often the goal:

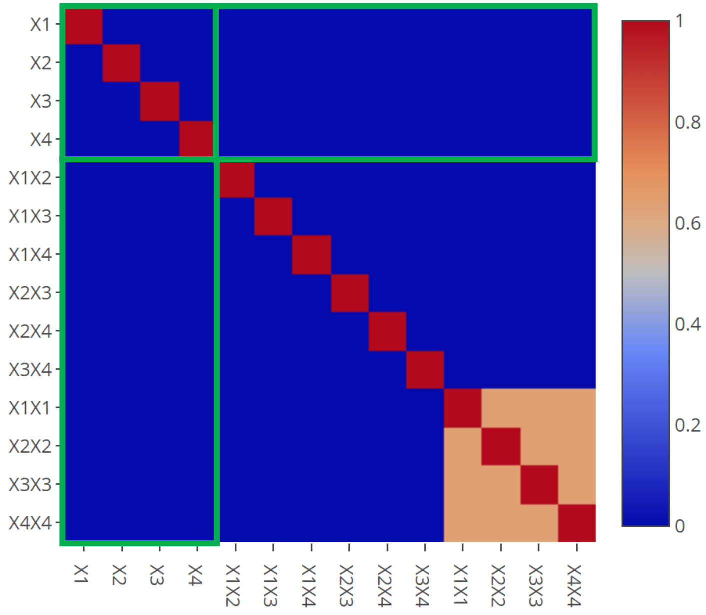
  Main effects

  Some Second-order effects (SOEs)
- Best-known designs is:

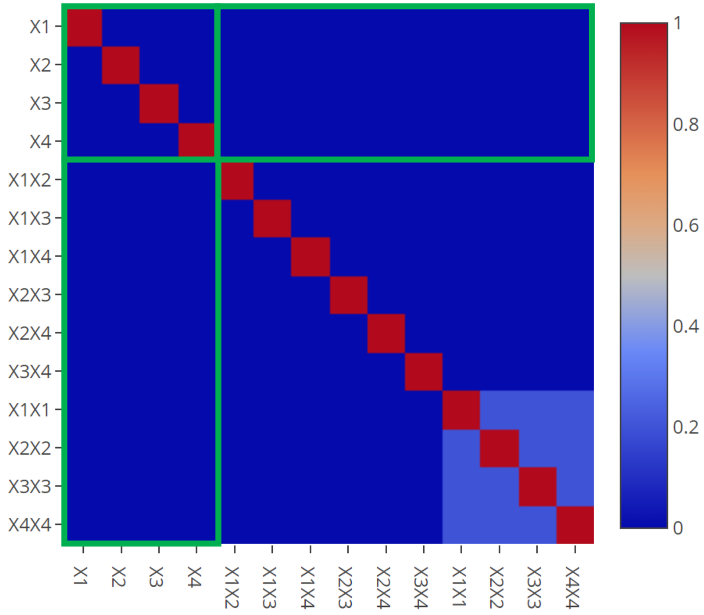
  Definitive Screening Design

The most popular 3-level designs

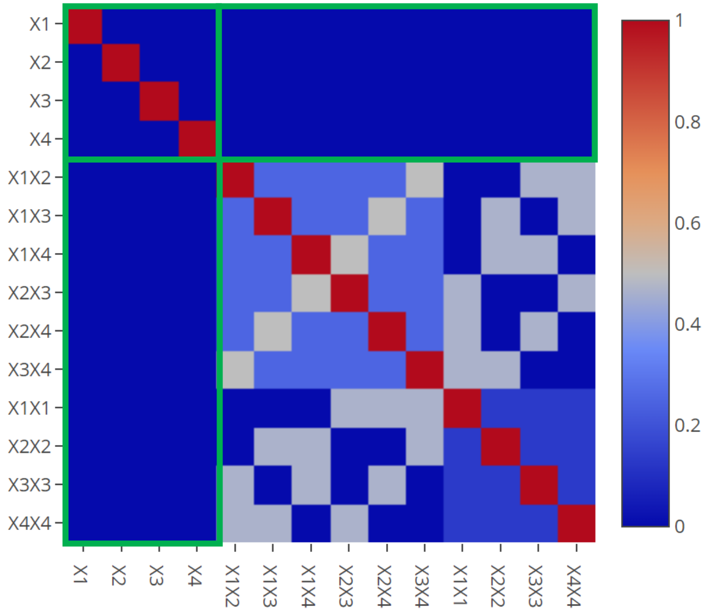
Central composite design



Box-Behnken design



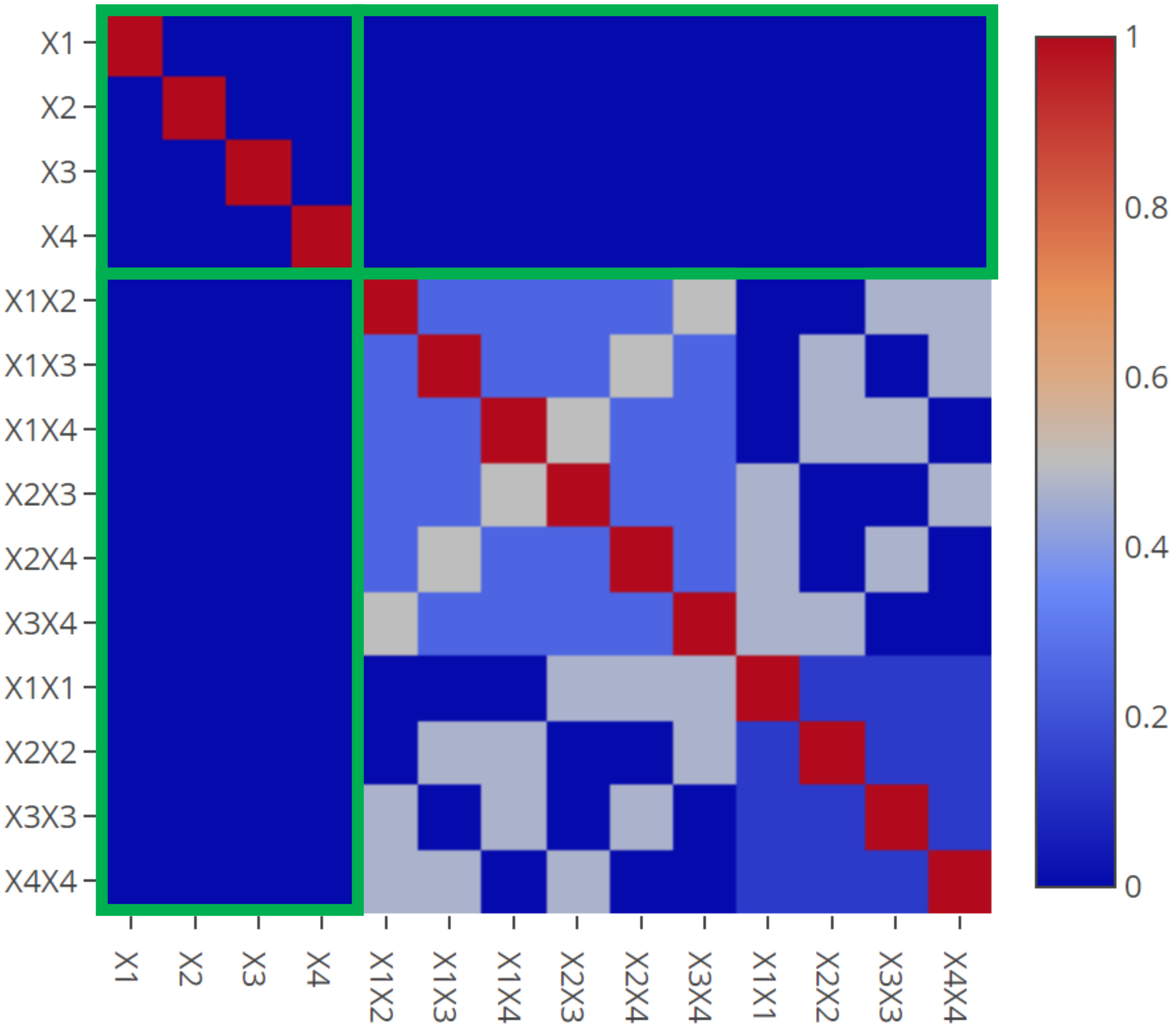
Definitive screening design



All these designs belong to the family of OMARS designs

[Núñez Ares, Goos 2020 & Núñez Ares, Schoen, Goos 2023]

OMARS designs



***O**rthogonal*

main effects estimated independently

from each other

***M**inimally **A**liased*

main effects estimated independently

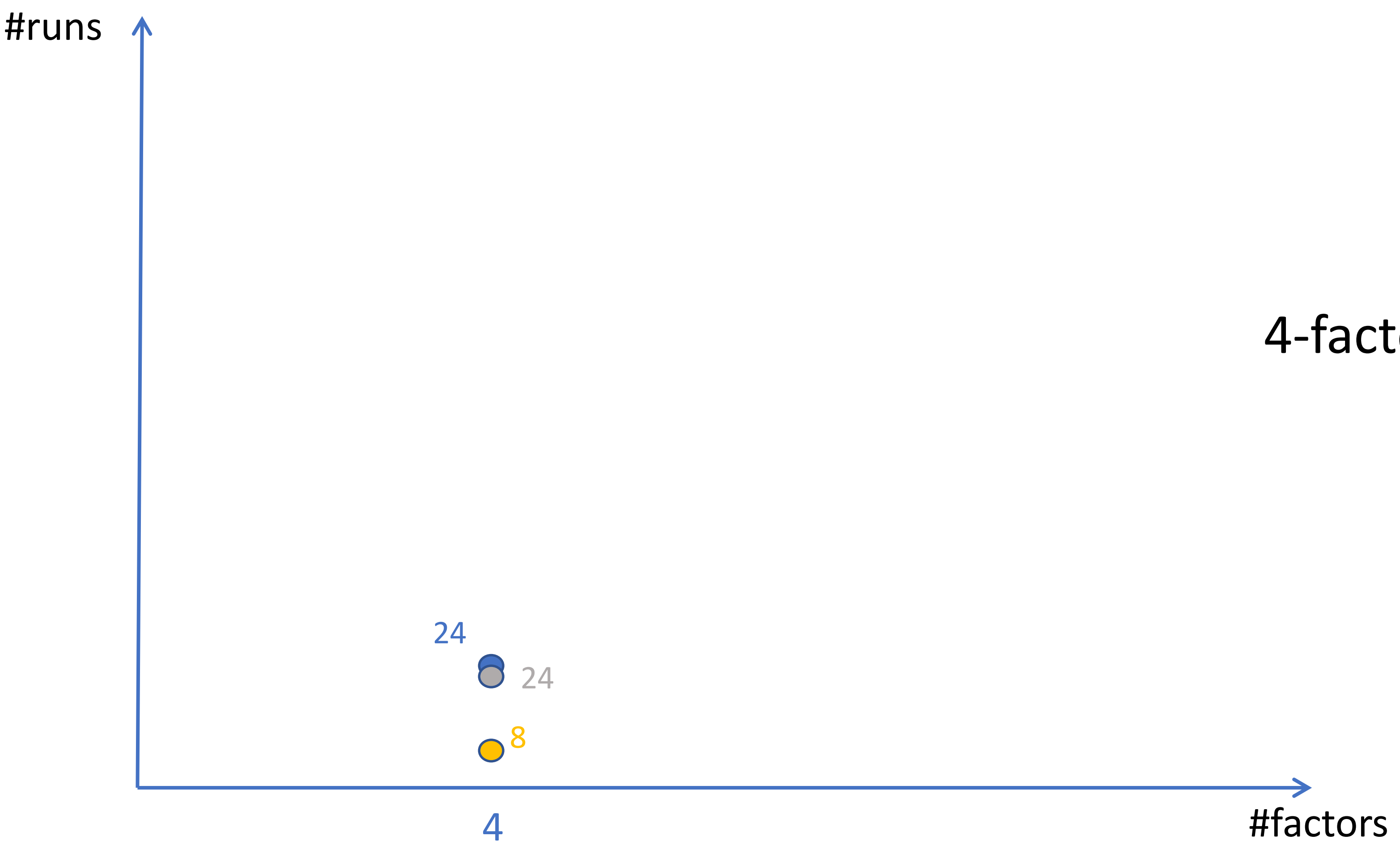
from all second-order effects

R**esponse **S**urface **Designs

allow the estimation of a partial or

complete second-order effects model

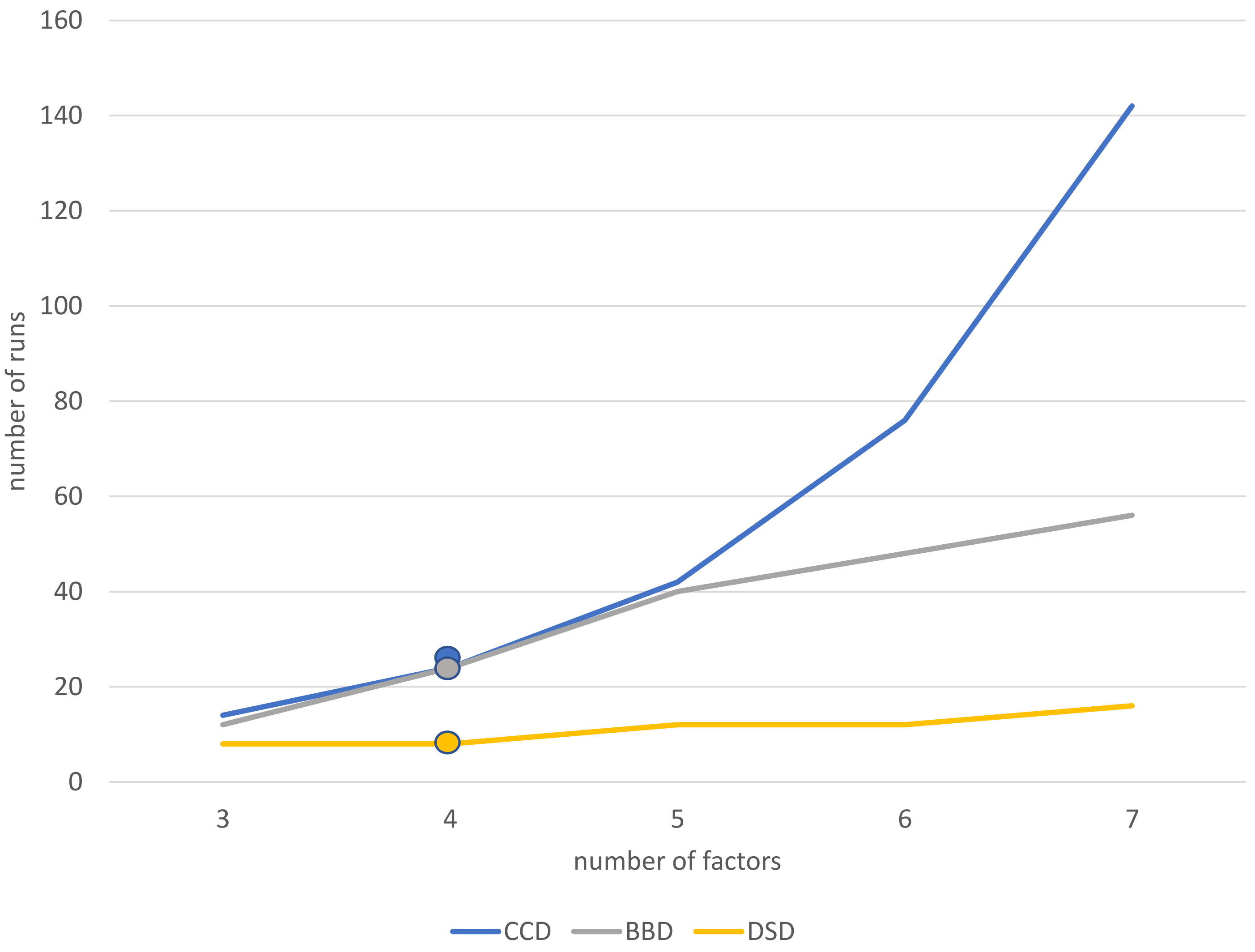
Choosing a standard 3-level design



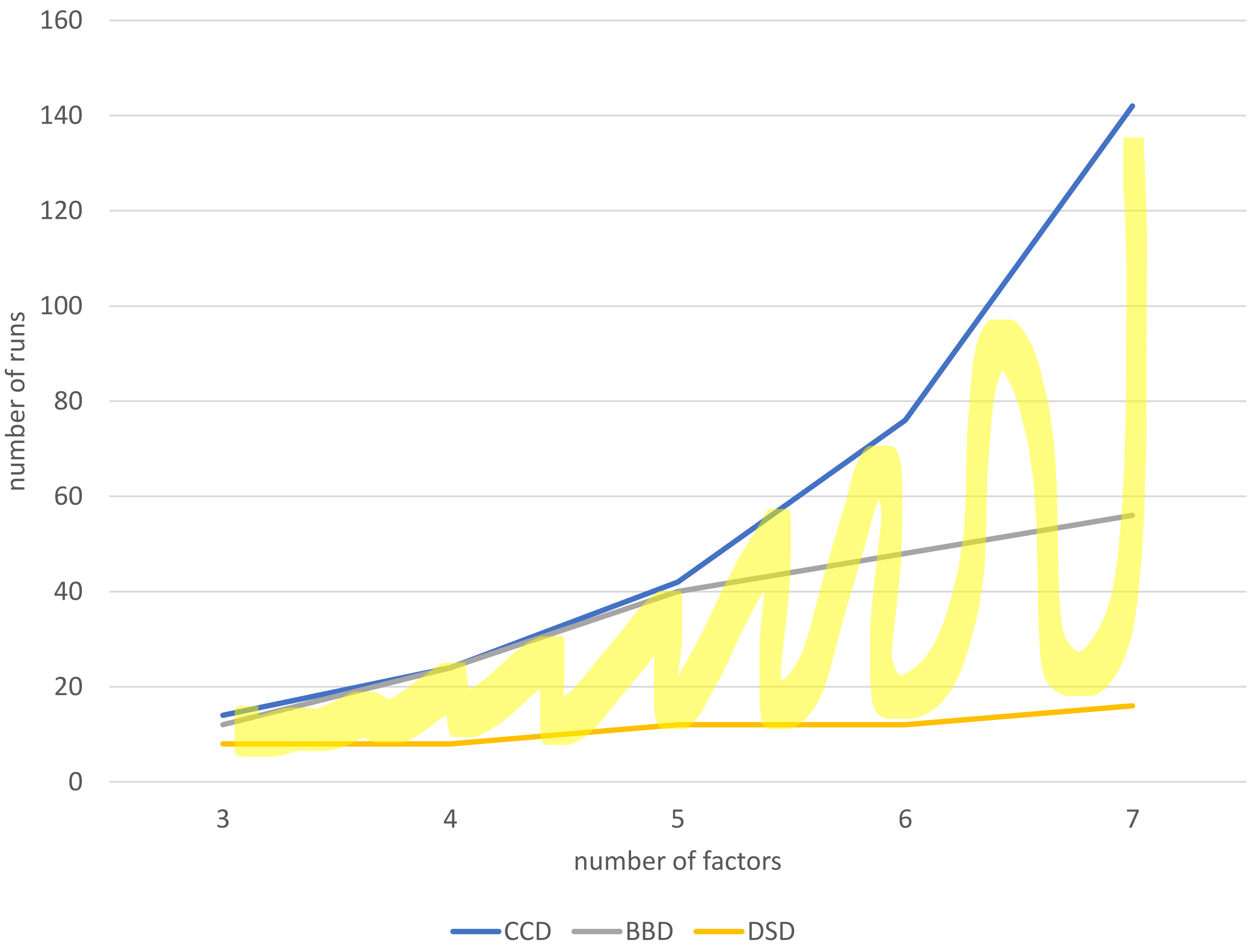
4-factor designs

Box-Behnken design   Central composite design   Definitive screening design

Limited number of standard designs



Motivation of the present work



Are there more OMARS designs with a number of runs between the small DSDs and the large CCDs?

Numerous OMARS designs exist!

#runs/#factors	3	4	5	6	7	8	9	10	11	12	13	14	15	16
14	46	128	11	4	2									
16	159	190	152	61	8	3								
18	198	359	552	171	30	11								
20	572	1,621	5,569	5,117	997	171	7	3						
22	1,438	5,788	42,262	97,792	37,941	3,021	145	6						
24	1,921	12,765	168,045	886,015	1,919,652	142,192	12,637	1,658	152	35				
26	2,235	21,482	807,530	9,611,789	5,086,943	1,815,173	898,596	287,208	298,799	1,426	7			
28	492	3,285	91,111	1,022,895	1,255,206	265,213	37,228	7,676	1,505	487	93			
30	1,263	18,761	1,822,824	27,311,163	55,340,120	26,620,971	3,231,476	60,050	560	31	8	1		
32	33	656	5,177	47,237	114,145	99,398	47,574	17,237	3,594	430				
34	38	651	8,564	139,985	171,785	15,654	878	177	27	15	4	4	1	1
36	64	2,157	38,368	1,926,480	4,971,761	1,646,150	53,536	669	11	1	1	1		
38	95	4,420	137,380	15,097,844	7,034,284	3,086,804	28,877	232	27	15	4	4	1	1
40	129	9,688	919,100	59,240,843	66,439,987	7,590,489	983,545	12,560	26	13	3	3	1	1
TOTAL	8,683	81,951	4,046,645	115,387,396	142,372,861	41,285,250	5,294,499	387,476	304,701	2,453	120	13	3	3
GRAND TOTAL	309,172,054													

How did we find them?

Our enumeration method:

Properties

- Enumerates non-isomorphic designs
- All enumerated designs are OMARS

Approach

- Integer programming
- High throughput computing

Execution

- HPC and HTC infrastructures
- High total computation time

Example 1: 5-factor 22-run design

	X1	X2	X3	X4	X5
1	-	-	-	-	-
2	-	-	+	0	-
3	-	-	+	+	+
4	-	0	-	0	0
5	-	0	0	-	+
6	-	+	-	+	+
7	-	+	0	-	0
8	-	+	+	+	-
9	0	-	-	+	0
10	0	-	0	0	+
11	0	0	-	+	-

	X1	X2	X3	X4	X5
12	0	0	+	-	+
13	0	+	0	0	-
14	0	+	+	-	0
15	+	-	-	-	+
16	+	-	0	+	0
17	+	-	+	-	-
18	+	0	0	+	-
19	+	0	+	0	0
20	+	+	-	-	-
21	+	+	-	0	+
22	+	+	+	+	+

Foldover

Balanced for MEs

No center runs

Example 2: 4-factor 23-run design

	X1	X2	X3	X4
1	-	-	-	-
2	-	0	0	+
3	-	0	0	+
4	-	0	0	0
5	-	0	+	-
6	-	+	0	0
7	0	-	-	+
8	0	-	0	0
9	0	-	+	+
10	0	-	+	0
11	0	0	-	0
12	0	0	0	-

	X1	X2	X3	X4
13	0	0	+	-
14	0	+	-	-
15	0	+	-	+
16	0	+	0	-
17	0	+	+	+
18	+	-	0	-
19	+	0	-	0
20	+	0	0	-
21	+	0	0	+
22	+	0	0	+
23	+	+	+	0

Non-foldover

Balanced for MEs

No center runs

Are they any good? How to choose?

Optimization second-order design for 4 quantitative factors

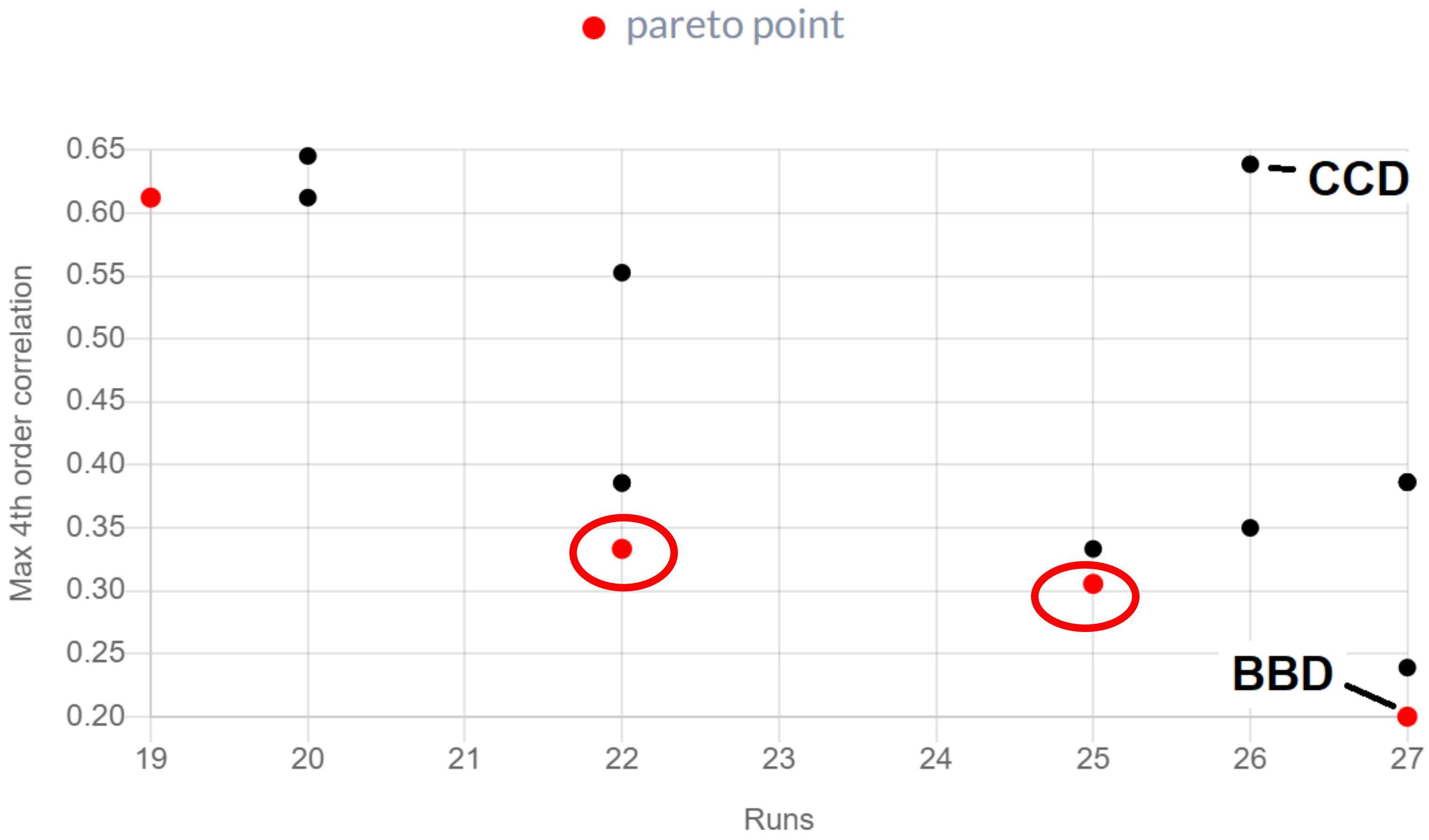
Consider the standard designs:

- Central composite design: 26 runs with 2 center points
- Box-Behnken design: 27 runs with 3 center points

	CCD	BBD
Power interaction effect	0.952	0.452
Power quadratic effect	0.309	0.564
Maximum 4th order correlation	0.639	0.2
G-efficiency	75.07	23.8
Prediction variance	0.325	0.4
Pure error	YES	YES

Second-order designs for 4 factors

We select 14 4-factor second-order OMARS designs, and we compare them to the CCD and the BBD

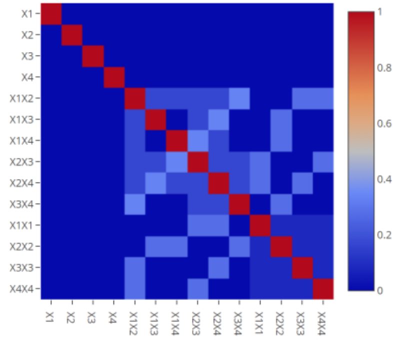


Two OMARS designs for optimization

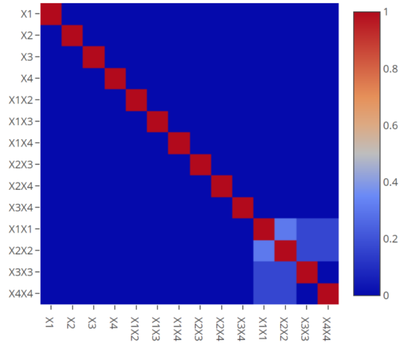
22- and 25-run OMARS designs

	OMARS 1	OMARS 2	CCD	BBD
Number of runs	22	25	26	27
Power interaction effect	0.699/0.641	0.948/0.876	0.952	0.452
Power quadratic effect	0.373/0.345	0.528/0.423	0.309	0.564
Maximum 4th order correlation	0.333	0.305	0.639	0.2
G-efficiency	40.21	73.13	75.07	23.8
Prediction variance	0.455	0.429	0.325	0.4
Pure error (number of replicates)	NO	YES (2)	YES (1)	YES (1)

22-run OMARS



25-run OMARS



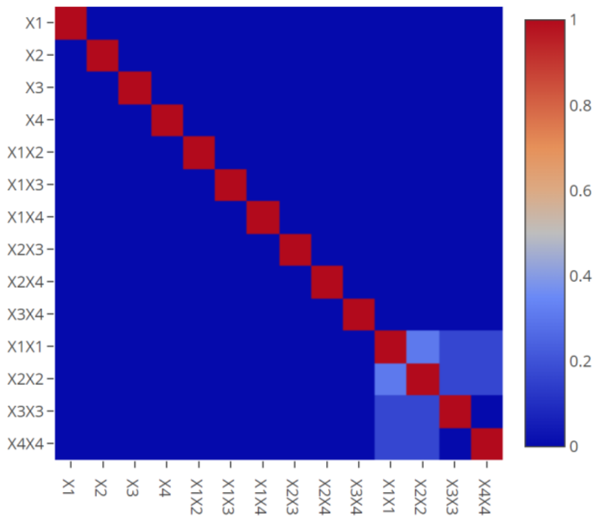
Strong OMARS

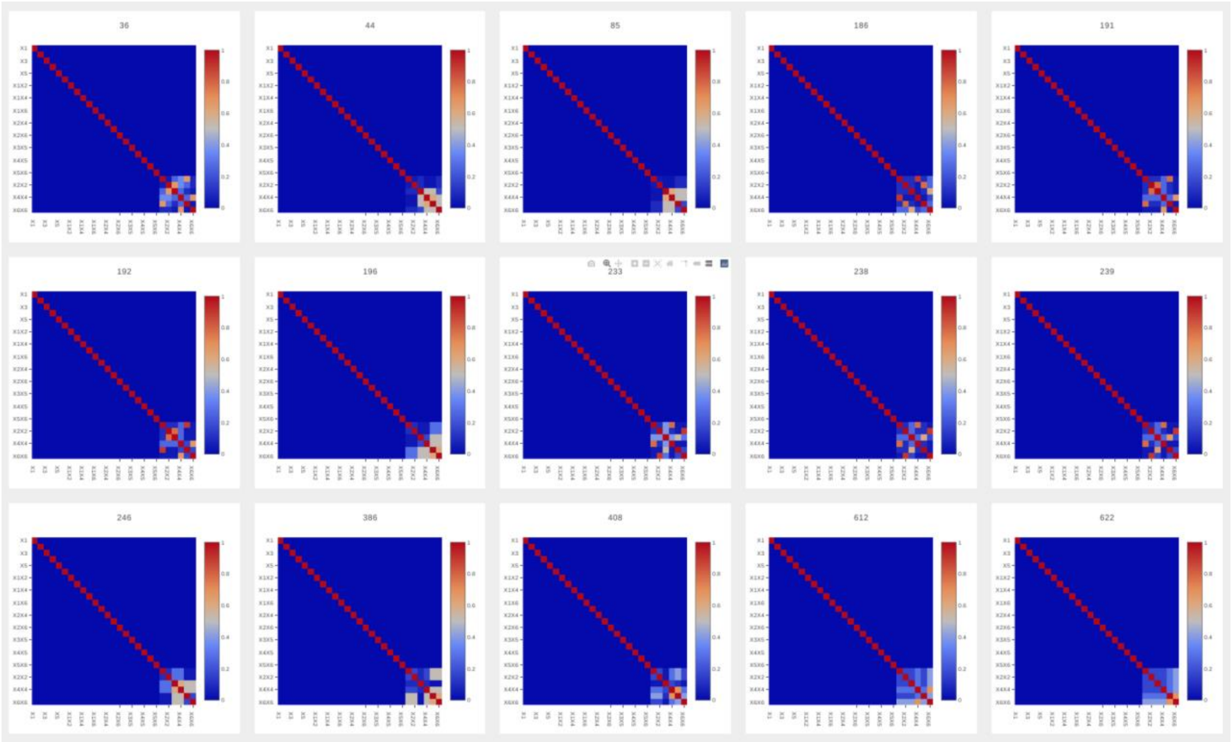
Two-factor interactions are orthogonal to each other and to the quadratic effects

Optimization designs, competing with CCDs and BBDs

Very few exist

4-factor 25-run strong OMARS





6-factor 40-run strong OMARS

A screening experiment

Screening second-order design for 6 quantitative factors, no more than 22 runs.

Benchmark designs: Definitive screening designs with 16 to 22 runs.

Projection estimation capacity equals **3**:

- 6 factors: X1, X2, X3, X4, X5, X6
- There are $\binom{6}{3} = 20$ subsets of 3 factors out of the six
- With these designs we can fit a full second-order effects model on any subset of **3** factors

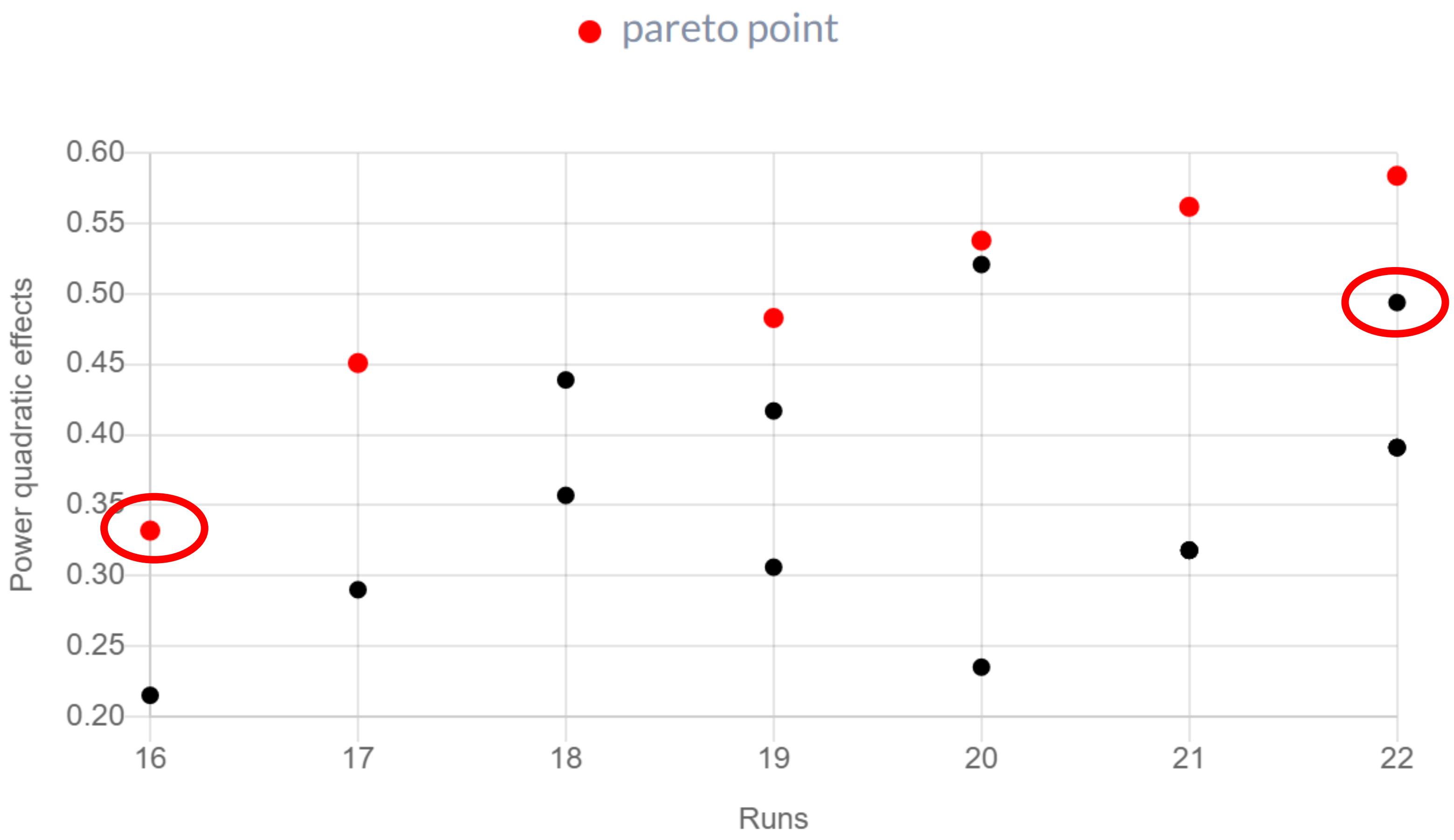
Benchmark designs

Characteristics of the benchmark definitive screening designs:

	DSD#1	DSD#2	DSD#3	DSD#4	DSD#5	DSD#6	DSD#7
Number of runs	16	17	18	19	20	21	22
Power interaction effect	0.857	0.868	0.876	0.882	0.935	0.958	0.96
Power quadratic effect	0.215	0.29	0.357	0.417	0.29	0.318	0.391
Maximum 4th order correlation	0.666	0.666	0.666	0.666	0.75	0.75	0.75
Projection estimation capacity	3	3	3	3	3	3	3
Projection information capacity D-eff (3)	41.81	44.43	44.25	43.39	44.43	44.51	44.8
Projection prediction variance (3)	1.25	1.21	0.41	0.36	0.53	0.5	0.38

Pareto analysis

We select 15 6-factor screening OMARS designs, and we compare them to the DSDs

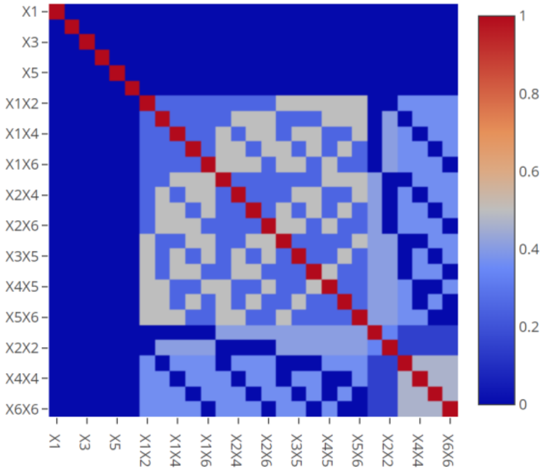


DSDs are not in the Pareto front

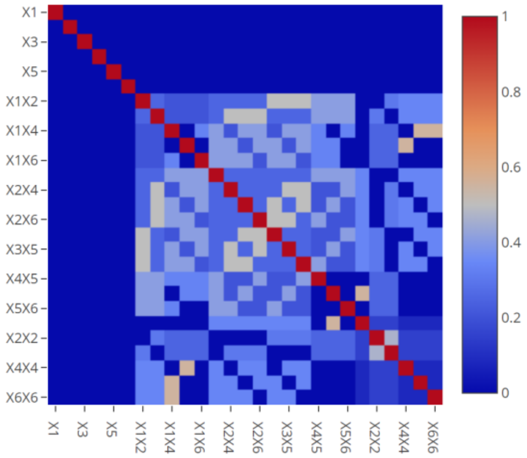
Two OMARS for screening

	OMARS 1	DSD#1	DSD#2	DSD#3	DSD#4	DSD#5	DSD#6	DSD#7	OMARS 2
Number of runs	16	16	17	18	19	20	21	22	22
Power interaction effect	0.698	0.857	0.868	0.876	0.882	0.935	0.958	0.96	0.748
Power quadratic effect	0.332	0.215	0.29	0.357	0.417	0.29	0.318	0.391	0.494
Maximum 4th order correlation	0.5	0.666	0.666	0.666	0.666	0.75	0.75	0.75	0.552
Projection estimation capacity	3	3	3	3	3	3	3	3	3.8
Projection information capacity D-eff (3)	40.34	41.81	44.43	44.25	43.39	44.43	44.51	44.8	39.99
Projection prediction variance (3)	0.46	1.25	1.21	0.41	0.36	0.53	0.5	0.38	0.33

16-run OMARS



22-run OMARS



Weak points of standard designs

Central composite designs

- No flexibility in the number of runs
- Expensive designs
- High correlation between quadratic effects
- Low power to detect quadratic effects

Box-Behnken designs

- No flexibility in the number of runs
- Expensive designs
- Low power to detect interaction effects

Definitive screening designs

- High correlation between second-order effects
- Low power to detect quadratic effects
- Limited projection estimation capacity

Advantages of OMARS design catalog

Flexibility in terms of number of runs.
All standard OMARS designs are included in the catalog.
Consider multiple criteria while choosing a design

Optimization

- There are cheaper alternatives to CCDs and BBDs.
- The weak points of CCDs and BBDs can be overcome
- More OMARS have 2FIs orthogonal to each other and to QEs.

Screening

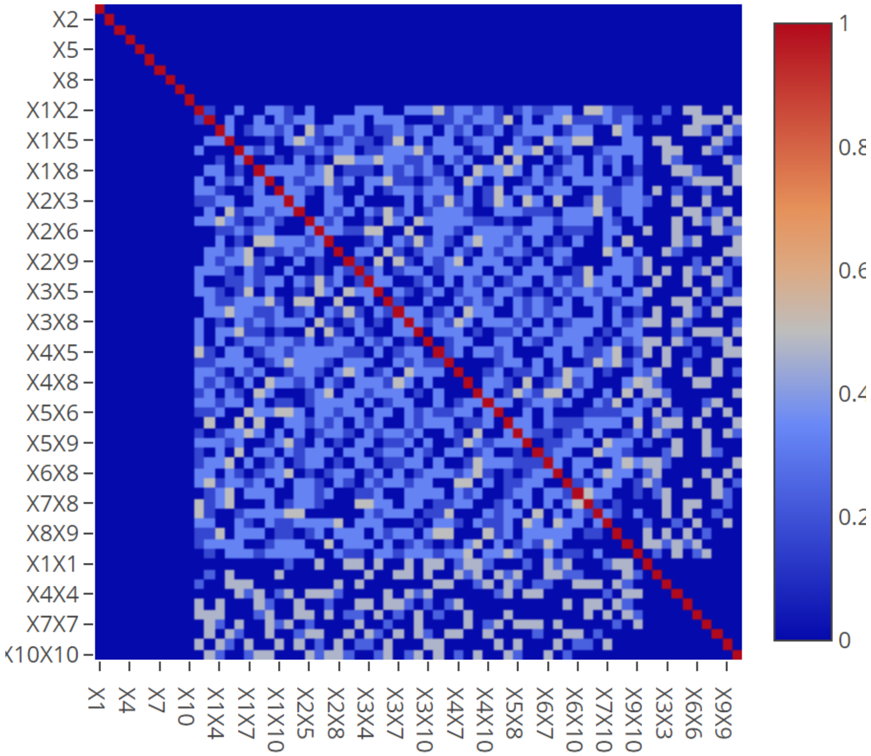
- Higher projection estimation capacity than DSDs.
- Higher powers to detect curvature than DSDs
- Lower correlation between SOEs than DSDs

Application 1: complex problems

Chemical experiment.

Extremely expensive and high estimation quality requirements

10-factor 27-run design with Projection estimation capacity = 4



Projection information capacity

#factor projections	D-eff	A-eff	G-eff	PV
3	42.04	27.61	62.85	0.244
4	35.37	17.79	33.44	0.907

Max 4^{th} order correlation = 0.5
Quadratic effects orthogonal to each other
Min power to detect an IE: 0.898
Min power to detect a QE: 0.629

Software demo

“never give a software demo” (popular saying)

Extensions 1: mixed-level OMARS

OMARS with quantitative and two-level categorical factors

The orthogonality structure is preserved

We improve the previous work on mixed-level DSDs.

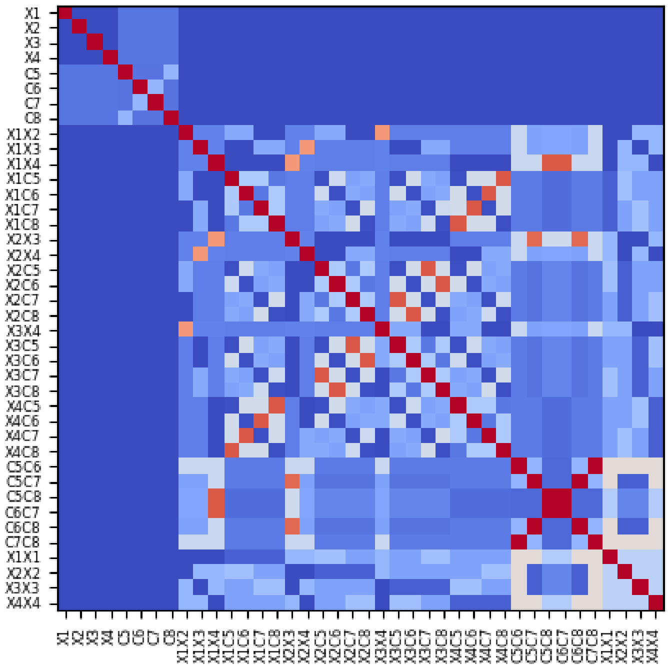
We built a large catalog of mixed-level OMARS for both screening and optimization.

A similar design selection approach can be followed for mixed-level designs too.

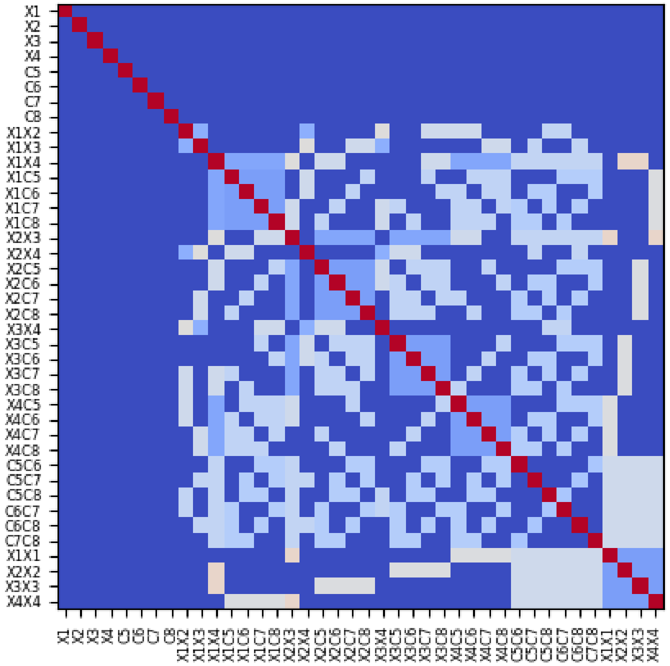
Mixed-level OMARS: example

Screening design with 4 quantitative factors and 4 two-level categorical factors.
Two DSDs (22 and 26 runs) and one 24-run OMARS comparison.

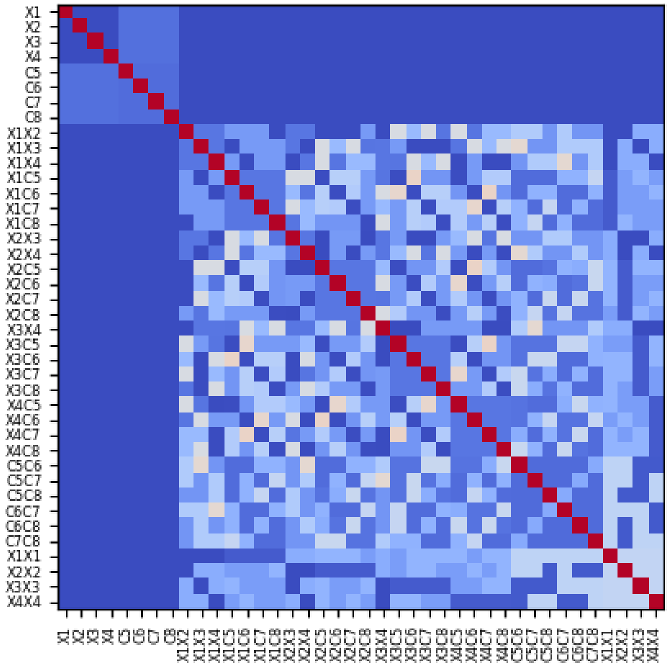
22-run DSD



24-run OMARS



26-run DSD



Application 2: mixed-level design

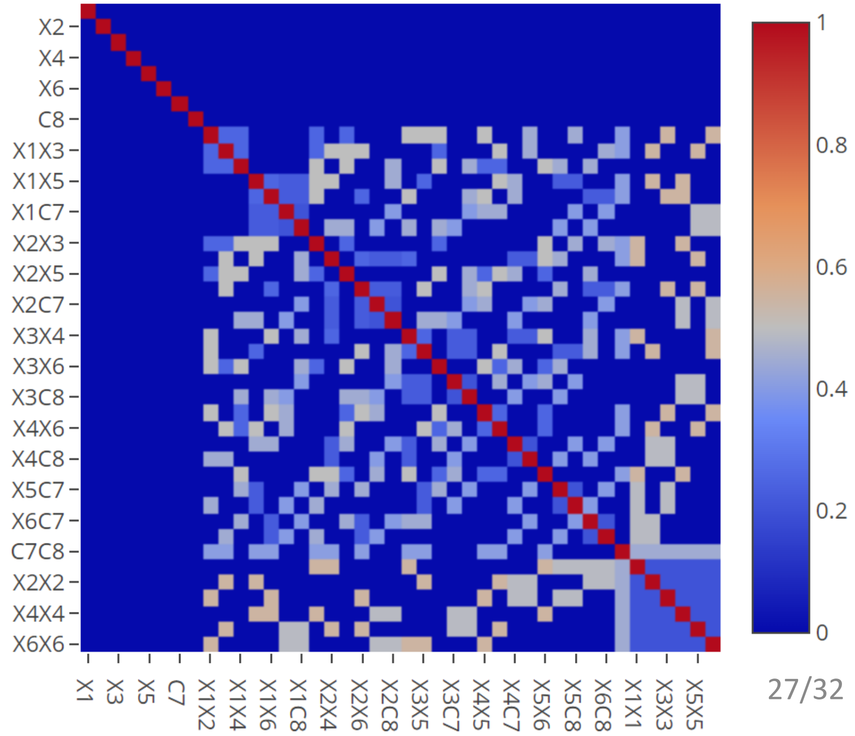
Chemical experiment in the health sector.

Screening + optimization experiment

6 quantitative factors and 2 two-level categorical factors

Budget of 24 runs

Max 4th order correlation = 0.54
Good projection properties
Twice the power to detect quadratic effects
than alternative DSDs from JMP



Extensions 2: blocked OMARS

(Mixed-level) OMARS usually can be blocked in different ways.

Our blocked designs have the following properties:

- Block effect is orthogonal to main effects
- Minimal aliasing between the blocks and the second-order effects

Our approach is based on integer programming

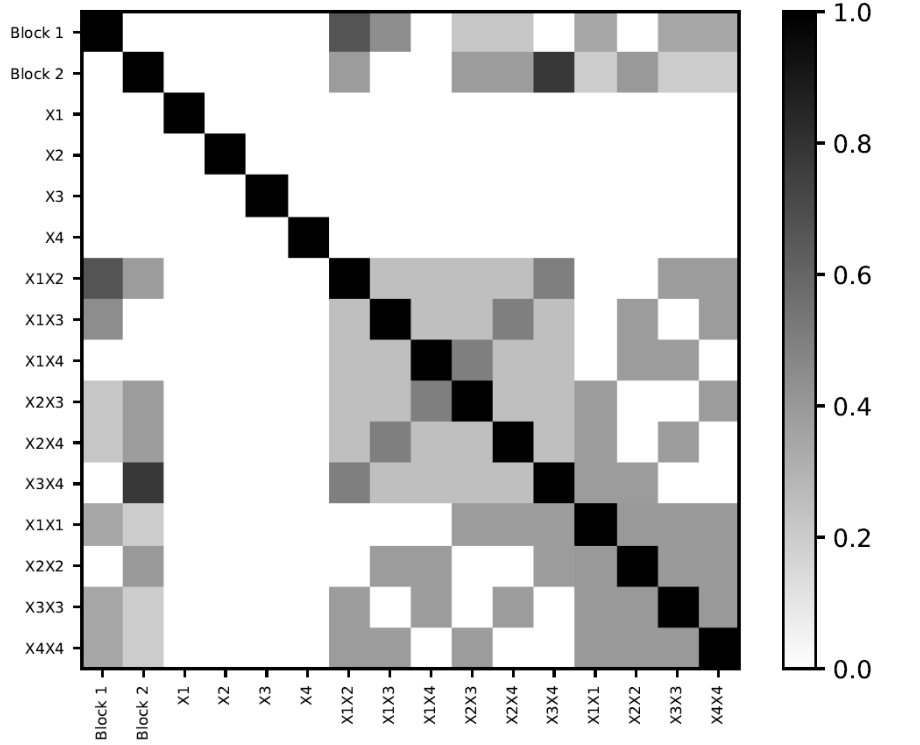
We built a large catalog of blocked (mixed-level) OMARS for both screening and optimization.

A similar design selection approach can be followed for blocked designs too.

Blocked OMARS: example

4-factor 15-run definitive screening design

block 1	block 2	block 3
- - + 0	+ + + -	+ - 0 -
0 + + +	- 0 + -	+ - + +
0 - - -	+ 0 - +	- + - -
+ + - 0	- - - +	- + 0 +
0 0 0 0	0 0 0 0	0 0 0 0

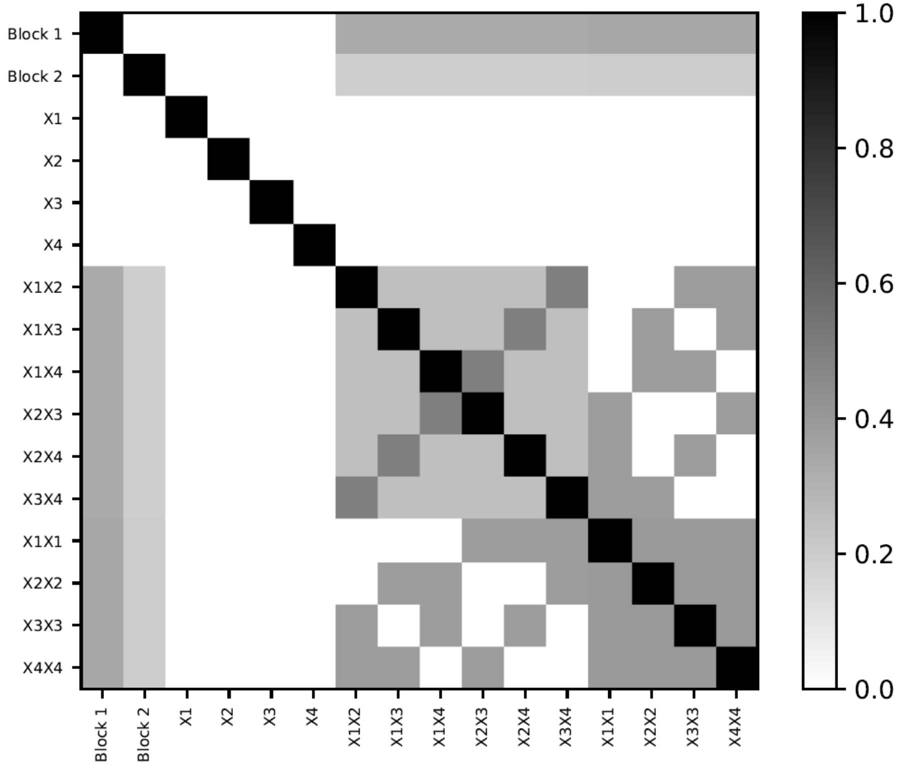


Blocking scheme using JMP16

Blocked OMARS: example

4-factor 15-run definitive screening design

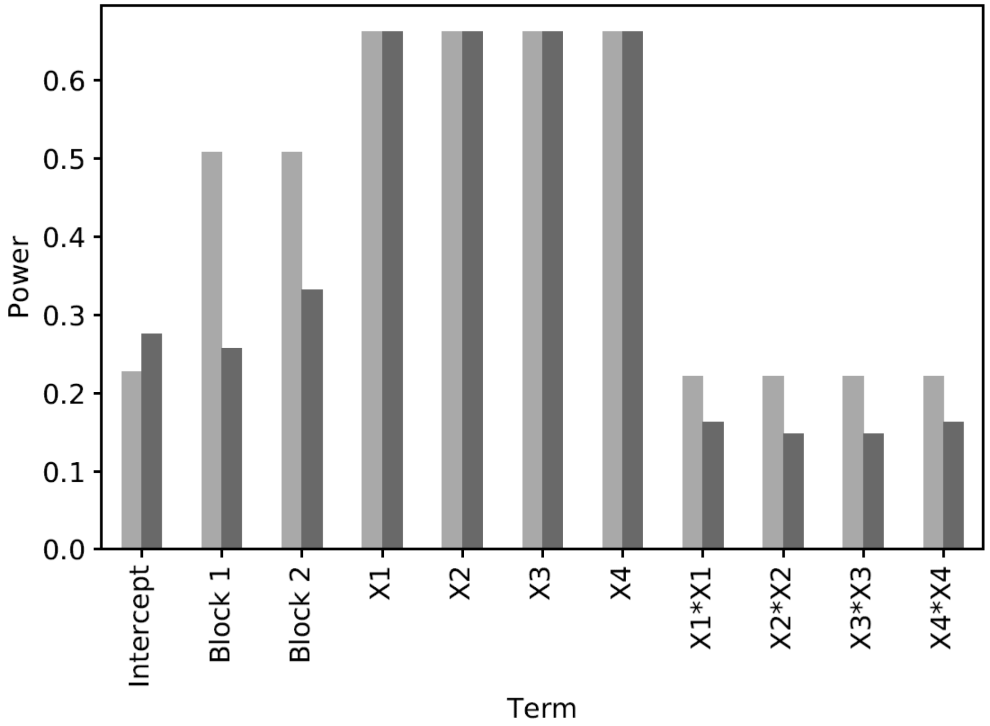
block 1	block 2	block 3
0 + + +	0 - - -	0 0 0 0
- - + 0	+ + - 0	+ + + -
+ 0 - +	- 0 + -	- - - +
+ - 0 -	+ - + +	0 0 0 0
- + - -	- + 0 +	0 0 0 0



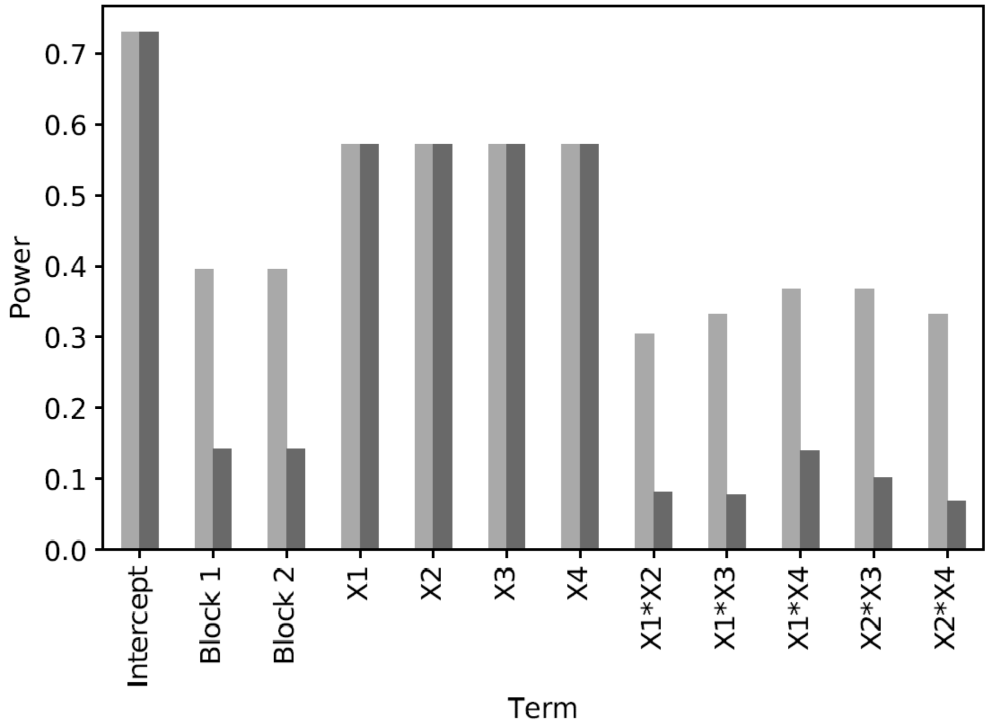
Blocking scheme using our approach

Blocked OMARS: example

Powers to detect the effects in two models



Model 1



Model 2

Summary

The catalog offers much flexibility in choosing a design.

Often improves DSDs for screening and CCDs and BBDs for optimization.

Our catalog allows finding a design for novel problems, like, for example, a screening design in blocks with a high power to detect QEs.

The availability of a complete catalog allows us to develop a multi-criteria selection approach.

Thank you!