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OMARS Designs: Bridging the Gap between Definitive Screening Designs and Standard Response Surface Designs

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Response surface designs (RSDs)

- Experimental designs for process optimization
- Allow the study of several quantitative factors
  - Main effects
  - Quadratic effects
  - Two-factor interactions
- Best-known designs are
  - Central composite designs (CCDs)
  - Small central composite designs (SCCDs)
  - Box-Behnken designs (BBDs)

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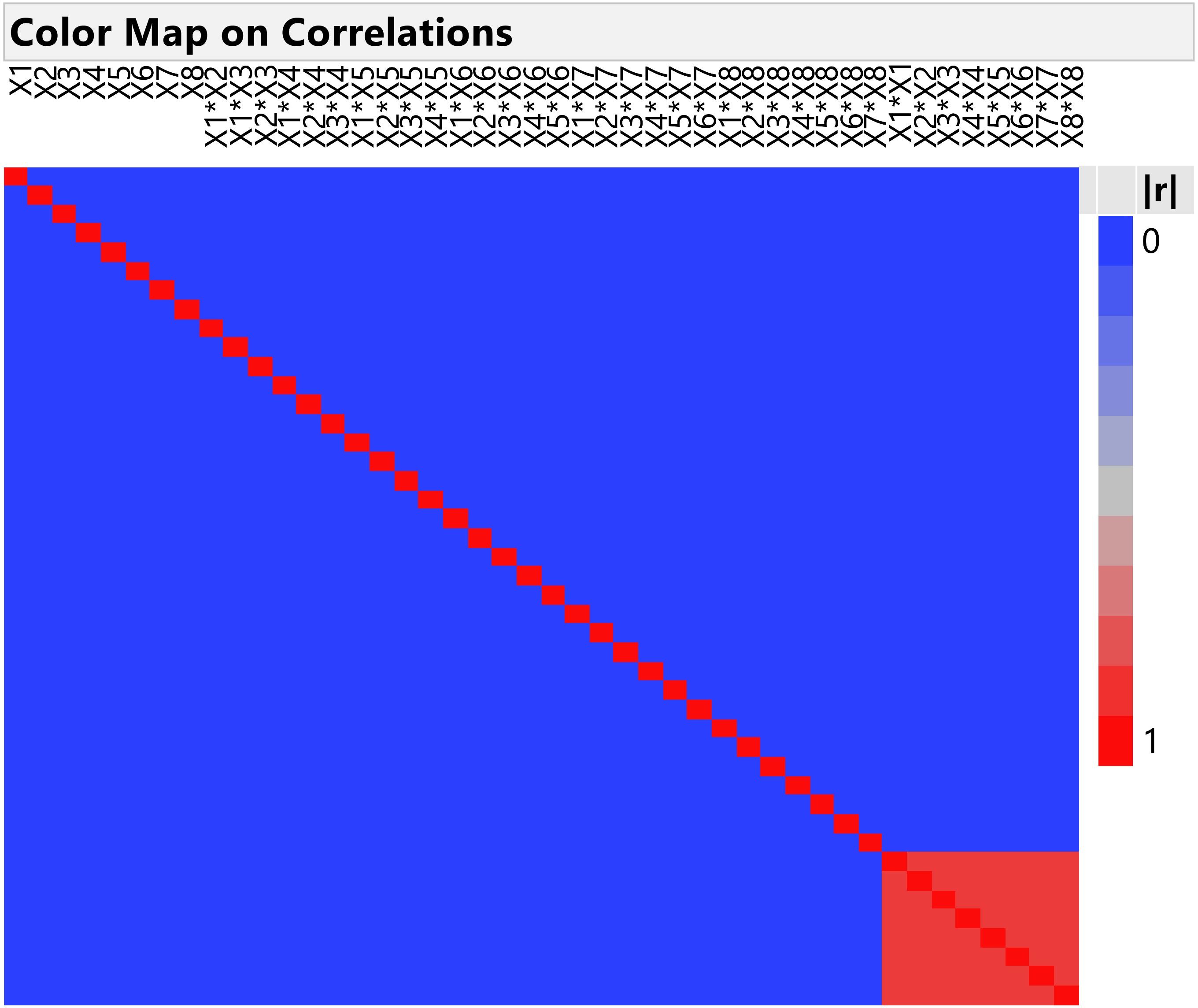
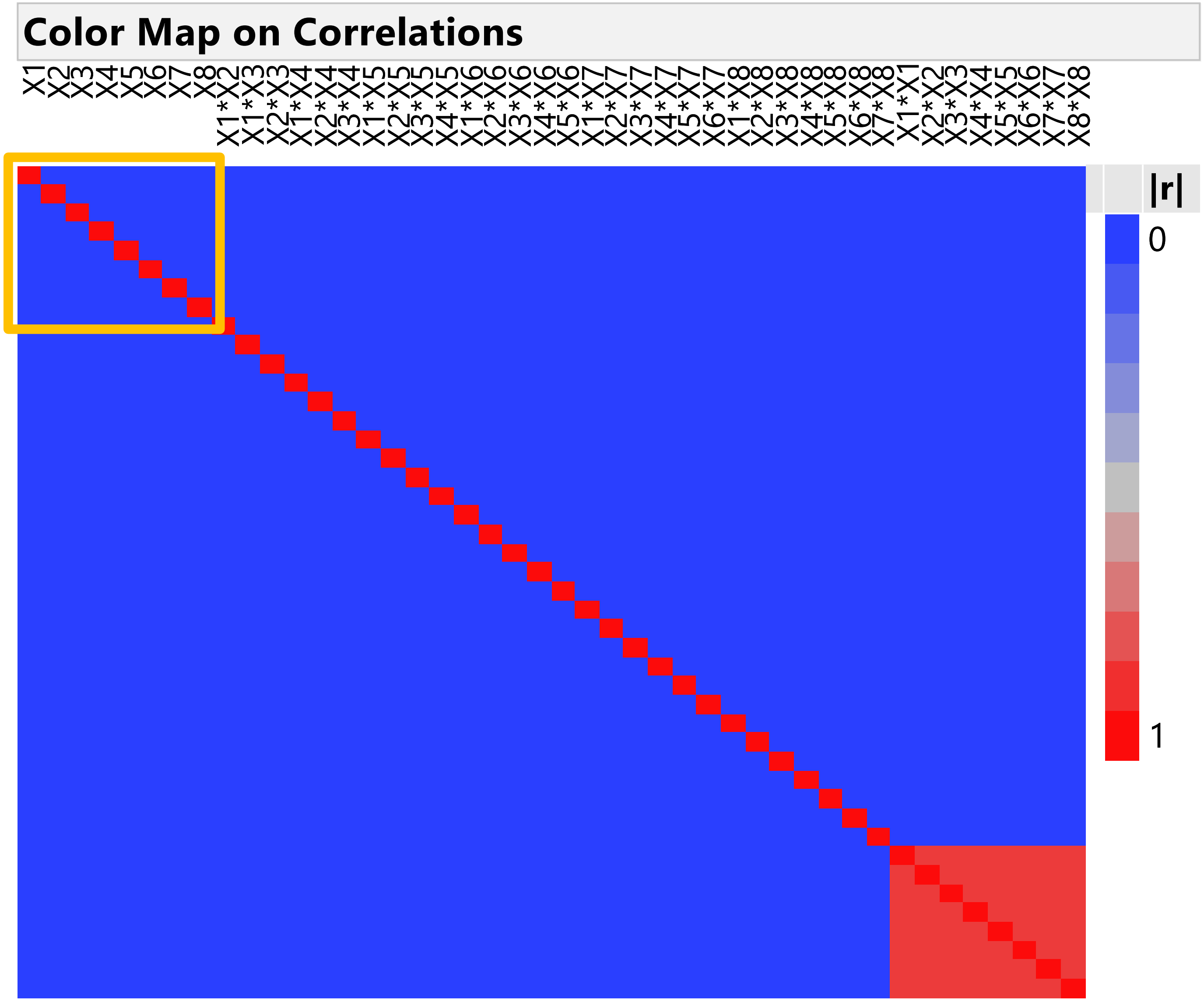
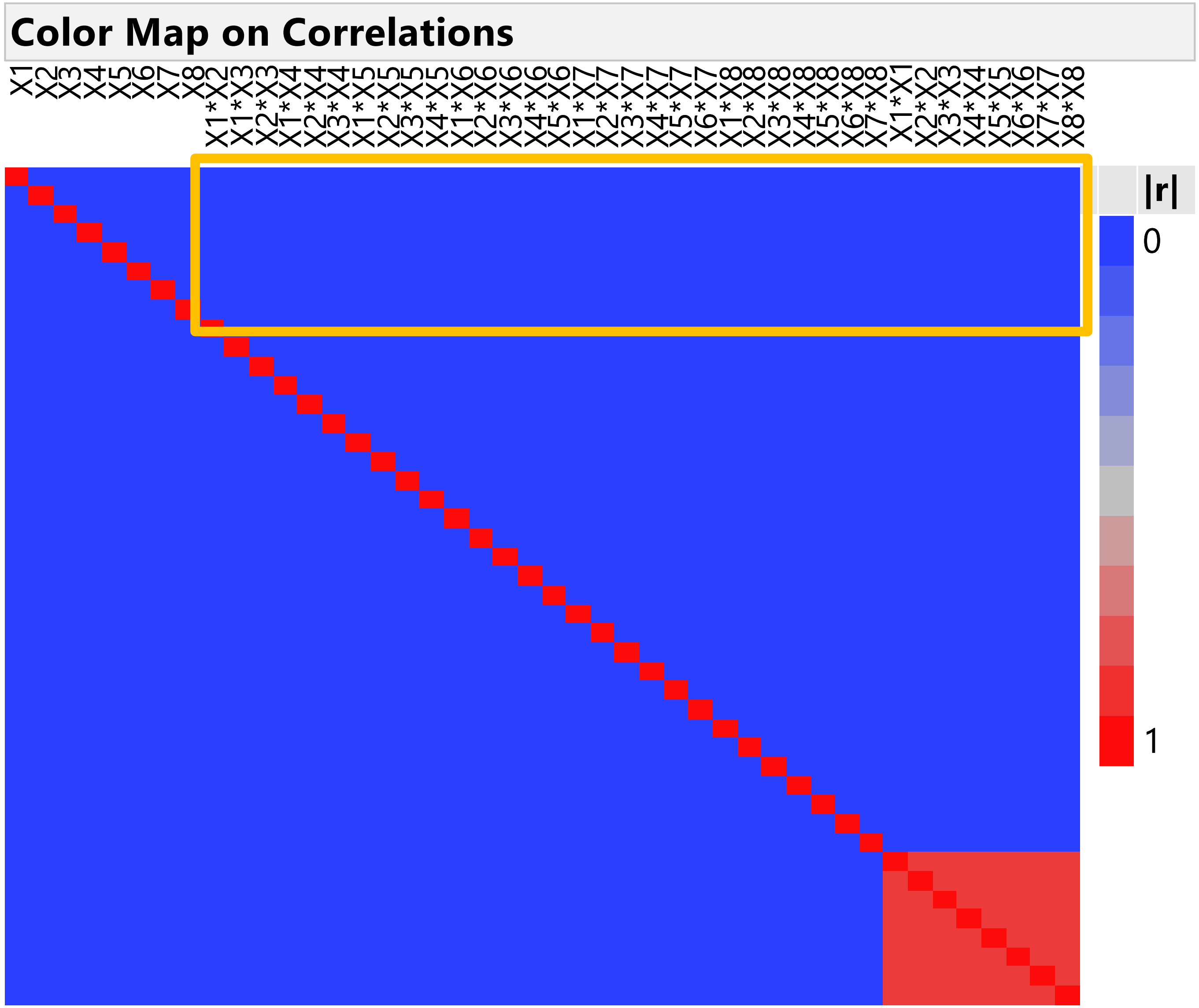
Central composite design



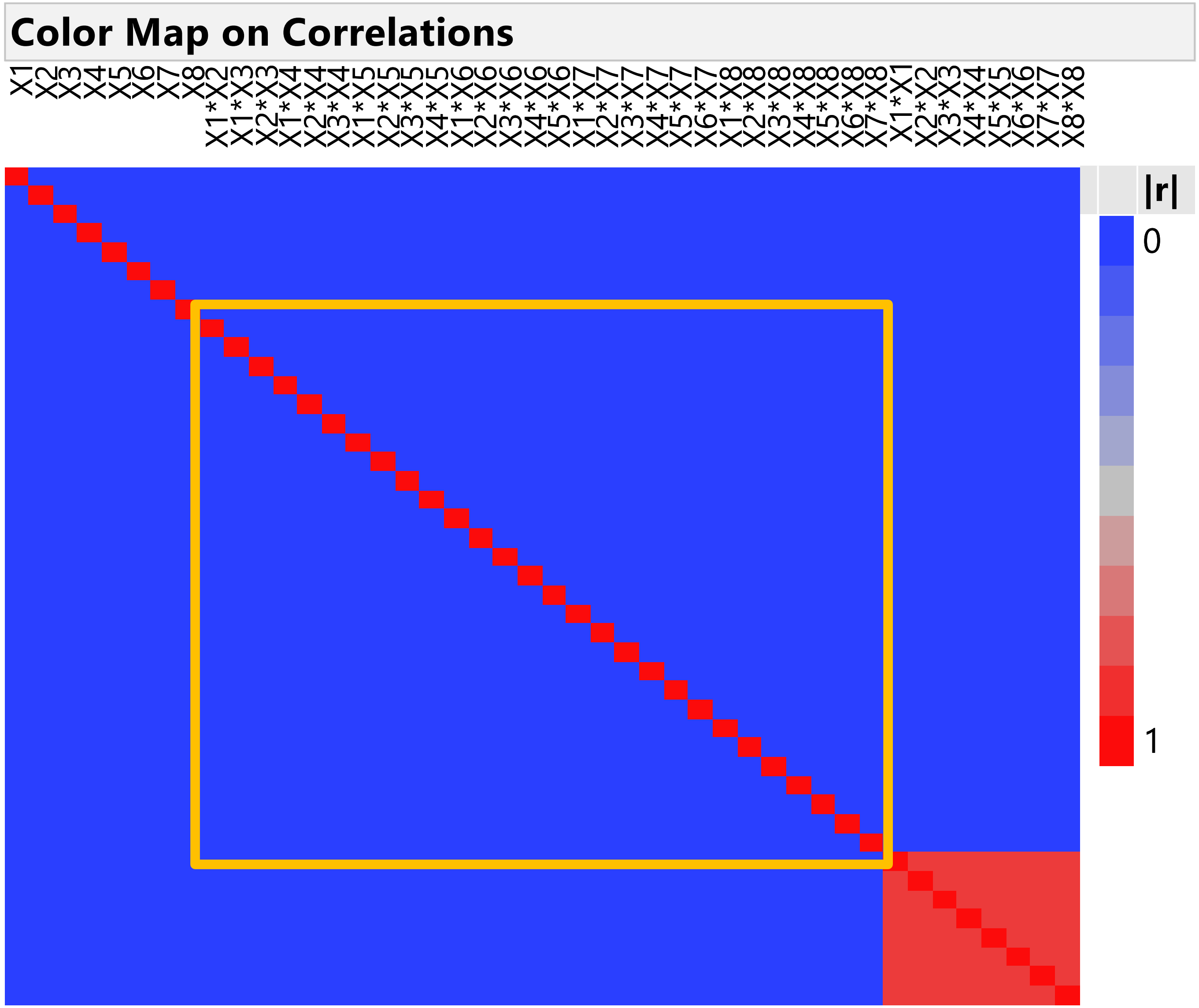
Central composite design



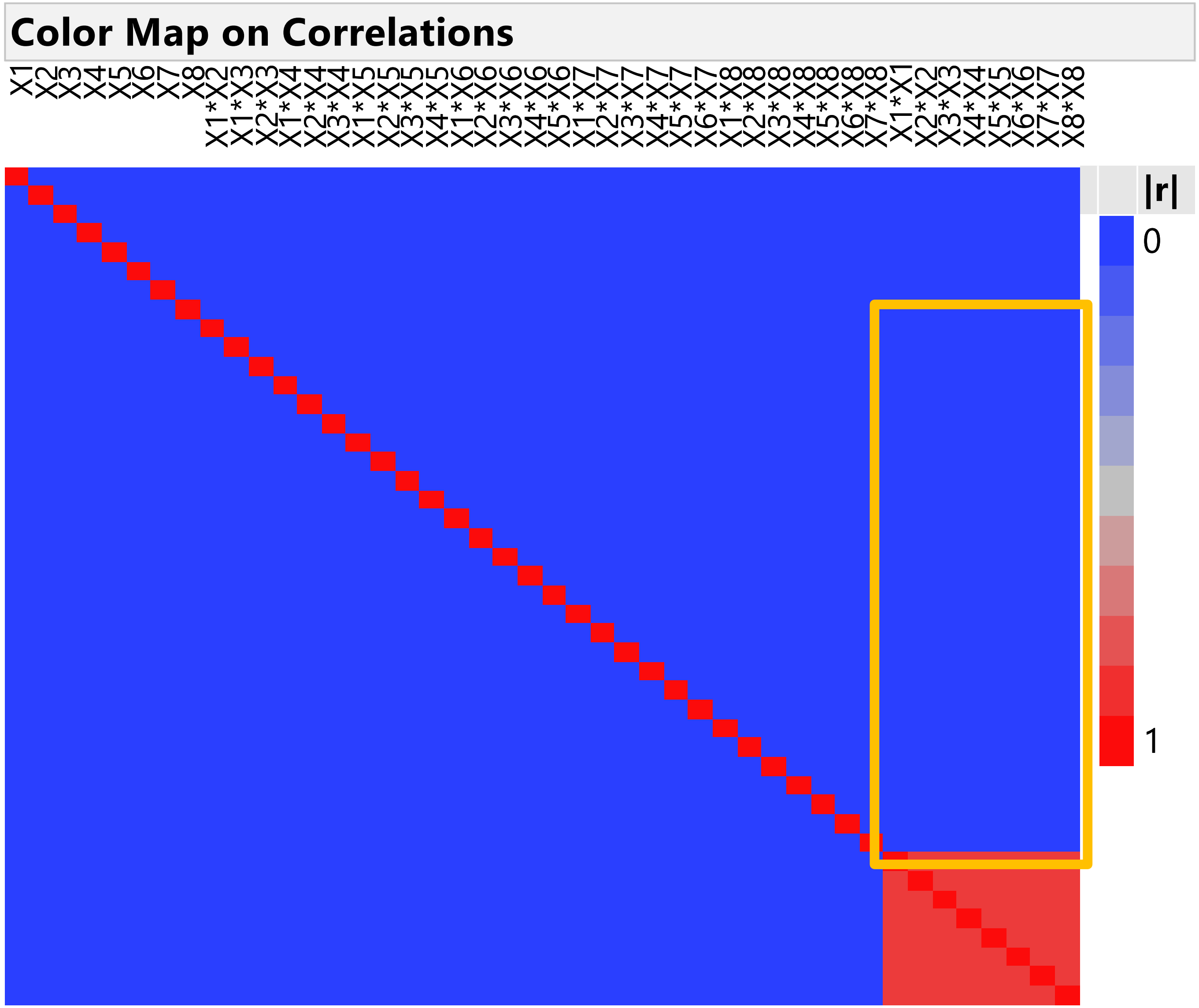
Central composite design



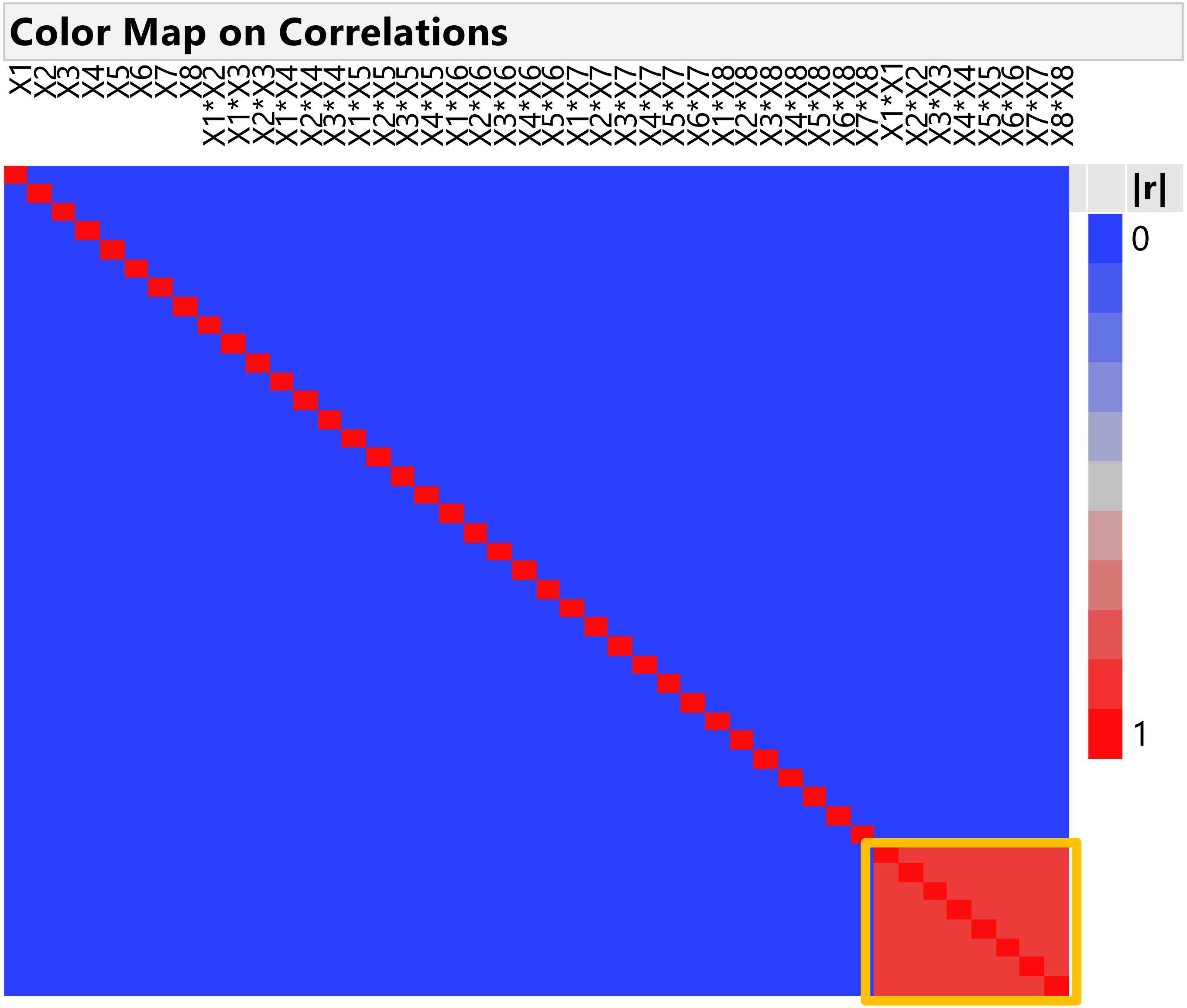
Central composite design



Central composite design



Central composite design



Properties

- Traditional response surface designs have nice orthogonality properties
  - Main effects are orthogonal to each other
  - Main effects are orthogonal to two-factor interactions and to quadratic effects
  - Two-factor interactions are orthogonal to quadratic effects
- Offer large powers for main effects and two-factor interactions
- Run size increases rapidly with the number of factors
- Guarantees a painless data analysis, at a large experimental cost

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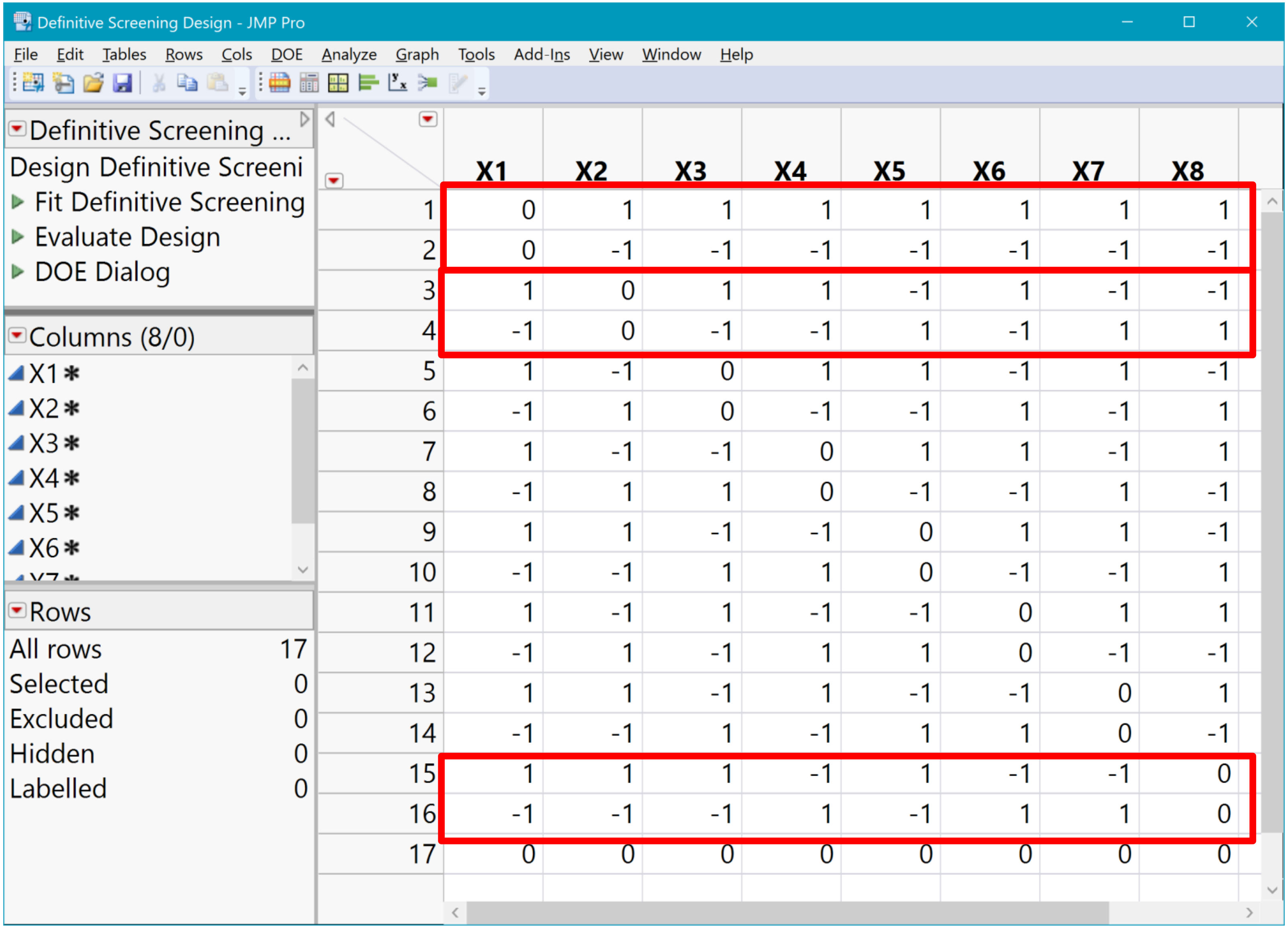
Definitive screening designs

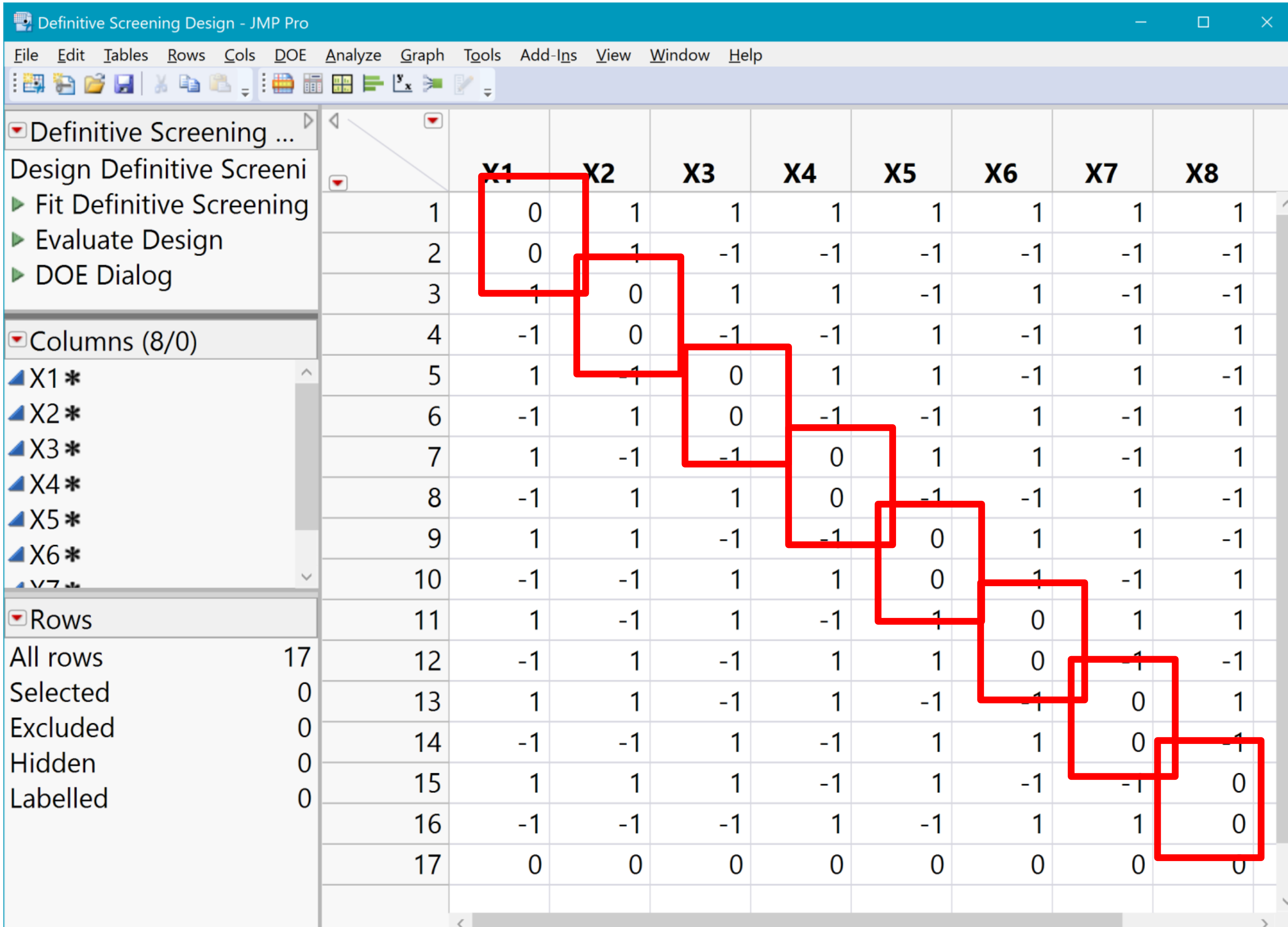
- Three-level experimental designs for screening large numbers of quantitative factors
- Allow the estimation of
  - Main effects
  - Quadratic effects
  - Two-factor interactions
- Introduced by Jones & Nachtsheim (Technometrics, 2011)
- A fast construction based on conference matrices was proposed by Xiao, Lin & Bai (Journal of Quality Technology, 2012)
- Designs based on that construction are available in commercial software

8-factor definitive screening design



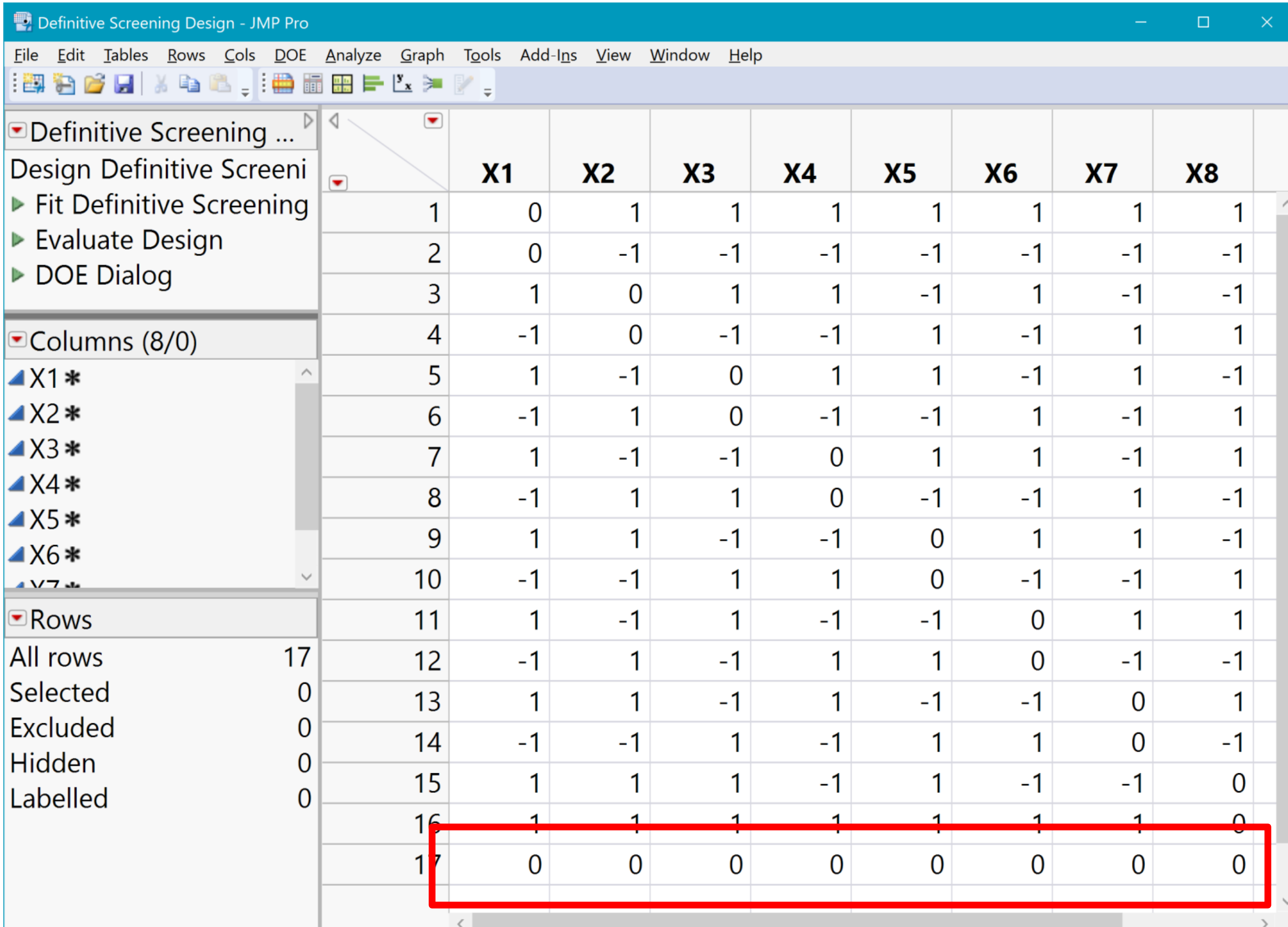
	X1	X2	X3	X4	X5	X6	X7	X8
1	0	1	1	1	1	1	1	1
2	0	-1	-1	-1	-1	-1	-1	-1
3	1	0	1	1	-1	1	-1	-1
4	-1	0	-1	-1	1	-1	1	1
5	1	-1	0	1	1	-1	1	-1
6	-1	1	0	-1	-1	1	-1	1
7	1	-1	-1	0	1	1	-1	1
8	-1	1	1	0	-1	-1	1	-1
9	1	1	-1	-1	0	1	1	-1
10	-1	-1	1	1	0	-1	-1	1
11	1	-1	1	-1	-1	0	1	1
12	-1	1	-1	1	1	0	-1	-1
13	1	1	-1	1	-1	-1	0	1
14	-1	-1	1	-1	1	1	0	-1
15	1	1	1	-1	1	-1	-1	0
16	-1	-1	-1	1	-1	1	1	0
17	0	0	0	0	0	0	0	0

8-factor definitive screening design



	X1	X2	X3	X4	X5	X6	X7	X8
1	0	1	1	1	1	1	1	1
2	0	1	-1	-1	-1	-1	-1	-1
3	1	0	1	1	-1	1	-1	-1
4	-1	0	-1	-1	1	-1	1	1
5	1	-1	0	1	1	-1	1	-1
6	-1	1	0	-1	-1	1	-1	1
7	1	-1	-1	0	1	1	-1	1
8	-1	1	1	0	-1	-1	1	-1
9	1	1	-1	-1	0	1	1	-1
10	-1	-1	1	1	0	1	-1	1
11	1	-1	1	-1	1	0	1	1
12	-1	1	-1	1	1	0	-1	-1
13	1	1	-1	1	-1	-1	0	1
14	-1	-1	1	-1	1	1	0	-1
15	1	1	1	-1	1	-1	-1	0
16	-1	-1	-1	1	-1	1	1	0
17	0	0	0	0	0	0	0	0

8-factor definitive screening design



	X1	X2	X3	X4	X5	X6	X7	X8
1	0	1	1	1	1	1	1	1
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3	1	0	1	1	-1	1	-1	-1
4	-1	0	-1	-1	1	-1	1	1
5	1	-1	0	1	1	-1	1	-1
6	-1	1	0	-1	-1	1	-1	1
7	1	-1	-1	0	1	1	-1	1
8	-1	1	1	0	-1	-1	1	-1
9	1	1	-1	-1	0	1	1	-1
10	-1	-1	1	1	0	-1	-1	1
11	1	-1	1	-1	-1	0	1	1
12	-1	1	-1	1	1	0	-1	-1
13	1	1	-1	1	-1	-1	0	1
14	-1	-1	1	-1	1	1	0	-1
15	1	1	1	-1	1	-1	-1	0
16	1	1	1	1	1	1	1	0
17	0	0	0	0	0	0	0	0

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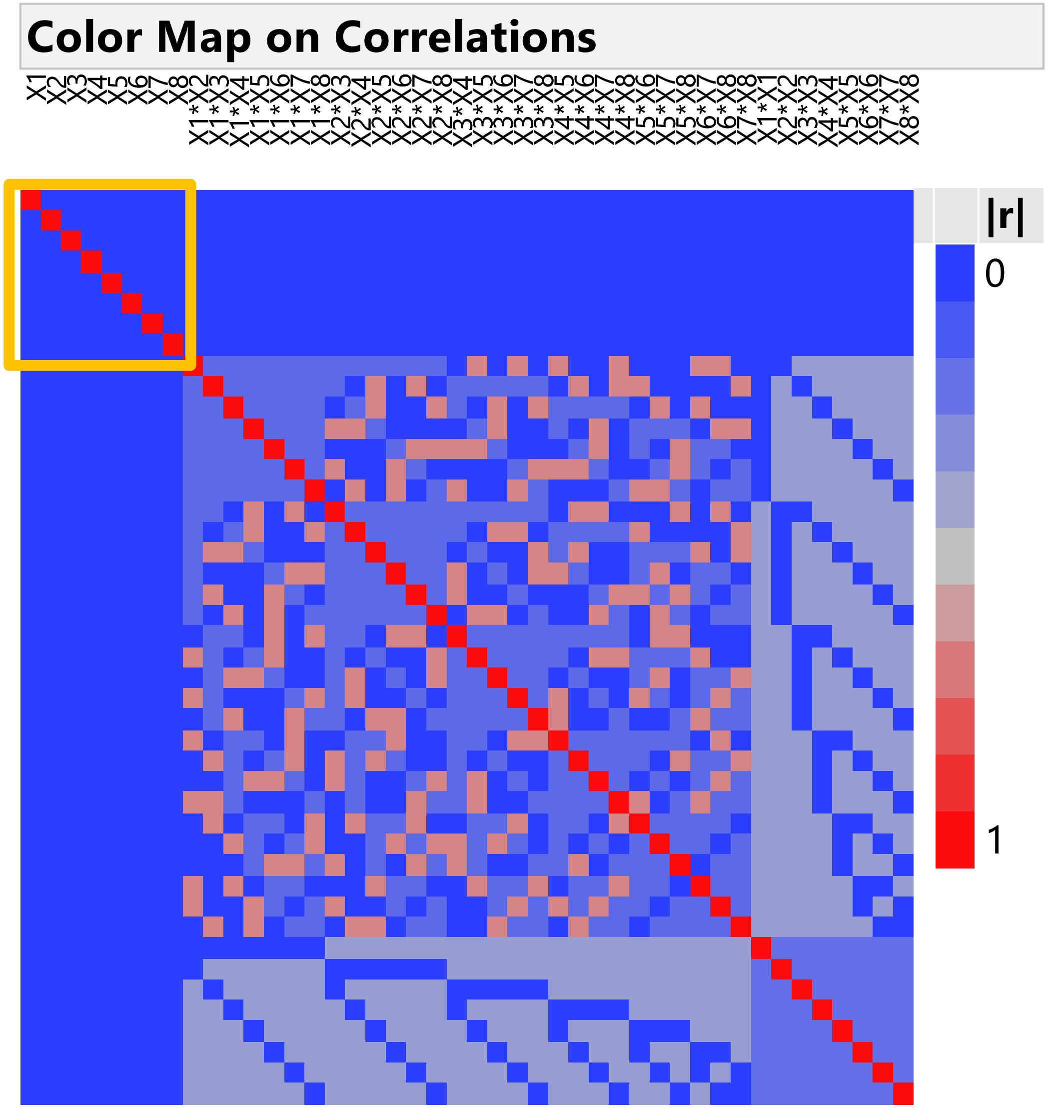

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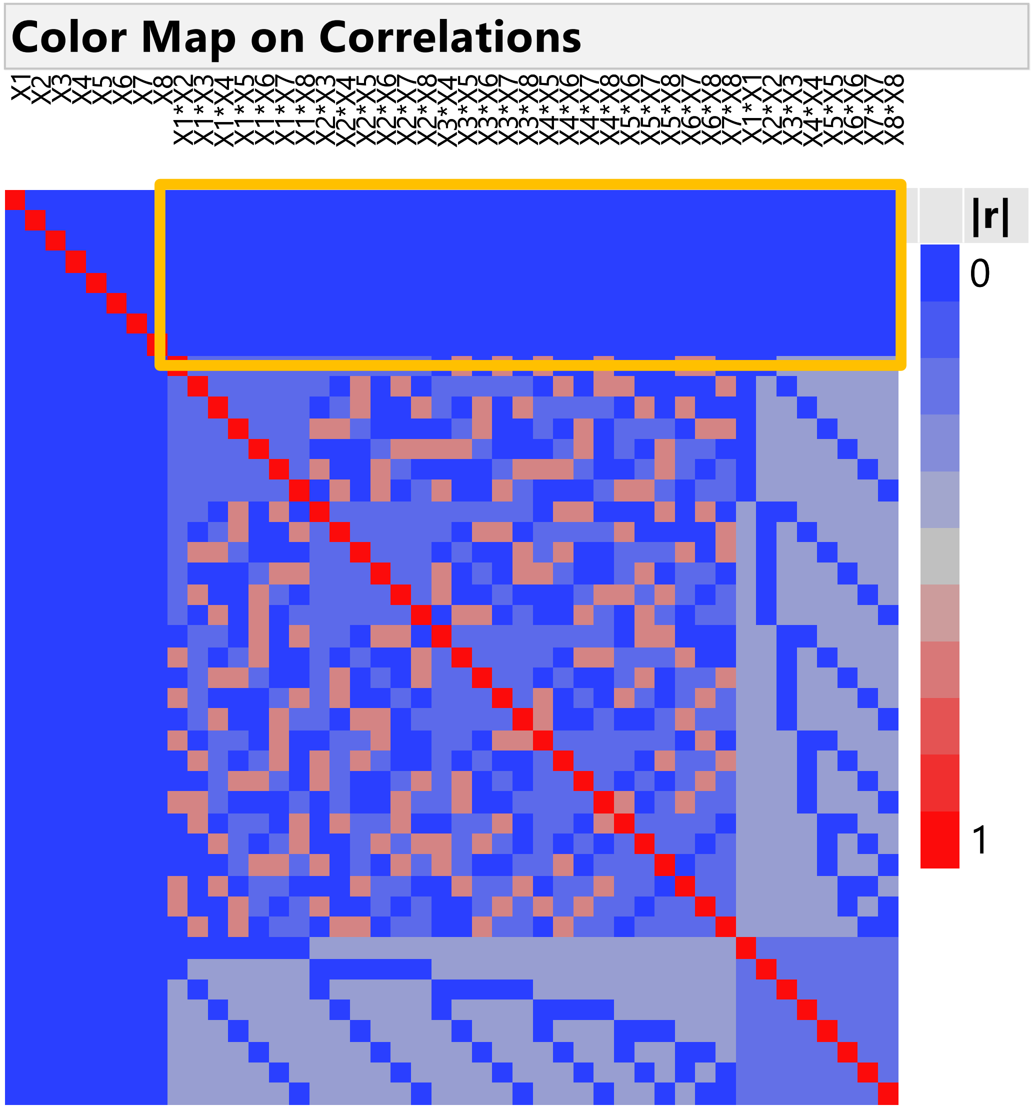

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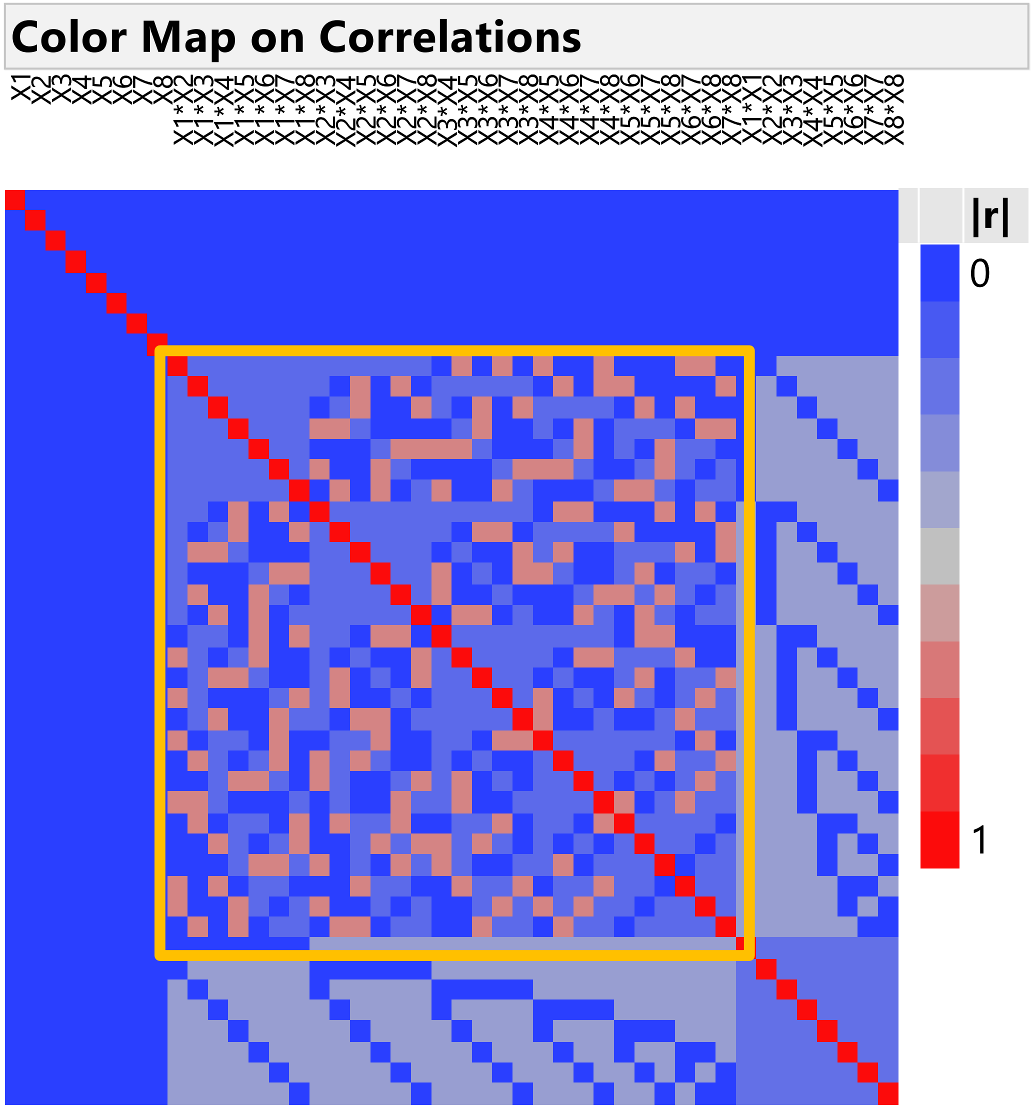

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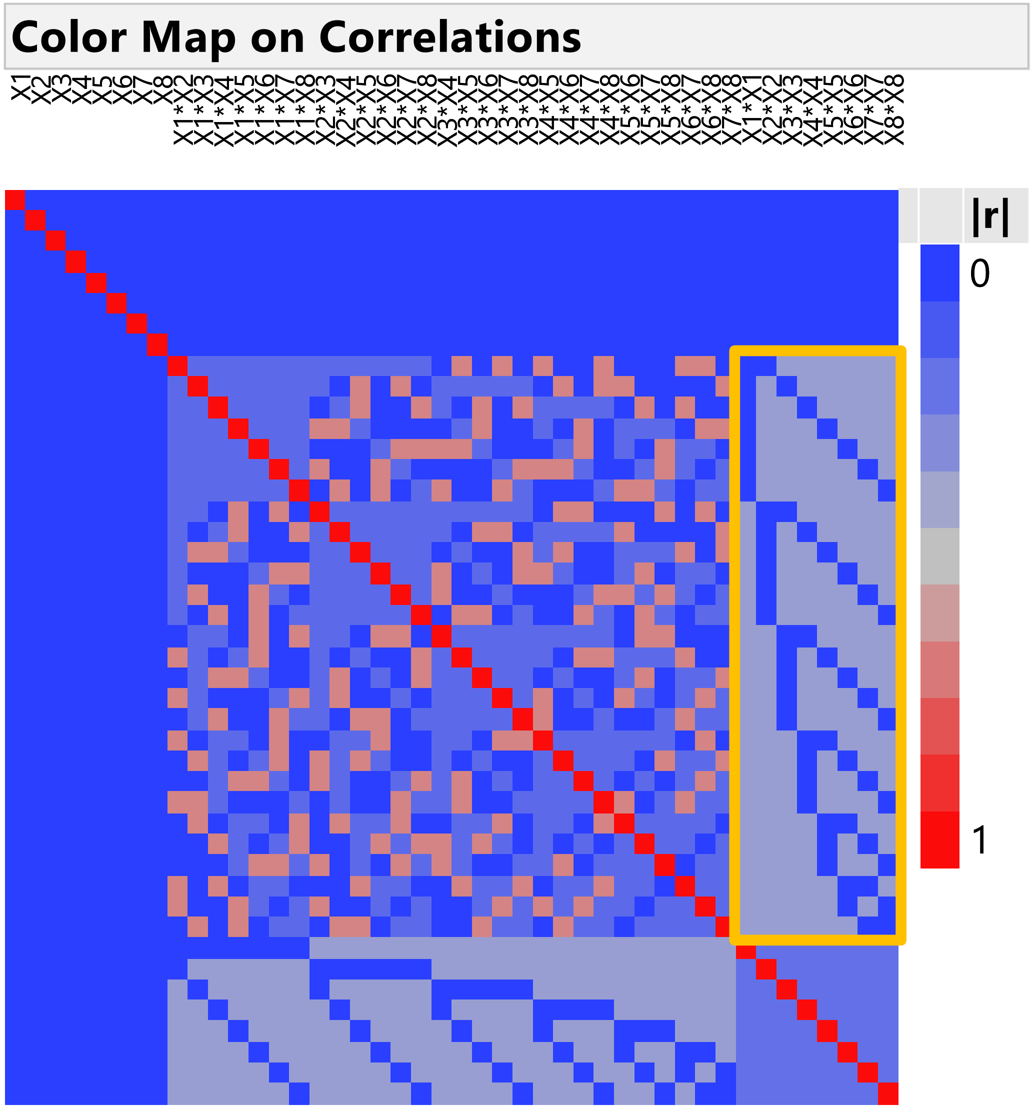

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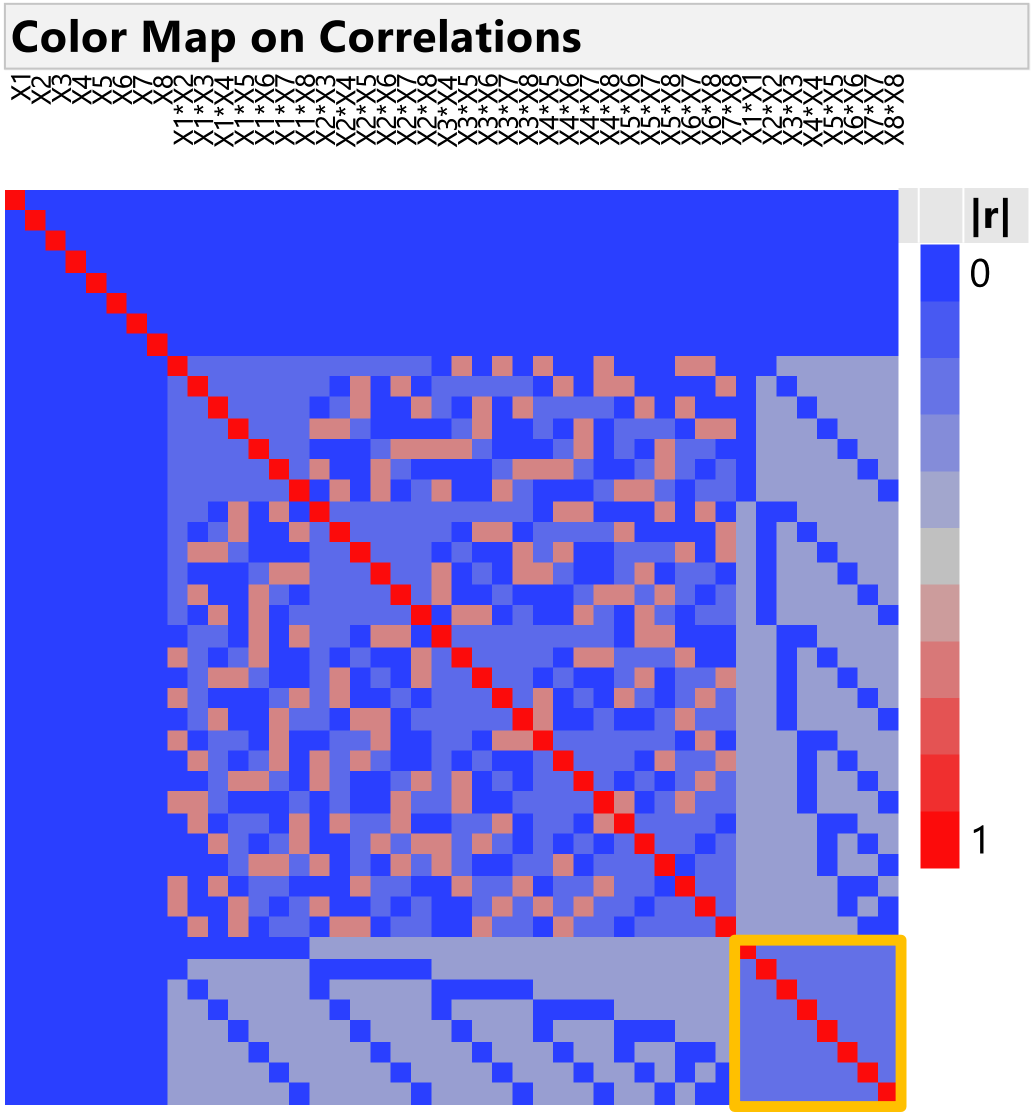

Properties

- Definitive screening designs also have nice orthogonality properties
  - Main effects are orthogonal to each other
  - Main effects are orthogonal to two-factor interactions and to quadratic effects
  - Therefore, they are called minimally aliased designs
- Two-factor interactions are sometimes very strongly aliased with each other
- Two-factor interactions are sometimes strongly aliased with quadratic effects as well
- Run size increases linearly with the number of factors

Discussion

- DSDs are sometimes marketed as a screening design and a response surface design in one
- If only a few factors matter, definitive screening designs project onto a response surface design in these factors
- DSDs are viewed as the smallest kind of response surface designs
- While (S)CCDs and BBDs involve more than enough runs to fit all main effects, interaction effects and quadratic effects, DSDs by far do not have enough runs to achieve this goal
- Analysis can be painful and leave ambiguity if more than a few factors matter
- Exist only for certain numbers of runs

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Conclusion

- On the one hand, we have traditional RSDs
  - With attractive properties
  - With a lot of runs
- On the other hand, we have DSDs
  - With a very small number of runs
  - With some attractive and some unattractive properties
- We wondered whether designs exist with similar orthogonality properties and intermediate numbers of runs
- We discovered a new family of designs that fill the gap between the large RSDs and the small DSDs

Orthogonal

Minimally

Aliased

Response

Surface

designs

Properties

- OMARS designs are three-level designs for quantitative factors
- Therefore, they are called **response surface** designs
- In OMARS designs, main effects are orthogonal to each other
- Therefore, they are called **orthogonal**
- In OMARS designs, main effects are orthogonal to two-factor interactions and to quadratic effects
- Therefore, they are called **minimally aliased**
- The designs have a uniform precision property in the sense that all main effects can be estimated equally well

How many OMARS designs exist?

# Factors	3	4	5	6	7
# Runs	8-14	8-24	12-44	12-50	14-70
# Designs	5	41	5399	1406	1082
Even # Runs (foldover)	5	41	5350	1349	1082
Even # Runs (non-foldover)	-	-	23	49	-
Odd # Runs	-	-	26	8	-

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How did we find the OMARS designs?

- We used integer linear programming techniques
- For each number of runs, we set up a system of linear equalities the solution of which is an OMARS design
- As soon as an OMARS design is found, we solve the system again preventing that the original OMARS design is found again (or any design that is isomorphic to it)
- As soon as the second OMARS design is found, we solve the system again preventing that the two first OMARS designs are found again (or any designs that are isomorphic to them)
- This process is continued until there are no feasible solutions any more

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OMARS designs

- The initial OMARS designs we enumerated did not have center runs
- But we can add as many center runs as we want, since center runs do not affect the orthogonality properties
- The family of OMARS designs generalizes the families of CCDs, BBDs and DSDs
- So, we have a new catalog of designs with the same kinds of attractive properties as CCDs, BBDs and DSDs
- These results appeared in Technometrics

More OMARS designs

		nruns								
		14	16	20	22	24	26	27	28	30
$m = 6$	#sol	1	1	2	4	25	519	7	485	8,864
	#nodes	82	250	502	2,532	16,252	718,458	704,220	1,173,594	39,415,295
	time	6s	13s	20s	69s	457s	7.7h	6.9h	12h	15.9d
$m = 7$	#sol	1	1	1	1	5	549	0	106	20,019
	#nodes	60	262	634	832	13,726	2,053,001	372,331	4,263,183	555,221,657
	time	25s	100s	158s	128	1702s	5.4d	21.1h	8.9d	4.4y
$m = 8$	#sol	-	1	1	0	3	853	-	9	11
	#nodes	-	110	646	236	11,985	6,807,971	-	9,497,041	11,900,209
	time	-	113s	572s	99s	3.1h	3m	-	6.2m	5.6m

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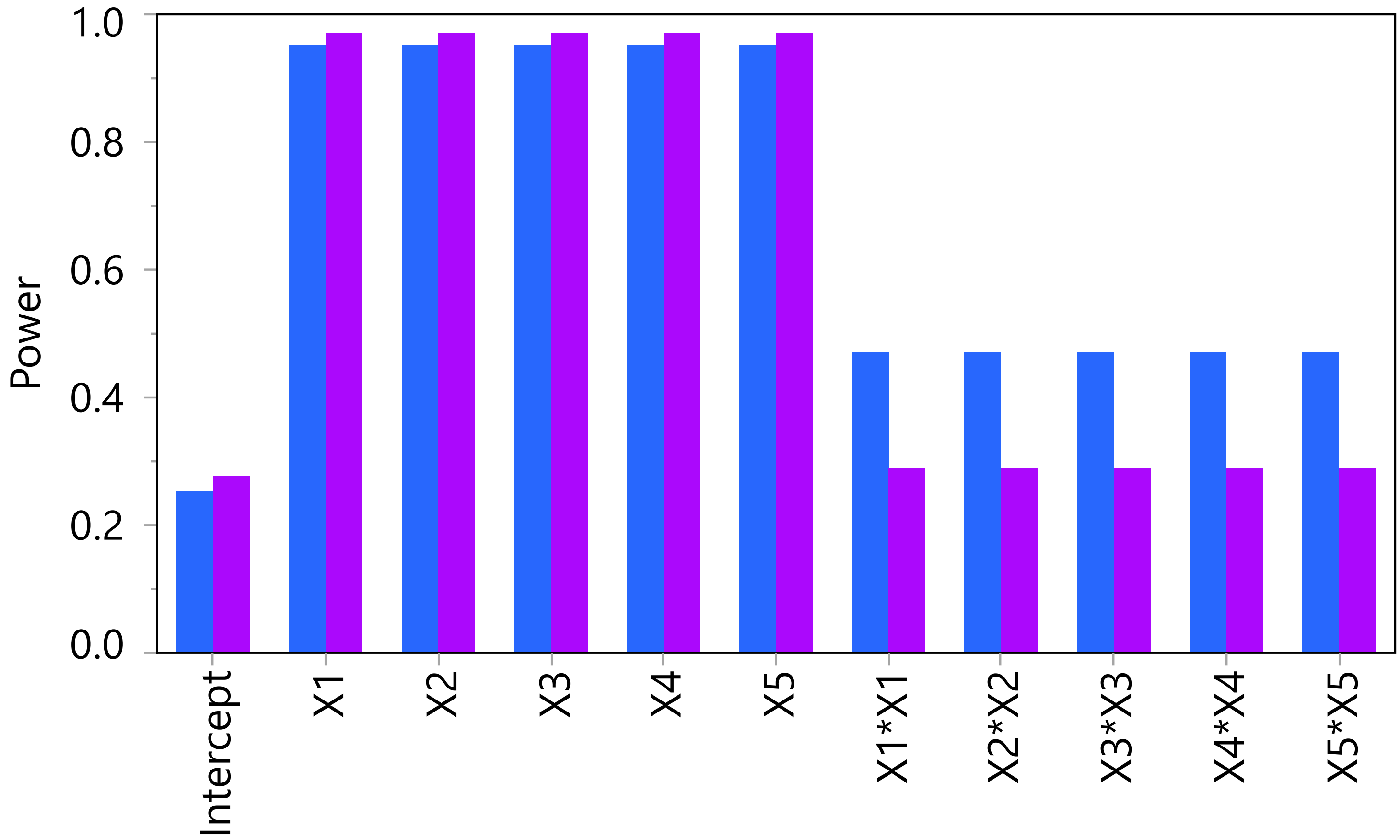
More OMARS designs

		nruns					
		31	32	34	35	36	40
$m = 6$	#sol	37	69,677	227,902	258	65,836	-
	#nodes	50,649,649	358,608,938	976,161,360	1,644,770,934	226,213,340	-
	time	16.5d	5m	1.9y	4.4m	2.8m	-
$m = 7$	#sol	9	49,269	16,952	3	57,727	1,656
	#nodes	712,279,617	280,674,367	430,079,736	3,140,152,715	3,366,592,634	72,419,243,247
	time	4.7y	19.7y	3.5y	20.2y	22.2y	2.3y
$m = 8$	#sol	-	31	0	-	0	284
	#nodes	-	981,101,888	86,365	-	269,792,124	23,824,792,213
	time	-	106.5y	16.4h	-	25.3y	28.8y

Are OMARS designs any good?

- Let us compare the following designs
  - the 22-run 5-factor OMARS design from our Technometrics paper
  - the 22-run 5-factor DSD with two center runs, obtained using the JMP software by asking for 8 extra runs
- The OMARS design is able to fit all two-factor interactions while the DSD is not
- The OMARS design has better projection properties
- The OMARS design has a much larger power for the quadratic effects, at the expense of a slightly smaller power for the main effects

Are OMARS designs any good?



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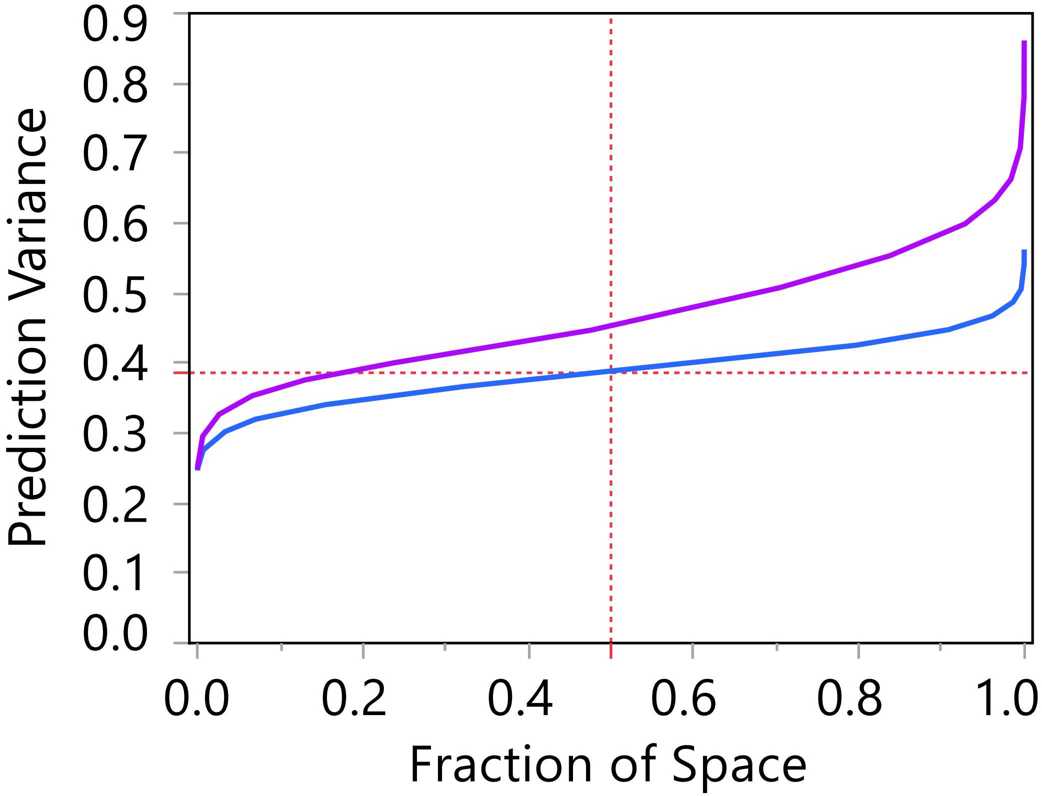

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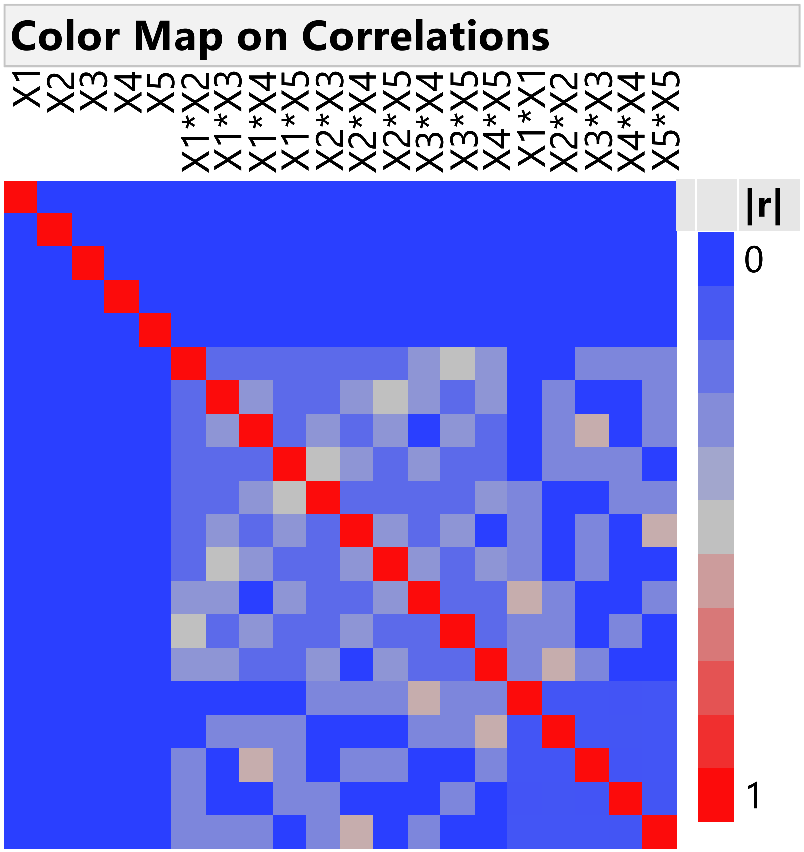
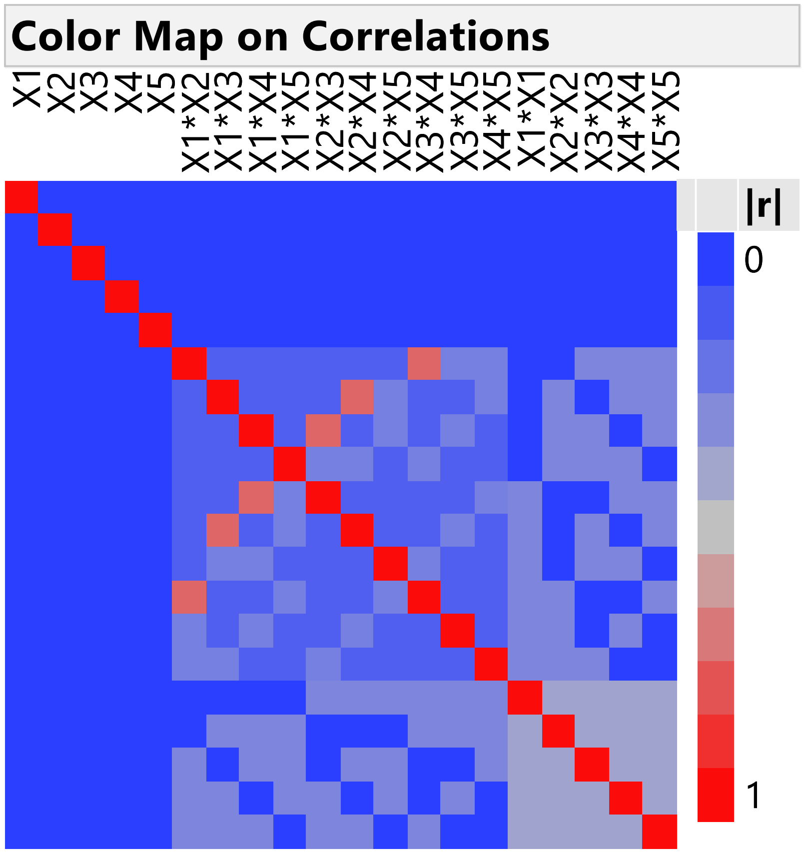


OMARS



DSD

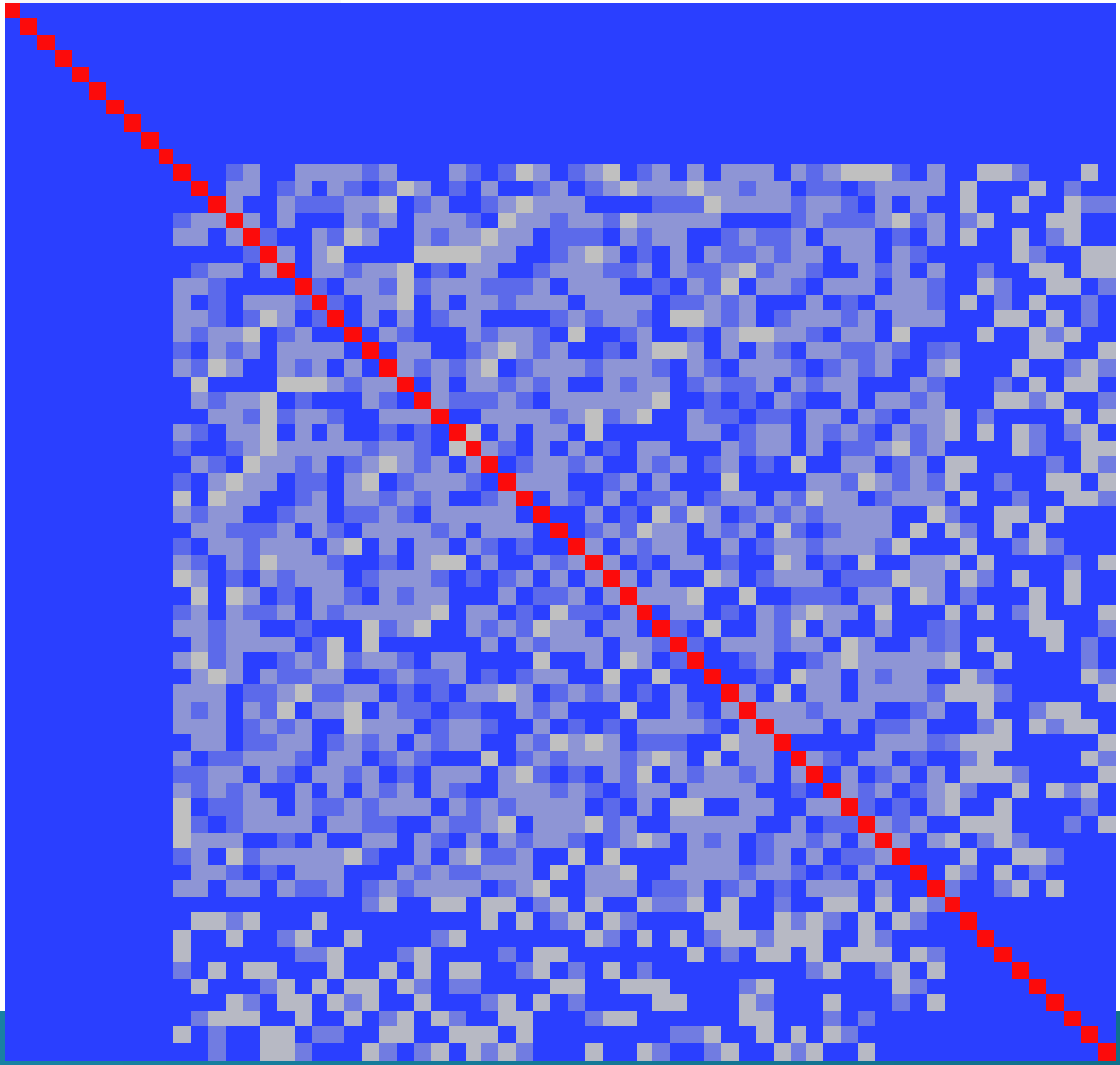
The design

- Foldover design
- Balanced: as many +1s as −1s in every column
- No center runs
- Six 0s in every column (as a result of which the precisions for the main effects are identical)
- Can be blocked orthogonally in two blocks of 11 runs

X1	X2	X3	X4	X5
-1	-1	-1	-1	-1
-1	-1	1	0	-1
-1	-1	1	1	1
-1	0	-1	0	0
-1	0	0	-1	1
-1	1	-1	1	1
-1	1	0	-1	0
-1	1	1	1	-1
0	-1	-1	1	0
0	-1	0	0	1
0	0	-1	1	-1
0	0	1	-1	1
0	1	0	0	-1
0	1	1	-1	0
1	-1	-1	-1	1
1	-1	0	1	0
1	-1	1	-1	-1
1	0	0	1	-1
1	0	1	0	0
1	1	-1	-1	-1
1	1	-1	0	1
1	1	1	1	1

The Engie experiment

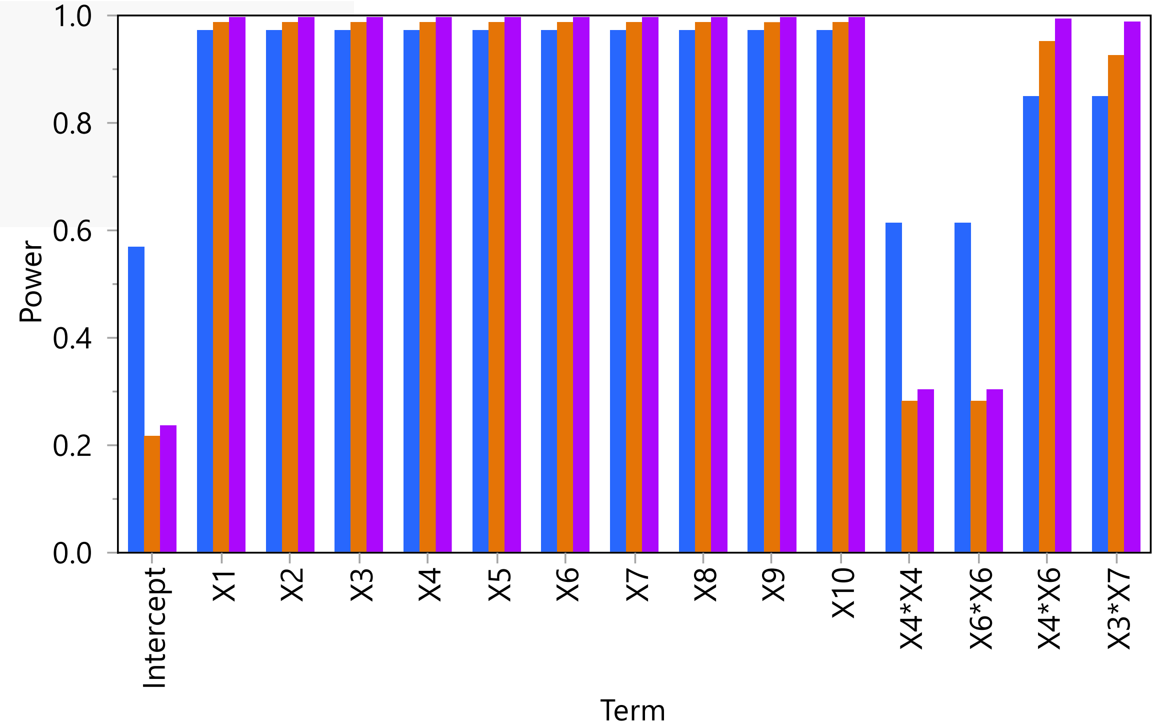
- .



The Engie example

- 27 runs for 10 factors
- three levels of every factor are equireplicated
- therefore, the OMARS design provides more information and a larger power for quadratic effects
- the OMARS design allows any response surface model in 4 factors to be estimated, unlike the benchmark definitive screening designs
- the OMARS design has a 100% projection estimation capacity for 4 factors (the benchmarks have projection estimation capacities of 33% and 73% for 4 factors)

Power to detect effects (S/N ratio = 1)



Blue: OMARS 27R
Orange: DSD 25R
Purple: DSD 29R

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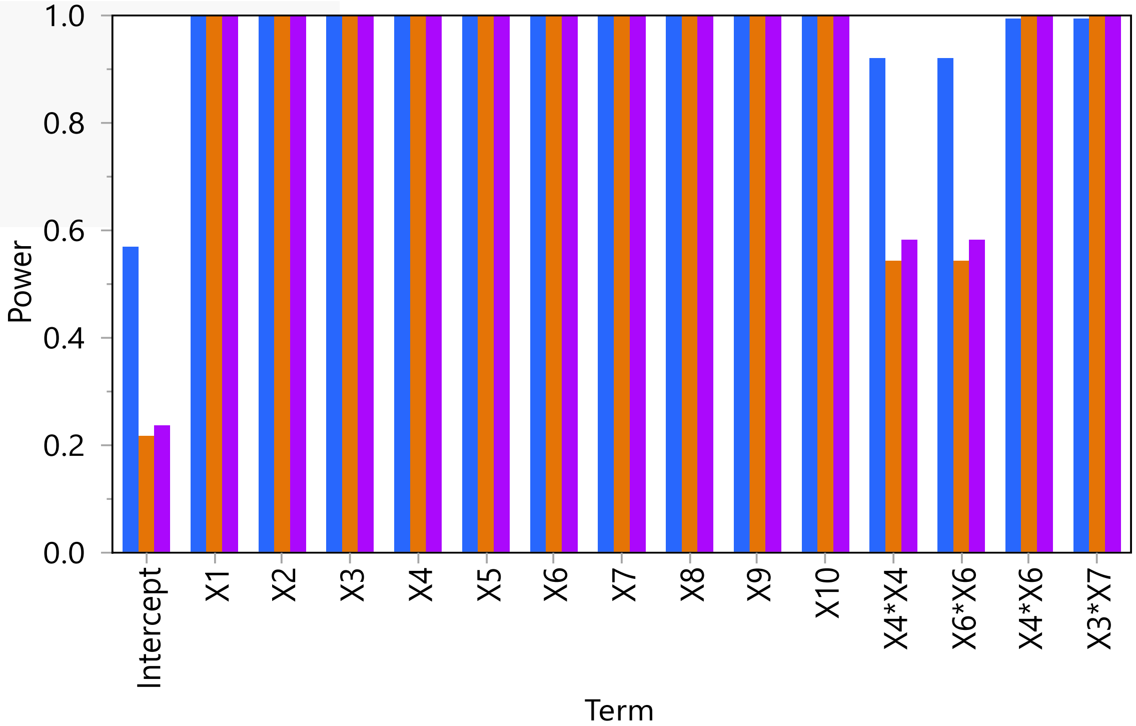
Power to detect effects (S/N ratio = 1.5)



Blue: OMARS 27R
Orange: DSD 25R
Purple: DSD 29R

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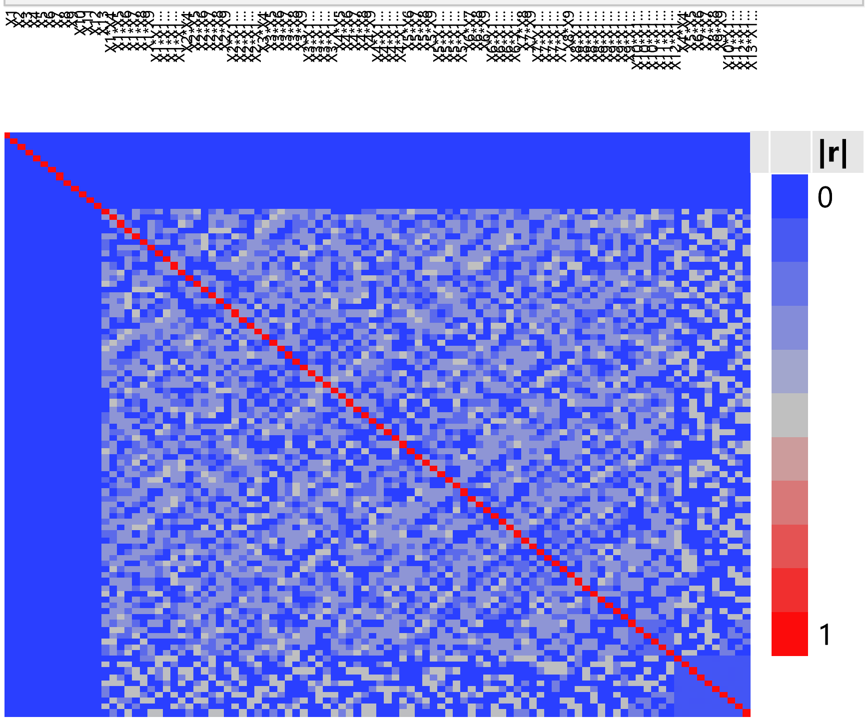
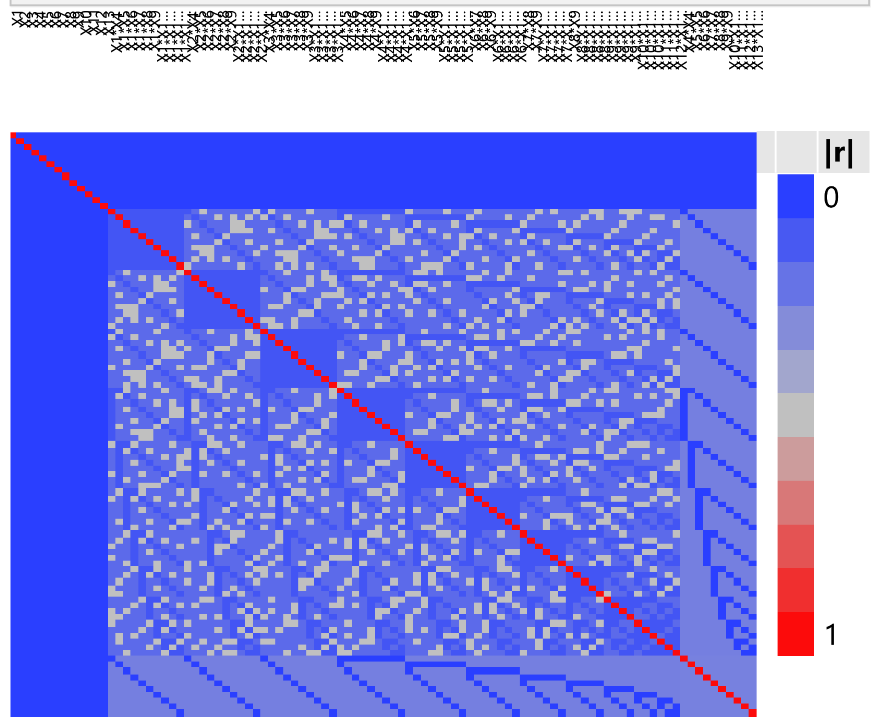
13-factor example

13-factor OMARS



13-factor DSD



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How to choose an OMARS design?

- We have characterized the OMARS designs in many different ways
  - D-, I- and A-optimality
  - Power for detecting active main effects, interaction effects and quadratic effects
  - Standard errors of estimates
  - Projection properties: can they fit all models with 2, 3, 4, 5, … factors
  - …
- We are developing a web-based application to select OMARS designs taking into account multiple criteria

Multi-criteria design selection algorithm

satisficing → dominance → utopia method / manual comparison

Select designs which meet certain acceptability criteria

Multi-criteria design selection algorithm

Discard designs which are dominated by others for a user-specified subset of the design characteristics

Select the set of Pareto optimal designs

Multi-criteria design selection algorithm

The utopia design is a fictitious design whose characteristics are the best ones possible among the surviving designs

Select the design whose characteristics are closest to this utopia design

Multi-criteria design selection algorithm

The algorithm can also output all Pareto optimal designs for manual comparison

Summary

- We created a brand new catalog of orthogonal RSDs
- OMARS designs certainly challenge DSDs
- Offer much flexibility in terms of run size
- OMARS designs will be especially useful when the number of runs is too small to generate D- or I-optimal designs for the full quadratic model (main effects, interactions and quadratic effects)
- The availability of a complete catalog allows us
    - to take many different criteria into account when picking a design
    - to develop a novel kind of design selection approach

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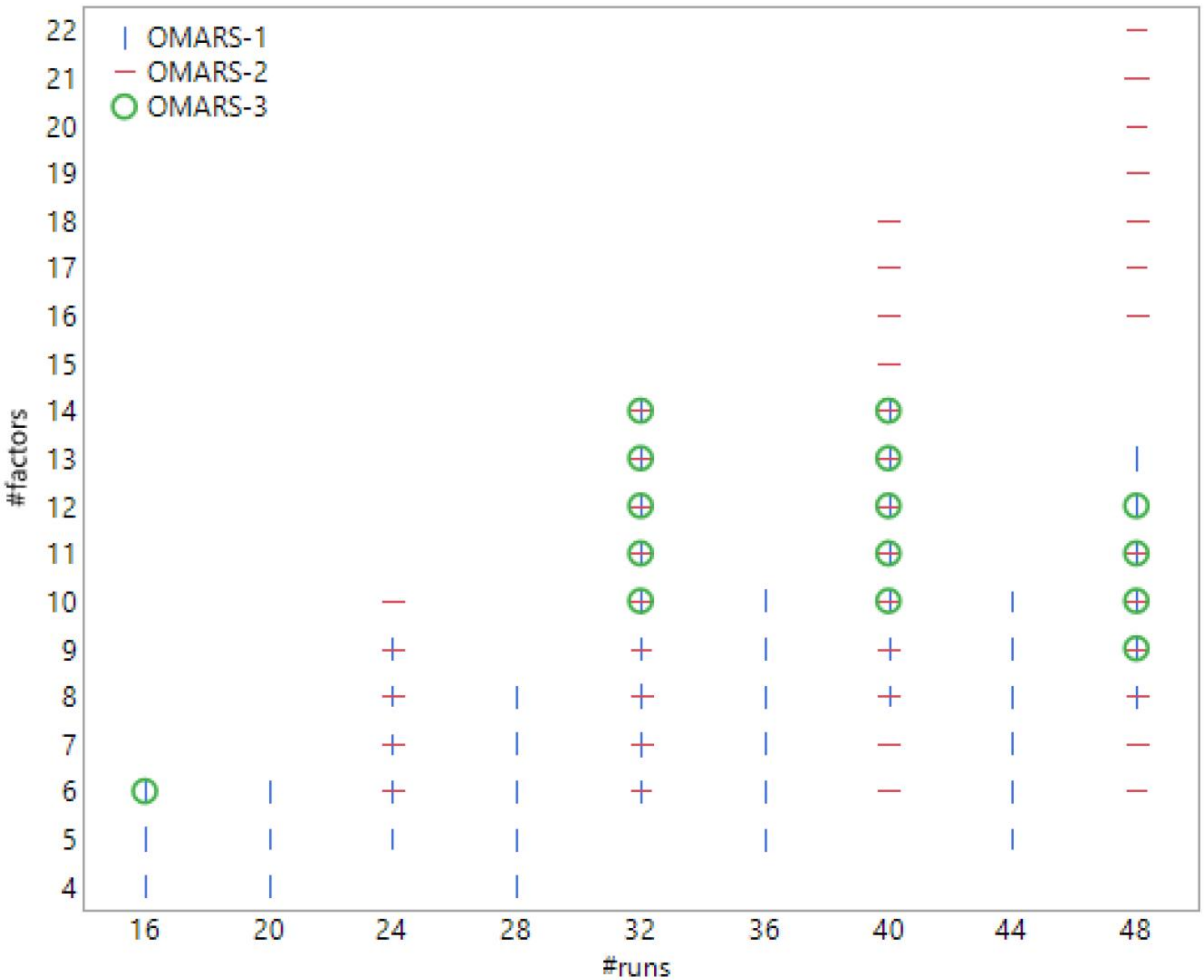
What else?

- Many experiments involve categorical factors too
- The combination of traditional RSDs and categorical factors has not received much attention
- DSDs can be extended to incorporate two-level categorical factors, but the resulting designs are no longer orthogonal
- Our proof-of-concept computations indicate that certain OMARS designs can be extended with one or more categorical factors, without losing the orthogonality properties of the designs
- We found quite a lot of these already …

OMARS designs with 2-level factors



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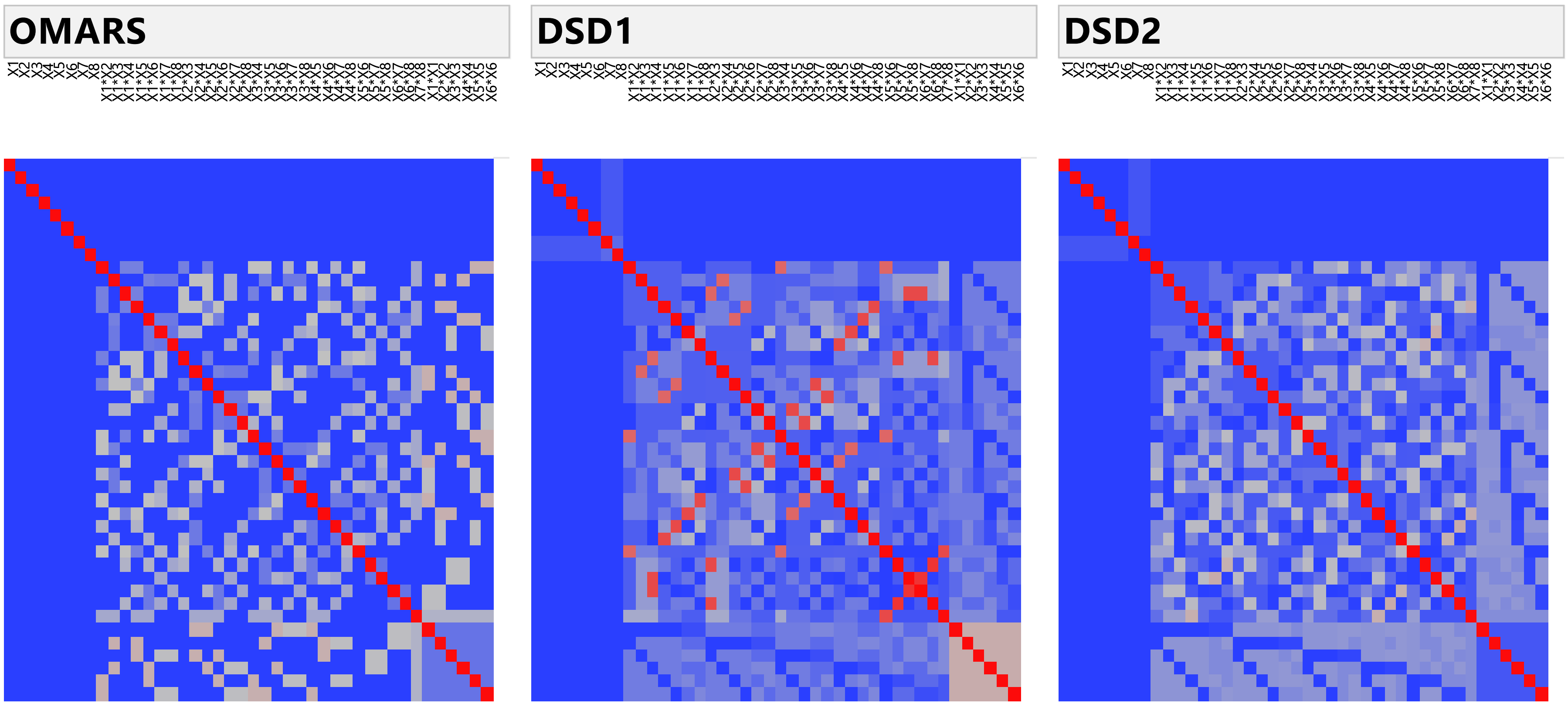
24-run example with 6 quantitative and 2 categorical factors



What else?

- All OMARS designs I've shown
  - Have the same precision for main effects of quantitative factors …
  - … and for the quadratic effects
- We therefore call the design "uniform precision" OMARS designs
- We have now also enumerated OMARS design that do not possess the "uniform precision" property
- There are many of these …
- … offering more and more opportunities for tailoring OMARS designs to your needs

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