Constructing two-level Q_B-optimal screening designs using mixed integer programming and heuristic algorithms

Alan R. Vazquez

Department of Industrial Engineering

University of Arkansas

alanv@uark.edu

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Outline

1. Introduction: The Q_B criterion

2. Mixed integer programming for finding optimal designs

3. A heuristic algorithm for constructing efficient designs

4. Results and conclusions

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Introduction

Two-level screening designs allow us to identify the active main effects and two-factor interactions of many factors under study, using an economical number of runs.

Some recent applications of these designs include:

- Investigating the regulation of specific cells (Barminko et al., 2014).
- Developing treatments that inhibit tuberculosis (Silva et al., 2016).
- Tuning the hyperparameters of machine learning algorithms (Lujan-Moreno et al., 2018)

Criteria to evaluate two-level designs

Criteria	Favors designs that:

(Mee et al., 2017)

A unifying criterion

Criteria
G_2-aberration (Tang & Deng, 1999)
D- and A-optimality (Atkinson et al., 2007)
Estimation and Information Capacities (Sun, 1999; Li & Nachtsheim, 2000)
Projection Estimation and Information Capacities (Loeppky et al., 2007)
Among others

Q_B criterion

(Tsai & Gilmour, 2010; Mee et al., 2017)

Example

Compare two-level screening designs with 24 runs and 7 factors.

Design 1.
Folded-over Plackett-Burman design
(Miller & Sitter, 2001)

X1	X2	X3	X4	X5	X6	X7
1	-1	1	1	1	-1	-1
1	-1	-1	-1	1	-1	1
1	-1	1	1	-1	1	1
1	1	1	-1	-1	-1	1
-1	1	-1	1	1	-1	1
-1	1	1	-1	1	1	1
-1	1	1	1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1
-1	-1	1	-1	1	1	-1
1	1	-1	-1	-1	1	-1
1	1	-1	1	1	1	-1
-1	-1	-1	1	-1	1	1
-1	1	-1	-1	-1	1	1
-1	1	1	1	-1	1	-1
-1	1	-1	-1	1	-1	-1
-1	-1	-1	1	1	1	-1
1	-1	1	-1	-1	1	-1
1	-1	-1	1	-1	-1	-1
1	-1	-1	-1	1	1	1
1	1	1	1	1	1	1
1	1	-1	1	-1	-1	1
-1	-1	1	1	1	-1	1
-1	-1	1	-1	-1	-1	1
1	1	1	-1	1	-1	-1

Design 2.
Obtained from
http://neilsloane.com/hadamard/

X1	X2	X3	X4	X5	X6	X7
-1	-1	1	1	1	1	1
1	-1	1	-1	-1	-1	-1
-1	1	1	1	1	1	-1
-1	-1	-1	-1	-1	-1	-1
1	1	1	1	-1	1	-1
1	1	-1	1	-1	1	1
1	1	1	1	1	-1	1
1	-1	-1	-1	-1	1	1
-1	1	-1	1	-1	-1	-1
1	-1	-1	1	-1	1	-1
1	-1	-1	1	1	-1	-1
-1	1	-1	-1	-1	-1	1
-1	-1	-1	-1	1	1	1
-1	1	1	-1	-1	1	-1
-1	-1	1	-1	1	-1	-1
1	-1	1	-1	1	1	-1
-1	-1	-1	1	1	1	1
-1	-1	1	1	-1	-1	1
1	1	-1	-1	1	-1	1
1	1	1	-1	1	-1	1
1	-1	1	1	-1	-1	1
-1	1	1	-1	-1	1	1
1	1	-1	-1	1	1	-1
-1	1	-1	1	1	-1	-1

The Q_B criterion

Measures the efficiency to estimate many potential models.

1. Maximal model with the intercept, all main effects and all two-factor interactions.
2. Sub-models of interest satisfy functional marginality.

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_{12} X_1 X_2 + \beta_{13} X_1 X_3 + \beta_{23} X_2 X_3 + \varepsilon$$

(Tsai, Gilmour & Mead, 2007)

The $\boldsymbol{Q_B}$ criterion

Measures the efficiency to estimate many potential models.

1. Maximal model with the intercept, all main effects and all two-factor interactions.
2. Sub-models of interest satisfy functional marginality.
3. A_s criterion to measure the estimation efficiency of sub-models.

$$\boxed{A_s = \sum_{i=1}^{p_s} \mathrm{Var}(\hat{\beta}_i)}$$

(Tsai, Gilmour & Mead, 2007)

The $\boldsymbol{Q_B}$ criterion

Measures the efficiency to estimate many potential models.

4. Prior probabilities:
   - π_1: Active main effect.
   - π_2: Active interaction given that <u>both</u> main effects of the factors involved are active too.
   - π_3: Active interaction given that <u>one</u> of the main effects of the factors involved is active.

   Under this framework, we can calculate the prior probability that sub-model is the best.

Li et al. (2006): $\pi_1 = 0.41$, $\pi_2 = 0.33$ and $\pi_3 = 0.045$

(Tsai, Gilmour & Mead, 2007)

The $\boldsymbol{Q_B}$ criterion

Weighted average of the A_s criterion over all sub-models of interest.

Weights: prior probability of a sub-model being the best.

Example (cont.): 24-run 7-factor designs.

Consider $\pi_1 = 0.41$, $\pi_2 = 0.33$ and $\pi_3 = 0.045$.

Design 1

$$Q_B = 0.246$$

Design 2

$$Q_B = 0.255$$

Minimizing Q_B is equivalent to maximizing the estimation efficiency for the sub-models of the maximal model.

Research question

+ The Q_B criterion unifies several statistical criteria for screening designs.
+ The Q_B criterion seeks for designs that are model-robust.

- The only available algorithm for generating Q_B-optimal designs is the columnwise search algorithm (Tsai et al., 2000), which is computationally-inefficient for moderate and large designs.

In this talk, we introduce two effective algorithms for finding two-level Q_B-optimal designs from scratch.

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Mixed Integer Programming

To construct two-level Q_B-optimal designs, we introduce a Mixed Integer Programming (MIP) algorithm.

The MIP algorithm consists of

- A problem formulation for finding two-level Q_B-optimal designs.
- The use of state-of-the-art optimization software to solve this problem formulation.

Encoding of two-level designs

2^m

X_1	X_2	X_3	…	X_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

Two-level full factorial design in *m* factors

The variables z_u are binary:

- $z_u = 1$ if the test combination is included in the design.
- $z_u = 0$ otherwise.

Let n be the desired run size of the design. We have that

$$\sum_{u=1}^{2^m} z_u = n$$

Calculation of the $\boldsymbol{Q_B}$ criterion I

Consider an n-run m-factor design given by $\mathbf{z} = (z_1, z_2, \ldots, z_{2^m})^T$.

Let $\mathbf{X}_k$ be the matrix including all k-th factor interaction contrast vectors of the *two-level full factorial design*.

We define the vector $\mathbf{y}_k = \frac{1}{2^m}\mathbf{X}_k^T\mathbf{z}$ and use $\mathbf{y}_1$, $\mathbf{y}_2$, $\mathbf{y}_3$ and $\mathbf{y}_4$.

$\mathbf{y}_1^T\mathbf{y}_1 \propto$ Aliasing between intercept and main effects
$\mathbf{y}_2^T\mathbf{y}_2 \propto$ Sum of squared correlations among main effects
$\mathbf{y}_3^T\mathbf{y}_3 \propto$ Sum of squared correlation between main effects and interactions
$\mathbf{y}_4^T\mathbf{y}_4 \propto$ Sum of squared correlations among interactions

Calculation of the $\boldsymbol{Q_B}$ criterion II

For a maximal model including the intercept, all main effects and all two-factor interactions, minimizing the Q_B criterion is equivalent to minimizing

$$w_1\mathbf{y}_1^T\mathbf{y}_1 + w_2\mathbf{y}_2^T\mathbf{y}_2 + w_3\mathbf{y}_3^T\mathbf{y}_3 + w_4\mathbf{y}_4^T\mathbf{y}_4,$$

where w_k's depend on π_1, π_2 and π_3.

(Vazquez et al., 2022; Mee et al. 2016; Tsai & Gilmour, 2010)

The problem formulation

$$\min_{\mathbf{y}_k,\mathbf{z}} w_1\mathbf{y}_1^T\mathbf{y}_1 + w_2\mathbf{y}_2^T\mathbf{y}_2 + w_3\mathbf{y}_3^T\mathbf{y}_3 + w_4\mathbf{y}_4^T\mathbf{y}_4$$

Subject to:

(1).	$\mathbf{y}_k = \frac{1}{2m}\mathbf{X}_k^T\mathbf{z}$
(2).	$\sum_{u=1}^{2m} z_u = n$
(3).	$z_u \in \{0, 1\}$

Solved by optimization solvers:
Gurobi, CPLEX or SCIP.

<u>Attractive features</u>:

- Find high-quality designs.
- Provide certificates of optimality.

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Perturbation-Based Coordinate Exchange (PBCE) algorithm

The algorithm is based on the metaheuristic called Iterated Local Search (Luorenço et al., 2019).

<u>Building blocks</u>:

1. Computationally-cheap version of the Q_B criterion.
2. Local search algorithm to construct locally-optimal designs.
3. Perturbation operator to escape from local optimality.

1. An alternative calculation of $\boldsymbol{Q_B}$

Let $\mathbf{D}$ be an *n*-run *m*-factor two-level design matrix. Consider the row-coincidence $\mathbf{T} = \mathbf{D}\mathbf{D}^T$ with elements T_{ij} . We define $M_k = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n} T_{ij}^k$ (Butler, 2003).

Theorem: For a maximal model including the intercept, all main effects and all two-factor interactions, minimizing the Q_B criterion is equivalent to minimizing

$$w_1 M_1 + w_2 M_2 + w_3 M_3 + w_4 M_4, \qquad (1)$$

where the w_k's depend on π_1, π_2 and π_3.

Computing the Q_B criterion using (1) is cheap!

(Vazquez et al., 2022)

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.071$

12 runs and 6 factors

$D =$

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

(Meyer & Nachtsheim, 1995)

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.064$

$D =$

-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

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.053$

$D =$

-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

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.051$

$D =$

-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

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.051$

$D =$

-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

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.051$

$D =$

-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

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.023$

$D =$

-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

2. Coordinate-Exchange Algorithm

- Local Search.
- One move: Sign switch a coordinate in the design *D*.

Example:

$\pi_1 = 0.41, \pi_2 = 0.11, \pi_3 = 0.0$

$Q_B = 0.023$

$D^* =$

-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

3. Perturbation Operator

$n = 12$ runs and $m = 6$ factors

Set the value of the tunning parameter $\alpha = 0.1$.

1. Compute the “contribution” of each row to the Q_B criterion value.

2. Select the $[n\alpha] = 2$ rows with the largest contribution.

$D^* =$

-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

3. Perturbation Operator

Set the value of the tunning parameter $\alpha = 0.1$.

1. Compute the “contribution” of each row to the Q_B criterion value.

2. Select the $[n\alpha] = 2$ rows with the largest contribution.

3. Switch the signs of $[m\alpha] = 1$ randomly chosen coordinates in these rows.

$n = 12$ runs and $m = 6$ factors

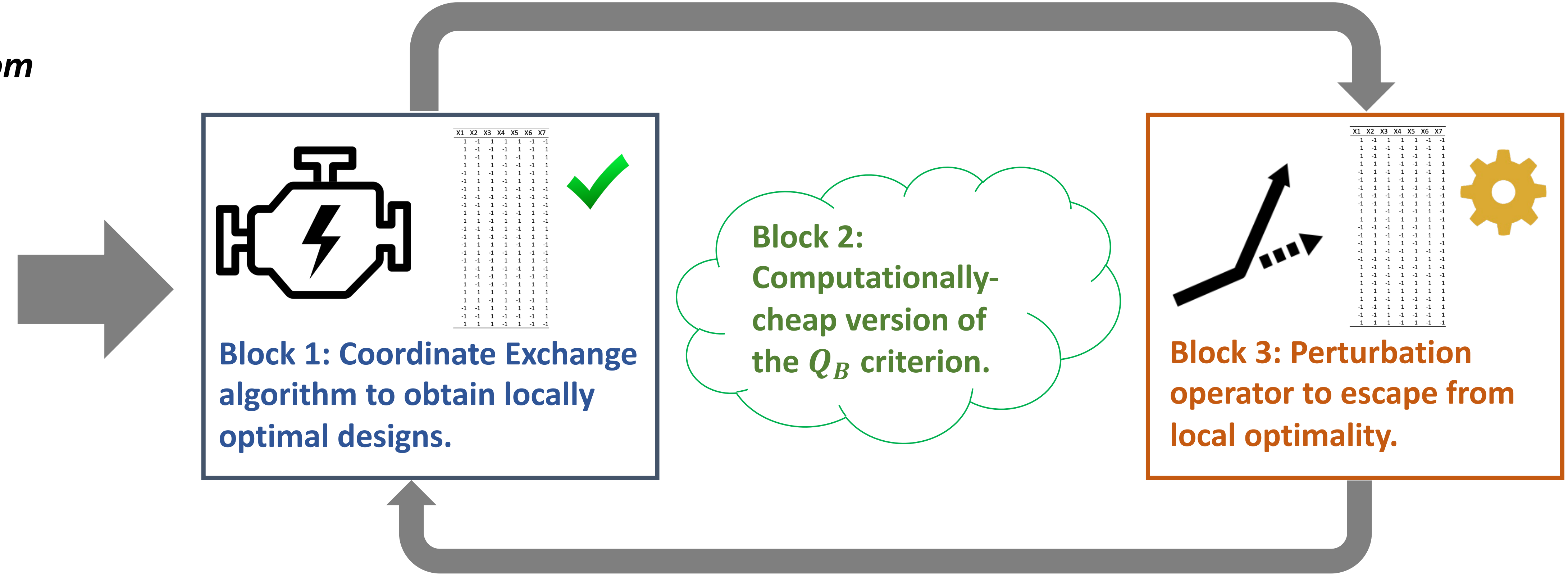
$D' =$

-1	-1	-1	1	-1	-1	0.153
-1	-1	1	1	1	-1	0.169
1	-1	1	1	-1	1	0.168
1	1	-1	1	1	-1	0.140
1	-1	1	1	1	1	0.188
-1	1	1	-1	1	-1	0.115
-1	1	1	-1	-1	1	0.115
-1	1	-1	1	1	1	0.195
-1	-1	-1	-1	1	1	0.088
-1	-1	**1**	-1	-1	-1	0.203
1	-1	1	-1	-1	-1	0.123
1	1	-1	-1	-1	1	0.141

Summary of the PBCE algorithm

Initial design matrix at random

X1	X2	X3	X4	X5	X6	X7
1	-1	1	1	1	-1	-1
1	-1	-1	-1	1	-1	1
1	-1	1	1	-1	1	1
1	1	1	-1	-1	-1	1
-1	1	-1	1	1	-1	1
-1	1	1	-1	1	1	1
-1	1	1	1	-1	-1	-1
-1	-1	-1	-1	-1	-1	-1
-1	-1	1	-1	1	1	-1
1	1	-1	-1	-1	1	-1
1	1	-1	1	1	1	-1
-1	-1	-1	1	-1	1	1
-1	1	-1	-1	-1	1	1
-1	1	1	1	-1	1	-1
-1	1	-1	-1	1	-1	-1
-1	-1	-1	1	1	1	-1
1	-1	1	-1	-1	1	-1
1	-1	-1	1	-1	-1	-1
1	-1	-1	-1	1	1	1
1	1	1	1	1	1	1
1	1	-1	1	-1	-1	1
-1	-1	1	1	1	-1	1
-1	-1	1	-1	-1	-1	1
1	1	1	-1	1	-1	-1



Repeat for a maximum number of iterations without improvement.

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Numerical comparisons

We obtain design problems with 7 and 11 factors from Mee et al. (2017).

Algorithms:

- MIP algorithm with Gurobi v9 and a maximum search time of 20 min.
- PBCE algorithm with $\alpha = 0.1$, Max_Iter = 100, and 5 repetitions.
- Coordinate-exchange algorithm with 1000 iterations (Meyer & Nachtsheim, 1995).
- Restricted columnwise-pairwise algorithm with 1000 iterations (Li, 2006).
- Point-exchange algorithm with 10 iterations (Cook and Nachtsheim, 1980).

Results

Factors	Runs	Coordinate-Exchange Algorithm	Restricted Columnwise-Pairwise Algorithm	PBCE Algorithm	Point-Exchange Algorithm	Mixed Integer Programming
$\pi_1 = 0.5, \pi_2 = 0.8$ and $\pi_3 = 0.0$						
7	16	**0.1050**	**0.1050**	**0.1050**	**0.1050**	**0.1050**
	20	**0.0652**	**0.0652**	**0.0652**	**0.0652**	**0.0652**
	24	**0.0333**	0.0351	**0.0333**	**0.0333**	**0.0333**
	28	**0.0203**	**0.0203**	**0.0203**	**0.0203**	**0.0203**
	32	**0.0075**	**0.0075**	**0.0075**	**0.0075**	**0.0075**

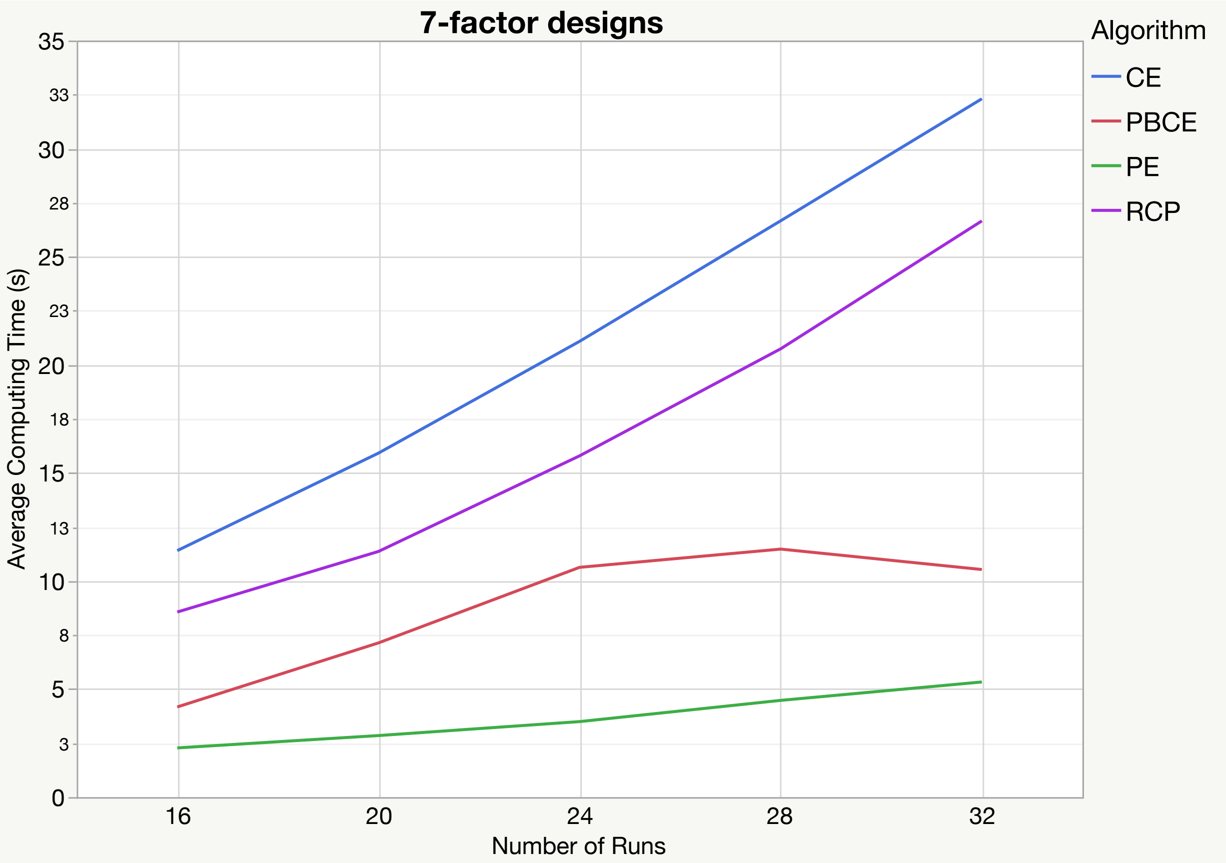
Smaller the better

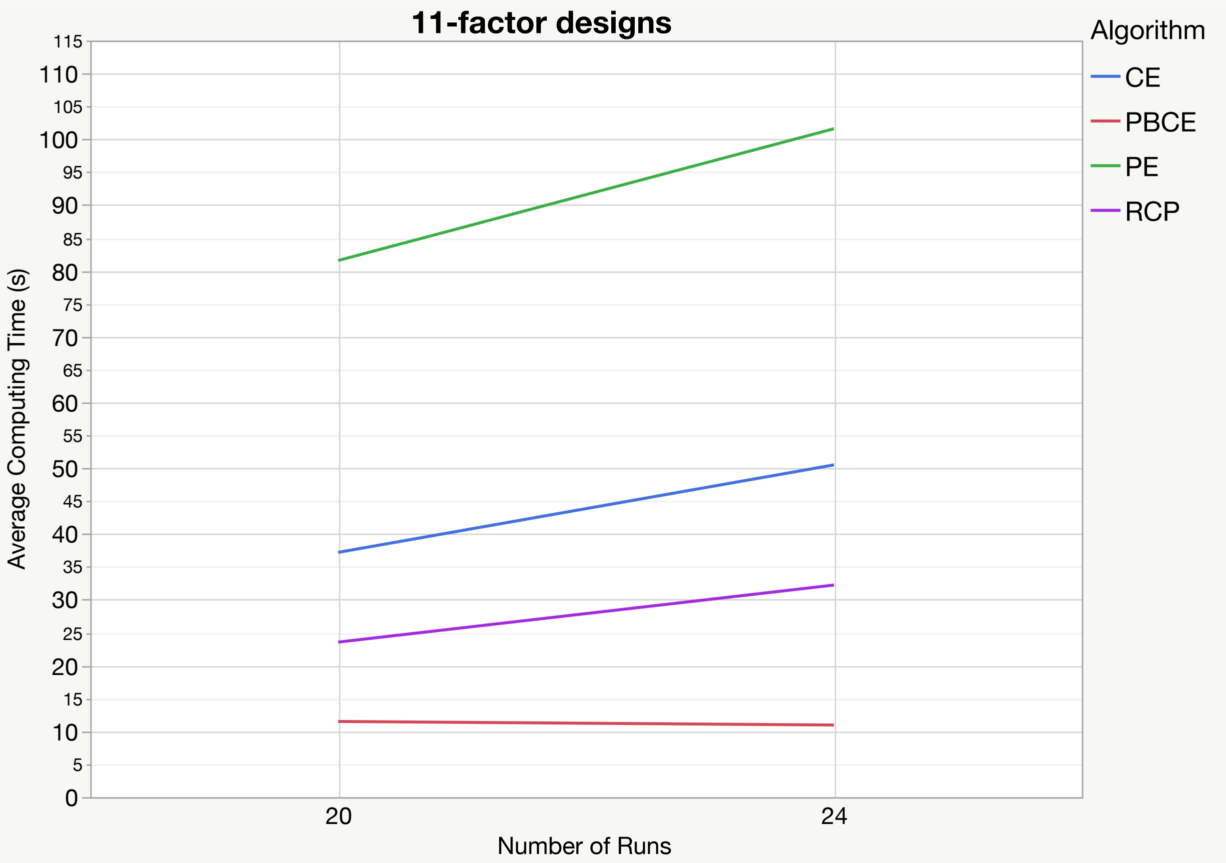
Conclusions

- The MIP and PBCE algorithms are computationally-effective to construct two-level screening designs that optimize the Q_B criterion.
- For up to 6 factors, our MIP algorithm obtains Q_B-optimal designs.
- For large numbers of factors, our PBCE algorithm outperforms benchmark algorithms in terms of design quality and computing time.
- Data analysis may be conducted using mixed integer programming, along the lines of Vazquez et al. (2021).

Appendix 1: Computing times of heuristics

Average computing times for 10 optimizations performed by the heuristic algorithms.





For the MIP approach, Gurobi did not finish within 20 min.

Appendix 3: Constructing some two-level Q_B-optimal designs

Using Gurobi v9

Priors: $\pi_1 = 0.82$, $\pi_2 = 0.66$ and $\pi_3 = 0.09$

Number of factors	# Coeff. in maximal model	Run size	Computing time (s)
4	11	11	1
		12	1
		13	1
5	16	16	1
		17	1
		18	1
6	22	22	165
		23	1120
		24	4136

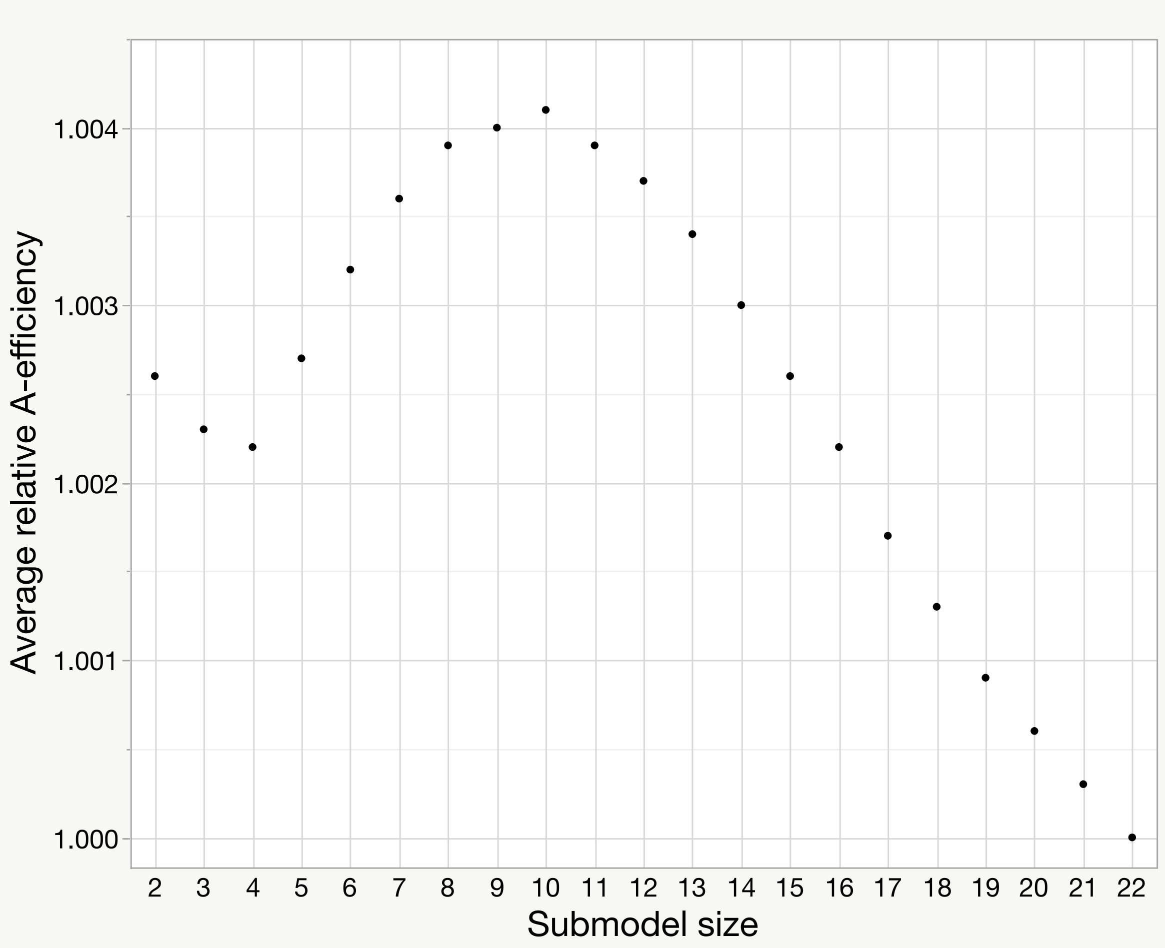
Appendix 2: The MIP algorithm in practice

Example:

- Construct a two-level design with 23 runs and 6 factors.
- Number of coefficients in the maximal model is 22.
- Prior probabilities: $\pi_1 = 0.82, \pi_2 = 0.66$ and $\pi_3 = 0.09$.

Benchmark design: A-optimal design for the maximal model constructed using JMP 16.

$A_S(\text{A-opt})/A_S(Q_B\text{-opt})$



Higher the better