An algorithm for blocking
regular fractional factorial 2-level designs with clear two-factor interactions

Who? Ulrike Grömping

From? Beuth University of Applied Sciences, Berlin

Full factorial 2-level designs

Basics

n treatment factors A,B,C,. . . ,H,J,K,. . .

- each with levels 0 and 1 from GF(2), and addition modulo 2 (used here)
- or each with levels -1 and $+1$, and multiplication (closer to conventional industrial statistics, automatically yields nice model matrices for estimation)

A full factorial has all 2^n conceivable level combinations.

A full model has 2^n effects (1 constant, n main effects, $\binom{n}{2}$ 2-factor interactions, ...).

Full model model matrix (n=4 factors)

	0	**1**	**2**	3	**4**	5	6	7	**8**	9	10	11	12	13	14	15
	I	**A**	**B**	AB	**C**	AC	BC	ABC	**D**	AD	BD	ABD	CD	ACD	BCD	ABCD
(1)	1	**0**	**0**	0	**0**	0	0	0	**0**	0	0	0	0	0	0	0
a	1	**1**	**0**	1	**0**	1	0	1	**0**	1	0	1	0	1	0	1
b	1	**0**	**1**	1	**0**	0	1	1	**0**	0	1	1	0	0	1	1
ab	1	**1**	**1**	0	**0**	1	1	0	**0**	1	1	0	0	1	1	0
c	1	**0**	**0**	0	**1**	1	1	1	**0**	0	0	0	1	1	1	1
ac	1	**1**	**0**	1	**1**	0	1	0	**0**	1	0	1	1	0	1	0
bc	1	**0**	**1**	1	**1**	1	0	0	**0**	0	1	1	1	1	0	0
abc	1	**1**	**1**	0	**1**	0	0	1	**0**	1	1	0	1	0	0	1
d	1	**0**	**0**	0	**0**	0	0	0	**1**	1	1	1	1	1	1	1
ad	1	**1**	**0**	1	**0**	1	0	1	**1**	0	1	0	1	0	1	0
bd	1	**0**	**1**	1	**0**	0	1	1	**1**	1	0	0	1	1	0	0
abd	1	**1**	**1**	0	**0**	1	1	0	**1**	0	0	1	1	0	0	1
cd	1	**0**	**0**	0	**1**	1	1	1	**1**	1	1	1	0	0	0	0
acd	1	**1**	**0**	1	**1**	0	1	0	**1**	0	1	0	0	1	0	1
bcd	1	**0**	**1**	1	**1**	1	0	0	**1**	1	0	0	0	0	1	1
abcd	1	**1**	**1**	0	**1**	0	0	1	**1**	0	0	1	0	1	1	0

Blocking full factorials

Basics

Purpose control for variation in the experimental material

Blocking $N = 2^n$ runs can be assigned to $N/2^q = 2^{n-q}$ blocks of size 2^q

Block factor has 2^{n-q} levels (needs $2^{n-q} - 1$ df)

Assumptions

- block effect active, but not of interest
- block factors do not interact with treatment factors
- in line with Godolphin, look at only a single block factor

Blocking a full factorial in n factors

Approach of FrF2

- pick $n - q$ independent effect columns for generating the levels of the block factor
  e.g. for $n = 4$ and $q = 2$: $b_1 = \text{ABC}$ and $b_2 = \text{ABD}$
- the remaining dfs of the block factor are implied by the generating columns
  e.g. $b_3 = (b_1 + b_2) \mod 2 = (\text{ABC} + \text{ABD}) \mod 2 = \text{CD}$

Approach in Godolphin (X approach)

- pick q independent rows without all-zero columns that generate a group of size 2^q,
  which is the *principal block* (pb)
- take the other blocks as the cosets of the principal block

X approach in detail

Example continued

$q \times n$ matrix $\mathbf{X}$, rank q, no all-zero columns

$$\mathbf{X} = \begin{array}{c} \\ \text{bcd} \\ \text{acd} \end{array} \begin{array}{c} \begin{array}{cccc} \text{A} & \text{B} & \text{C} & \text{D} \end{array} \\ \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix} \end{array} \Longrightarrow \text{pb} = \begin{array}{c} \\ \text{(1)} \\ \text{bcd} \\ \text{acd} \\ \text{ab} \end{array} \begin{array}{c} \begin{array}{cccc} \text{A} & \text{B} & \text{C} & \text{D} \end{array} \\ \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

Further blocks are the cosets:

pb + a: a, abcd, cd, b
pb + c: c, bd, ad, abc
pb + d: d, bc, ac, abd

Example: Blocking a full factorial

The four rows of the principal block for two different blockings of the full factorial in factors A, B, C and D.
Bold face: the 2×4 $\mathbf{X}$ matrix for the blocking.
The table shows columns for all factorial effects.

	1	**2**	3	**4**	5	6	7	**8**	9	10	11	12	13	14	15
	A	**B**	AB	**C**	AC	BC	ABC	**D**	AD	BD	ABD	CD	ACD	BCD	ABCD
blocking 1							b_1				b_2	b_3			
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	**1**	1	**1**	1	0	0	**1**	1	0	0	0	0	1	1
	1	**0**	1	**1**	0	1	0	**1**	0	1	0	0	1	0	1
	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0
blocking 2			b_1		b_2	b_3									
	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	0	**0**	0	**0**	0	0	0	**1**	1	1	1	1	1	1	1
	1	**1**	0	**1**	0	0	1	**0**	1	1	0	1	0	0	1
	1	1	0	1	0	0	1	1	0	0	1	0	1	1	0

Regular fractional factorial 2-level designs

Regular fractions (unblocked)

A regular *fraction* (2^pth fraction of the 2^n run full factorial) has $N = 2^k = 2^{n-p} = 2^n/2^p$ level combinations.

Example

$n = 6,\ p = 2,\ k = n - p = 4$

$N = 16$ runs, design matrix 16×6, model matrix 16×16

- A *regular* fraction is obtainable from a full factorial in $k = n - p$ basic factors by $p > 0$ defining contrasts, which declare the effects from the full model in the basic factors that define the levels of p additional factors.
  Example: E=ABC, F=ABD
- Equivalently, there is a group theoretic creation approach (not discussed).

Full model model matrix (n=4 basic factors)

	0	**1**	**2**	3	**4**	5	6	7	**8**	9	10	11	12	13	14	15
	I	**A**	**B**	AB	**C**	AC	BC	*ABC*	**D**	AD	BD	*ABD*	CD	ACD	BCD	ABCD
(1)	1	**0**	**0**	0	**0**	0	0	0	**0**	0	0	0	0	0	0	0
a	1	**1**	**0**	1	**0**	1	0	1	**0**	1	0	1	0	1	0	1
b	1	**0**	**1**	1	**0**	0	1	1	**0**	0	1	1	0	0	1	1
ab	1	**1**	**1**	0	**0**	1	1	0	**0**	1	1	0	0	1	1	0
c	1	**0**	**0**	0	**1**	1	1	1	**0**	0	0	0	1	1	1	1
ac	1	**1**	**0**	1	**1**	0	1	0	**0**	1	0	1	1	0	1	0
bc	1	**0**	**1**	1	**1**	1	0	0	**0**	0	1	1	1	1	0	0
abc	1	**1**	**1**	0	**1**	0	0	1	**0**	1	1	0	1	0	0	1
d	1	**0**	**0**	0	**0**	0	0	0	**1**	1	1	1	1	1	1	1
ad	1	**1**	**0**	1	**0**	1	0	1	**1**	0	1	0	1	0	1	0
bd	1	**0**	**1**	1	**0**	0	1	1	**1**	1	0	0	1	1	0	0
abd	1	**1**	**1**	0	**0**	1	1	0	**1**	0	0	1	1	0	0	1
cd	1	**0**	**0**	0	**1**	1	1	1	**1**	1	1	1	0	0	0	0
acd	1	**1**	**0**	1	**1**	0	1	0	**1**	0	1	0	0	1	0	1
bcd	1	**0**	**1**	1	**1**	1	0	0	**1**	1	0	0	0	0	1	1
abcd	1	**1**	**1**	0	**1**	0	0	1	**1**	0	0	1	0	1	1	0

Regular fractions

Fractionating counfounds the 2^n effects of the full model in groups of 2^p effects that cannot be separated.

Example

Column headers for the model matrix show the *confounding pattern*.

0	1	2	3	4	5	6	7
I	**A**	**B**	**AB**	**C**	**AC**	**BC**	ABC
ABCE ABDF CDEF	BCE BDF ACDEF	ACE ADF BCDEF	**CE** **DF** ABCDEF	ABE ABCDF DEF	**BE** BCDF ADEF	**AE** ACDF BDEF	**E** CDF ABDEF

8	9	10	11	12	13	14	15
D	**AD**	**BD**	ABD	**CD**	ACD	BCD	ABCD
ABCDE ABF CEF	BCDE **BF** ACEF	ACDE **AF** BCEF	CDE **F** ABCEF	ABDE ABCF **EF**	BDE BCF AEF	ADE ACF BEF	**DE** **CF** ABEF

Group of words and resolution

Words

- are effects that coincide with the constant I, e.g.:
  I
  ABCE
  ABDF
  CDEF
- constitute a group with 2^p elements (here: $2^2 = 4$).
- give rise to a WLP (word length pattern, frequency table of word lengths):
  e.g. $A_0 = 1, A_1 = 0, A_2 = 0, A_3 = 0, A_4 = 3$

Resolution

length of shortest non-trivial word, here IV
larger is better

Matrix notation for fractionating

Matrix notation for defining contrasts
E=ABC and F=ABD:

$$\mathbf{Z} = \begin{matrix} & \text{A} & \text{B} & \text{C} & \text{D} \\ \text{E} & 1 & 1 & 1 & 0 \\ \text{F} & 1 & 1 & 0 & 1 \end{matrix}$$

Z is used in Godolphin's blocking approach for fractional factorials.

Blocking a fractional factorial

n factors, $2^k = 2^{n-p}$ runs, $p > 0$, $k = n - p$ basic factors
$q \times n$ matrix $\mathbf{X}$ needed for creating $2^q \times n$ principal block

Change versus full factorial

cannot freely choose all n columns of $\mathbf{X}$,
k columns for the basic factors determine the entire $\mathbf{X}$

Approach

Choose $q \times k$ matrix $\mathbf{X}_{\text{I}}$, calculate $q \times p$ matrix $\mathbf{X}_{\text{II}} = \mathbf{X}_{\text{I}}\mathbf{Z}^\top$,

and use $\mathbf{X} = (\mathbf{X}_{\text{I}} \vdots \mathbf{X}_{\text{II}})$.

Example: Previous X as $\mathbf{X}_{\text{I}}$ with E=ABC and F=ABD

$$\mathbf{X}_{\text{I}} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{X}_{\text{II}} = \mathbf{X}_{\text{I}}\mathbf{Z}^\top = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

Problem

$\mathbf{X}_{\text{II}}$ may contain all-zero column(s)
$\rightarrow$ treatment main effect(s) would be confounded with the block effect.

Solution

brute force search over all $\mathbf{X}_{\text{I}}$ for permissible blockings

Example: Blocking a fractional factorial

The four rows of the principal block for two different blockings of the fractional factorial with basic factors A, B, C and D and added factors E=ABC and F=ABD.

Bold face: the 2×6 $\mathbf{X}$ matrix for the blocking: $\mathbf{X} = (\mathbf{X}_{\mathrm{I}} \vdots \mathbf{X}_{\mathrm{II}})$

0	**1**	**2**	3	**4**	5	6	7	**8**	9	10	11	12	13	14	15
I	**A**	**B**	AB	**C**	AC	BC	ABC **E**	**D**	AD	BD	ABD **F**	CD	ACD	BCD	ABCD
blocking 1							b_1				b_2	b_3			
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	**0**	**1**	1	**1**	1	0	**0**	**1**	1	0	**0**	0	0	1	1
0	**1**	**0**	1	**1**	0	1	**0**	**1**	0	1	**0**	0	1	0	1
0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0
blocking 2			b_1		b_2	b_3									
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	**0**	**0**	0	**0**	0	0	**0**	**1**	1	1	**1**	1	1	1	1
0	**1**	**1**	0	**1**	0	0	**1**	**0**	1	1	**0**	1	0	0	1
0	1	1	0	1	0	0	1	1	0	0	1	0	1	1	0

Clear two-factor interactions

Clear 2fis

are not confounded with main effects or other 2fis,
and neither with the block factor

Situation

- some 2fis are of special interest
- other 2fis may not be of interest, but must not be assumed negligible
- higher order interactions can be neglected

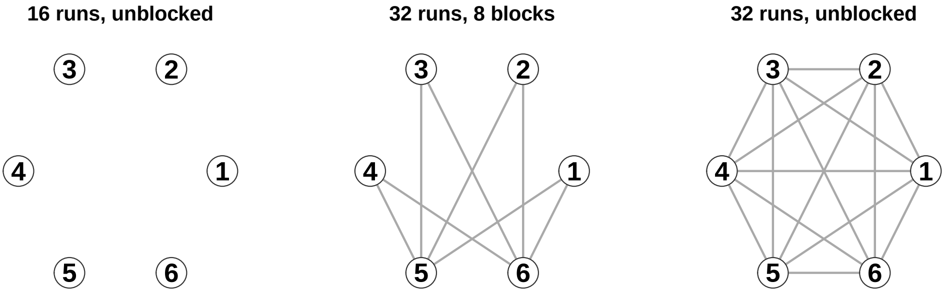
Goal fractionate and/or block such that required 2fis are clear

Sources

- Grömping (2012) provided an algorithm for unblocked fractions
- Godolphin (2021) provided the relation of the **X** approach to clear 2fis and a paper-catalogue for blocked fractions
- Grömping (2021) provided an automated algorithm for blocked fractions with clear 2fis, based on both Grömping (2012) and Godolphin (2021)

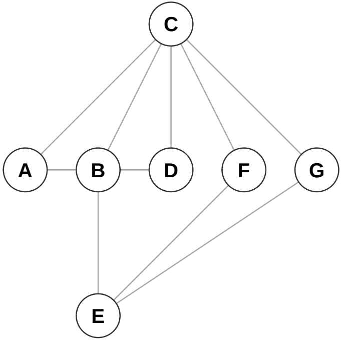
Clear interactions graphs (CIGs)

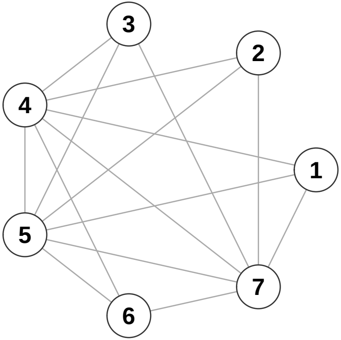
- each factor is the vertex of a graph
- there is an edge for each clear 2fi



Design CIG of best fraction for six factors

Using CIGs





left: requirement CIG, right: design CIG (7-2.1)

Task allocate treatment factors such that required 2fis are clear

Example allocate treatment factors A to G to design factors 1 to 7

- B, C and E must be on 4, 5 and 7
- **FrF2**: subgraph isomorphism checks automate the allocation

X approach for full factorial revisited

$\chi_{\mathbf{q}}$

$2^q - 1$ possibilities for the columns of **X**:
elements of $\chi_q = \{0,1\}^q - \mathbf{0}_q = \{\xi_1, \ldots, \xi_{2^q-1}\}$

Important Rule

The 2fi of a pair of factors is confounded with blocks
iff both factors have the same **X** column (Godolphin 2021).

Example: Blocking 1

$$\mathbf{X} = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{pmatrix}$$

CD is confounded with blocks,
the other five 2fis are clear.

Approach

- For a specific 2fi to be clear, assign different columns to its two factors.
- For a large number of clear 2fis, use the columns from χ_q in the highest possible balance $\rightarrow$ see "profiles" below.

Example: X approach for full factorial

The four rows of the principal block for two different blockings of the full factorial in factors A, B, C and D.

Bold face: the 2×4 **X** matrix for the blocking.

Highlighted : 2fis confounded with blocks

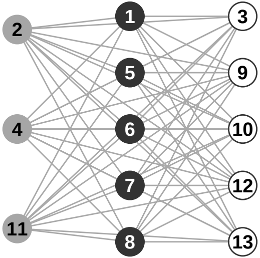
0	**1**	**2**	3	**4**	5	6	7	**8**	9	10	11	12	13	14	15
I	**A**	**B**	AB	**C**	AC	BC	ABC	**D**	AD	BD	ABD	*CD*	ACD	BCD	ABCD
blocking 1							b_1				b_2	b_3			
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	**0**	**1**	1	**1**	1	0	0	**1**	1	0	0	0	0	1	1
0	**1**	**0**	1	**1**	0	1	0	**1**	0	1	0	0	1	0	1
0	1	1	0	0	1	1	0	0	1	1	0	0	1	1	0
I	**A**	**B**	*AB*	**C**	*AC*	*BC*	ABC	**D**	AD	BD	ABD	CD	ACD	BCD	ABCD
blocking 2			b_1		b_2	b_3									
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	**0**	**0**	0	**0**	0	0	0	**1**	1	1	1	1	1	1	1
0	**1**	**1**	0	**1**	0	0	1	**0**	1	1	0	1	0	0	1
0	1	1	0	1	0	0	1	1	0	0	1	0	1	1	0

X approach for full factorial in graphs

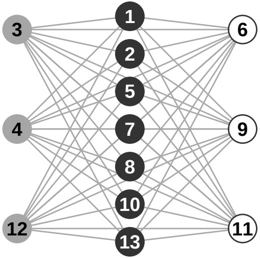
- **X** partitions the design factors into $2^q - 1$ sets,
  whose 2fis are confounded within sets (no edges),
  but not between sets (edges).
- The design CIG is a full $2^q - 1$-partite graph for the partitions,
  and thus $2^q - 1$ colourable.
- The sizes of the partition sets can be written in a *profile*,
  e.g. $<5,5,3>$ or $<9,3,1>$.

Four 3-partite graphs for 13 factors

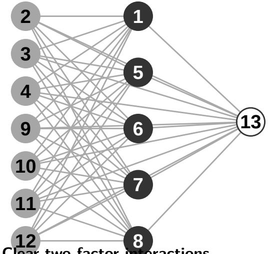
Profile <5,5,3>
55 clear 2fis



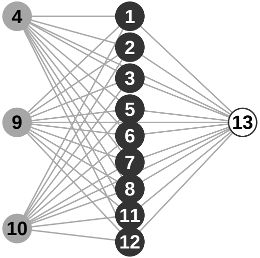
Profile <7,3,3>
51 clear 2fis



Profile <7,5,1>
47 clear 2fis

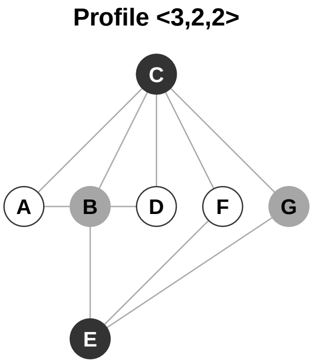


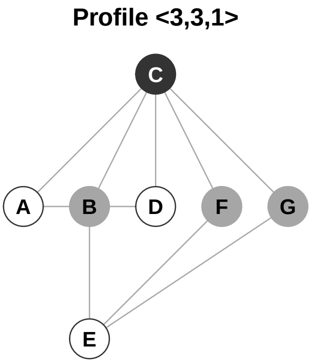
Profile <9,3,1>
39 clear 2fis



X approach for full factorial in graphs

A requirement CIG can be accommodated in blocks of size 2^q,
if it is $2^q - 1$-colourable.





Requirement CIG that can be accommodated in blocks of size 4

X approach for fractional factorial revisited

For a given **X**, the rule for confounding of 2fis *with the block effect* remains valid.

Resolution V fraction

If a suitable **X** has been found, the CIG coincides with that of a full factorial blocked by this **X**.
The structure of **Z** restricts the possible profiles.

> Example: for the best 256-run fraction for 13 factors in blocks of size 4, there are only four profiles
> (of 14 possible ones with three non-empty partitions).

Resolution IV fraction

2fis may already be confounded with other 2fis in the unblocked fraction.
The CIG from blocking an unblocked fraction by **X** is the *intersection*
of the *CIG of the unblocked fraction*
with the *CIG from blocking a full factorial* by the same **X**.
Deciding on a good **X** is thus more complicated.

Godolphin catalogues (blocks of size $2^2 = 4$)

Resolution V paper catalogues of partitions for combinations of n, N, q and profiles (up to 128 runs with up to 11 factors).

Resolution IV paper catalogues of partitions for selected numbers of factors,
in some cases with additional information of additional 2fis that are confounded already in the unblocked fraction,
for a few combinations of n, N, q and profiles

FrF2

- relieves practitioners from manual work with paper tables
- has a built-in algorithm that covers many situations
- allows R-savvy users to extend the situations for which blockings with estimable 2fis can be found (e.g. also extending Godolphin's paper catalogues)

Algorithmic implementation in FrF2

Catalogue Unblocked fractions sorted from better to worse WLP, with design CIGs

Algorithm

1. loop through unblocked fractions, until one can accommodate the requirement CIG (algorithm of Grömping 2012)
2. search for a suitable $q \times n$ matrix $\mathbf{X}$ for blocking that fraction without sacrificing required 2fis (see next slide)
3. if one is found: record number of clear 2fis
   if not maximum conceivable: try next $\mathbf{X}$ matrix
4. if $\mathbf{X}$ matrices have been found, use the one that keeps the largest number of 2fis clear;
   otherwise, manually restart the first step after discarding the unusable unblocked fraction

Search algorithm for a suitable X

Crucial for speed

It does not matter which column from $\mathcal{X}_q$ is used for which colour.

Denote $\mathcal{X}_q = \{\xi_1, \ldots, \xi_{2^q-1}\}$, i.e. assign an order to the elements. Then choose the columns of $\mathbf{X}_\mathrm{I}$ as follows:

- Fix the first column as ξ_1 (one choice).
- If $2^q - 1 \geq 2$, pick the second column from $\{\xi_1, \xi_2\}$ (two choices); otherwise pick it from $\mathcal{X}_q$ ($2^1 - 1 = 1$ choice).
- $\ldots$
- If $2^q - 1 \geq c$, pick the cth column from $\{\xi_1, \ldots, \xi_c\}$ (c choices); otherwise pick it from $\mathcal{X}_q$ ($2^q - 1$ choices).
- $\ldots$
- If $2^q - 1 \geq k = n - p$, pick the kth column from $\{\xi_1, \ldots, \xi_k\}$ (k choices); otherwise pick it from $\mathcal{X}_q$ ($2^q - 1$ choices).

Some Timings for impossible requests

Times[s] from function `FrF2` for attempting to block a suitable $(k+p)$–p fraction into blocks of size 4, while keeping a clique of size 4 clear

k	run size	$p=0$	$p=1$	$p=2$	$p=3$	$p=4$	$p=5$	$p=6$	$p=7$	$p=8$
5	32	0.12	0.12	0.13	0.02					
6	64	0.32	0.28	0.23	0.23	0.30	0.23			
7	128	0.91	0.75	0.64	0.53	0.47	0.58	0.66	0.41	0.43
8	256	2.67	2.46	1.97	1.63	1.39	1.15	0.99	0.90	0.82
9	512	8.64	7.16	5.89	5.19	4.06	3.56	3.24	3.05	2.91
10	1024	28.17	23.89	18.81	15.27	12.50	10.34	8.75	7.70	6.84
11	2048	91.36	72.41	59.92	48.57	40.22	33.42	27.35	22.61	18.86
12	4096	287.98	252.67	206.85	165.66	131.00	110.97	92.20	78.42	68.66

Back matter

Limitations

- Quality criteria for blocked designs are ignored - best (MA) unblocked fraction with most clear 2fis is found.
- There are not enough catalogues for large fractions (and some are huge!).
- The need of a manual restart of the algorithm is a nuisance.
- Searches can take a long time.

Concluding comments

- With Godolphin's (2021) approach, it became feasible to automate blocking with keeping a requirement set of 2fis clear.
- The approach is generally good for small blocks, even without a special interest in clear 2fis.
- For fractional factorial 2-level designs, play with **FrF2** and contact me in case of questions etc.
- I am interested in application show cases.

References

- Godolphin, J. (2021). Construction of blocked factorial designs to estimate main effects and selected two-factor interactions. *JRSS B* **83**, 5-29. DOI: https://doi.org/10.1111/rssb.12397.
- Grömping, U. (2007-2020). The **FrF2** Package (Fractional Factorial designs with 2-level factors). R package version 2.2-2.
- Grömping, U. (2012). Creating clear designs: a graph-based algorithm and a catalog of clear compromise plans. *IIE Transactions* **44**, 988-1001. DOI: https://doi.org/10.1080/0740817X.2012.654848.
- Grömping, U. (2021). An algorithm for blocking regular fractional factorial 2-level designs with clear two-factor interactions. *Computational Statistics and Data Analysis* **153**, 1-18. DOI: https://doi.org/10.1016/j.csda.2020.107059.
- and references in these papers