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R Package FrF2 for Creating and Analyzing Fractional Factorial 2-Level Designs

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Abstract

This article describes the R package **FrF2** for design and analysis of experiments with 2-level factors. The package offers both regular and non-regular fractional factorial 2-level designs, in the regular case with blocking and split plot facilities and algorithms for ensuring estimability of certain two-factor interactions. Furthermore, simple analysis facilities are on offer, first and foremost plotting functions for half normal plots, main effects and interaction plots, and cube plots. Package **FrF2** receives infrastructure support from package **DoE.base** and heavily builds on a subgraph isomorphism algorithm from package **igraph** for one of its estimability algorithms.

Keywords: design of experiments, DoE, fractional factorial 2-level designs, **DoE.base**, **FrF2**.

1. Introduction

Factorial experiments are very common in experimentation. Experiments with 2-level factors only are most widely spread, particularly in industrial experimentation. Both regular (fractional) factorial 2-level designs and non-regular ones are heavily used. The design and execution of industrial experiments is often done by subject matter experts during everyday work without support from a statistical expert – thus it is important to have a software available that can be safely used by non-statisticians. At the same time, statisticians are often involved in the more important experimental projects, and there are many facets to construction of (industrial) fractional factorial 2-level experiments for which a statistician very much appreciates support from a powerful software.

This article presents the R package **FrF2** (Grömping 2014) – implemented in the open-source programming environment R (R Core Team 2013) – that tries to serve non-statisticians and statistical experts alike: non-statisticians are supported in creating, conducting and analyzing valid experiments, whereas statistical experts find advanced tools for tailoring experiments to

the specific needs of the experimental situation. R package **FrF2** is part of a suite of several R packages: **DoE.base** provides the infrastructure for the suite and creates general factorial designs, **DoE.wrapper** interfaces to other packages for design of experiments on the Comprehensive R Archive Network (CRAN, http://CRAN.R-project.org/), and **RcmdrPlugin.DoE** provides graphical user interface (GUI) access to the suite (Grömping 2013b,c,e, 2011b). A fifth package **FrF2.catlg128** (Grömping 2013d) supports **FrF2** for non-standard design creation tasks in 128 runs. These packages and all further packages on which they depend are available from CRAN. The functionality implemented in **FrF2** is discussed in this article, with occasional digressions into relevant functions from **DoE.base** and subsequent use of **FrF2** designs by **DoE.wrapper**. The article provides an example-based discussion of the most important functionality aspects, as well as of the general philosophy regarding input and output structure. Details of algorithmic implementations are not covered, as this would exceed the scope of one article.

R provides various further packages for creating and analyzing regular fractional factorial 2-level designs. An overview is given in the CRAN task view "Design of Experiments (DoE) & Analysis of Experimental Data" (Grömping 2013a). Besides package **FrF2** (Grömping 2014), R packages **BHH2** (Barrios 2012a, companion package to Box, Hunter, and Hunter (2005)), **BsMD** (Barrios 2012b), **qualityTools** (Roth 2013) and **planor** (Kobilinsky, Bouvier, and Monod 2013) also allow creation of fractional factorial 2-level designs, however with less comfort and automatism: **FrF2** is the only package that relies on a comprehensive catalogue of designs, automatically determines the overall best design or the best design for a certain estimation purpose (option `estimable`) and offers automatic blocking and automatic creation of split plot designs. It should be mentioned here that the new package **planor** offers creation of regular fractional factorial designs not only for 2-level factors but also for factors at more than 2 levels and mixed levels. **planor** appears to be more flexible than **FrF2** regarding randomization structures; however, **planor** does not guarantee the quality criterion "minimum aberration" (see Section 3.1), is restricted to regular designs, offers less comfort and appears to be still in an early implementation phase as an R package. Regarding analysis features, **FrF2** offers various effects plots for fractional factorial 2-level designs. Packages **BsMD** and **qualityTools** also offer such functionality. One feature of **BsMD** is particularly noteworthy: it allows to conduct the Box and Meyer (1993) Bayesian assessment of effects in a screening design; this methodology is uniquely implemented in that package, to the author's knowledge; **FrF2** provides a function (`BsProb.design`) for convenient access to the methodology for designs created with the package.

The remainder of this article is organized as follows: Section 2 briefly explains general terminology and important experimental principles, Section 3 presents the mathematical background and terminology for fractional factorial 2-level designs. Section 4 provides two published examples that are used throughout the article for illustrating some design generation and analysis features. The implementation of regular fractional factorial 2-level designs in function `FrF2` is discussed in Section 5, while simple analysis tools are presented in Section 6. Design and analysis of non-regular fractional factorial 2-level designs is discussed in Section 7. Section 8 gives a brief overview of tools for augmenting or combining fractional factorial 2-level designs. Finally, a brief overview of interesting topics not covered in this article is provided. Appendix A provides some information on the class design (as far as relevant for fractional factorial 2-level designs), Appendix B discusses data export and import utilities provided by **DoE.base**, Appendix C gives details on the class `catlg` for catalogues of fractional factorial

2-level designs, and Appendix D provides details on the column orders used for screening designs with function `pb`.

2. Basic terminology for experimentation

This section briefly explains basic terminology for experimental design, using full factorial plans as a starting point. The principle of replication is explained and distinguished from repeated measurements, and randomization and randomization restrictions are discussed.

This article defines an experimental design as a rectangular table each row of which contains a prescription for the settings of all design factors (columns) in a particular run of the experiment. An unreplicated full factorial 2-level design in k factors is an experimental design in 2^k runs (= experimental setups) that contains each possible level combination exactly once. A replicated design contains each of its runs exactly r times, if r is the number of replications. It is helpful to distinguish between

- proper replications for which all sources of variability are newly set for the replicate runs,
- and repeated measurements, for which the settings of the experimental factors remain unchanged, and only the measurement process is repeated.

While proper replications are independent observations, it would be misleading to treat repeated measurements as such.

Two important principles of experimentation are blocking and randomization. The scientific community agrees that blocking should be used for keeping in check known influential factors that are not of interest in themselves (like batch variation), whereas randomization should be used as a safeguard against bias from unknown influences (see e.g., Box *et al.* 2005, p. 93: "Block What You Can and Randomize What You Cannot"). For blocking a 2-level factorial experiment, a block factor at two, four, eight, ... levels is defined such that the known influential factor can be kept constant within each block. For a useful experiment, the effect of the block factor need not be estimable itself, but can be aliased with other effects, as long as those are not of interest either. The design and analysis usually assumes that block factors do not interact with experimental factors.

Randomization means that the experimental runs are conducted in random order; if the order is completely randomized, all experimental runs can be treated as independent observations, and there is little risk of systematic bias from things like experimental order etc. For a blocked experiment, the experimental runs are randomized within each block only, which is a randomization restriction (blocks as a whole can also be randomized). Another randomization restriction occurs in case of repeated measurements: they are usually not separately randomized but conducted directly together, which is another way of distinguishing them from proper replications.

It can sometimes be necessary to keep some experimental factors fixed while changing others, mostly because of resource reasons. For example, when using a climate chamber for modifying two environmental factors at two levels each, it will be impractical to conduct the runs in random order, readjusting the climate chamber after each run. Instead, one will want to combine several runs with the same combination of levels of the environmental factors and

run them together, either in sequence or simultaneously, depending on the size and nature of the climate chamber. This is yet another type of randomization restriction: it is different from the blocking situation, since some factors *of interest* are kept fixed longer than the others. This situation is called a split plot design with so-called whole plot factors (the ones that are kept constant) and so-called split plot factors (the ones that change within whole plots). For split plot designs, the runs within whole plots are randomized, and the order of the whole plots is randomized. Split plot designs call for specific analysis strategies, e.g., mixed models.

3. Fractional factorial 2-level designs

This section provides the mathematical background for *fractional* factorial 2-level designs. There is a specific vocabulary that is reasonably straight-forward to grasp but may not be known to all readers. Readers interested in more detail are referred to Mee (2009), Box *et al.* (2005) or Montgomery (2001), for example.

3.1. Regular fractional factorial 2-level designs

For regular fractional factorial 2-level designs in m factors, like for full factorial 2-level designs, the number of runs must be a power of 2, but it is only a fraction of the number of runs (2^m) needed for a full factorial design (hence their name). Fractional factorial designs can also be replicated or run with repeated measurements and can also be completely randomized or subject to randomization restrictions. (Replicating a fractional factorial design is not recommended; it would usually be more useful to run a larger fraction without replication.)

The Yates matrix

For constructing a regular fractional factorial design for m factors in 2^k runs, one starts from the Yates matrix of a full factorial design for k 2-level factors (the base factors) and subsequently assigns $m - k$ additional factors (the generated factors) to interaction columns among the k base factors. For the construction of the Yates matrix, the base factors are denoted with $-1/1$ contrasts, and the Yates matrix is the model matrix of the full model up to the highest order interaction (except for the missing constant column of ones). The interaction columns are the elementwise products of the respective main effects columns and are arranged in a particular order, the so-called Yates order: Before a new base factor is added, all interactions of the base factors already present are included into the matrix, as shown for three factors in Table 1: the two-factor interaction (2fi) of factors A and B is added after the first two columns, the third base factor then sits on the fourth column ($= 2^{3-1}$), followed by the interactions of the third factor with the effects already present, in the order of the previous columns. For a regular fractional factorial 2-level design, all columns are orthogonal to each other. Note that the column ordering is important because regular fractional factorial designs are catalogued in terms of Yates matrix column numbers. The typical standard row ordering is the one shown in Table 1: The first base factor changes its levels with each run $(-1, +1, -1, +1, \dots)$, the second every other run $(-1, -1, +1, +1, -1, -1, +1, +1, \dots)$, the third every fourth run, and so forth. With this row ordering, the Yates matrix can easily be extended to arbitrarily many factors in an obvious way: for example, for extending the 8 run matrix in Table 1 to a 16 run full factorial matrix, the existing 8 run matrix is duplicated into 16 rows by stacking two copies on top of each other, an 8th column headed "D" is added with 8

	A	B	AB	C	AC	BC	ABC
	1	2	3	4	5	6	7
1	−1	−1	1	−1	1	1	−1
2	1	−1	−1	−1	−1	1	1
3	−1	1	−1	−1	1	−1	1
4	1	1	1	−1	−1	−1	−1
5	−1	−1	1	1	−1	−1	1
6	1	−1	−1	1	1	−1	−1
7	−1	1	−1	1	−1	1	−1
8	1	1	1	1	1	1	1

Table 1: Yates matrix for full factorial in 3 factors.

	1	2	3	4	5	6	7
I	A	B	AB	C	AC	BC	D
ABCD	BCD	ACD	CD	ABD	BD	AD	ABC

Table 2: Yates matrix column headers for (best) 8 run design in 4 factors.

−1 and 8 +1 entries each, and the subsequent columns 9 to 15 are obtained by appending the "D" to each header and multiplying the column headed with "D" with all previous columns.

There are different versions for the row order of the Yates matrix, all with the same column order and thus compatible with the design catalogues; the order of Table 1 is the most common, but it is convenient for some purposes to have runs sorted such that factor A changes slowest, factor B second slowest etc., or to even use the special run order proposed by Cheng, Martin, and Tang (1998).

Design generators and words

If a fourth factor is to be added to the design of Table 1 *without* increasing the number of runs, it is possible to use an existing interaction column for assigning the factor levels, e.g., – usually best – the column for the 3-factor interaction ABC, i.e., column 7. ABC (or column 7) is called the generator of factor D, which implies that ABC = D, i.e., the product of ABC and D is a constant column of ones. "I" is the usual notation for a constant column of ones, and ABCD = I is then called a "word". If ABCD = I, clearly, AB = CD, AC = BD, and AD = BC. Furthermore, A = BCD, B = ACD, C = ABD, and D = ABC (as we used initially). Thus, as a consequence of adding an additional factor, each column of the design now holds two effects instead of one effect only (see Table 2), which is called "aliasing".

If more than one factor is added to a design, things become slightly more complicated. For example, adding two factors to the full factorial in three factors will generate not two but three words, because the product of the two generating words is itself a word again. Generally, adding g factors implies g generators and $2^g - 1$ nontrivial words for the design. For example, adding a factor D to column 3 and E to column 5 of the Yates matrix in Table 1 implies the generators AB and AC, which in turn imply the words ABD and ACE, and consequently the additional word ABDACE = BCDE. Thus, this design has three words, and its complete alias structure is shown in the upper part of Table 3. The lower part shows the alias structure without interactions of order higher than two – assuming negligibility of higher order

	1	2	3	4	5	6	7
I	A	B	D	C	E	BC	CD
ABD	BD	AD	AB	AE	AC	DE	BE
ACE	CE	CDE	BCE	BDE	BCD	ABE	ABC
BCDE	ABCDE	ABCE	ACDE	ABCD	ABDE	ACD	ADE
	A	B	D	C	E	BC	CD
	BD	AD	AB	AE	AC	DE	BE
	CE						

Table 3: Yates matrix column headers for (best) 8 run design in 5 factors.

interactions. Such assumptions are often made and may be justified by a low order Taylor approximation, if the experimental area is reasonably small. In the following, the k factors originally spanning the 2^k full factorial design are called the "base factors", the $g = m - k$ additional factors are called the "generated factors".

Simple analysis tools

Generally, results from (fractional) factorial 2-level designs can be analyzed using a linear model. With regular fractional factorial experiments, the model with all conceivable interactions is not estimable, because of perfect aliasing of some effects. Of course, the number of estimable effects cannot exceed the number of different experimental runs. For example, the design of Table 2 allows estimation of the constant and the seven effects A+BCD, B+ACD, AB+CD, C+ABD, AC+BD, BC+AD and D+ABC. If one is prepared to assume negligibility of 3-factor interactions, main effects can be estimated without bias in that design. For a valid analysis, it is of course absolutely crucial to be aware of the alias structure of a design.

Some assessment of significance is needed in order to distinguish random variation from real experimental effects. For a design with proper replications, the estimable effects or effect sums can be tested for significance in the linear model. For unreplicated fractional factorial designs, significance tests from linear models often lack error degrees of freedom (dfs). For such cases, as linear model analysis does not work well, plotting methods for assessing effect significance have been proposed (Daniel 1959; Lenth 1989). These work reasonably well under an assumption of effect sparsity: If the majority of effects is not active (i.e., has the expected value zero), this non-active majority of effects can serve as an assessment of error variation. (Half) Normal plots of the effects show this majority of effects on a normality line and active effects as sticking out from that line. A half normal plot is often called Daniel plot, since it was proposed by Daniel (1959); Lenth (1989) proposed a numerical method for assessing effect significance. There are also approaches different from the one by Lenth (1989), which are, however, not implemented in **FrF2** and are therefore not discussed here. For an appropriate Daniel plot, it is crucial to include as many effects in the model as possible, i.e., as many as there are columns in the Yates matrix. Daniel plots work better for larger than for smaller designs – often a design in 8 runs with only seven effects will not yield a clear picture.

For effect interpretation, simple effects plots (main effects and interaction plots that visualize averages for each level of one factor or for each combination of levels of two factors) are helpful; cube plots visualize the occasional 3-factor interaction. Of course, awareness of the aliasing structure is again very important for drawing correct conclusions from any such plots.

Word length pattern and resolution

The less aliasing there is in a design, the more effects can be estimated without bias risk. The word list of a design summarizes all the aliasing that has been caused by adding g generated factors to the k base factors of the design. Words with three letters (= words of length 3) imply aliasing of main effects with 2fis; for example, the design in Table 3 has the word ABD, which implies confounding of the main effect of factor A with the BD interaction, and likewise B with AD and D with AB. Words with four letters imply aliasing of main effects with 3-factor interactions (3fis), and of 2fis with each other. Often, 3fis are assumed to be negligible, so that interest in 4-letter words results from their consequences for the aliasing of 2fis with each other (e.g., the word BCDE implies aliasing of BC with DE, of BD with CE and of BE with CD). Longer words have less severe consequences for usability of a design than shorter words, if one is prepared to accept the rationale that low order effects like main effects and 2fis are much more likely to be "active" than higher order effects.

It is customary to consider frequency tables of the word lengths of a design, the so-called "word length patterns" (WLPs): These are usually denoted as $(A_3, A_4, \dots)$. (Note that there cannot be words of length 2, because this would contradict orthogonality of the array.) For example, the WLPs for the designs of Tables 2 and 3 are $(A_3, A_4, A_5) = (0, 1, 0)$ and $(A_3, A_4, A_5) = (2, 1, 0)$. The length of the shortest word of a design is called the "resolution" of the design. Resolution is usually denoted in roman numerals and can be directly inferred from the WLP: it is the smallest word length with non-zero frequency. For example, the designs in Tables 2 and 3 have resolution IV and III, respectively.

Regular fractional factorial designs of resolution III are quite risky to use, because they confound main effects with 2fis: Even if interest is in main effects only, active 2fis can invalidate inference on these main effects. If the resolution is IV, main effects are no longer aliased with 2fis and can be estimated without bias, as long as interactions of order three or higher are negligible. However, 2fis can be aliased with each other. If all 2fis must be estimable (given that no effects of order three or higher exist), a design of resolution V is needed.

Minimum aberration

For larger designs, there are many different possibilities for adding g factors to an existing full factorial in k base factors. Some of these possibilities are structurally identical (= "isomorphic"), i.e., can be obtained from each other by swapping rows and/or columns and/or levels within columns. A lot of work has been invested in cataloguing non-isomorphic designs. Existing catalogues assess the comparative quality of catalogued designs by comparing their WLPs: a design D_1 is better than a design D_2, if it has smaller A_3, or in case of equal A_3 smaller A_4 or ... Thus, a design with higher resolution (see previous section) is always better, and in case of identical resolution, the word length pattern is successively minimized. This criterion is called "minimum aberration" (MA). Within **FrF2**, a catalogue of non-isomorphic designs ordered by the minimum aberration criterion is available (see Section 3.2 for more detail).

Maximum number of clear two-factor interactions, and MA clear designs

It has also been suggested to consider the number of "clear" 2fis as a quality criterion (Wu and Hamada 2000; Wu and Wu 2002). 2fis are called clear, if they are not aliased with main effects or other 2fis (usually, this criterion is used for resolution IV and higher only).

Design	Generator columns	A_3, A_4, A_5, ...	No. of clear 2fis
8 runs			
4-1.1	7	0 1 0	0
4-1.2	3	1 0 0	3
5-2.1	3 5	2 1 0	0
6-3.1	3 5 6	4 3 0	0
7-4.1	3 5 6 7	7 7 0 0 1	0
16 runs			
5-1.1	15	0 0 1	10
5-1.2	7	0 1 0	4
5-1.3	3	1 0 0	7
6-2.1	7 11	0 3 0	0
6-2.2	3 13	1 1 1	6
6-2.3	3 12	2 0 0 1	9
6-2.4	3 5	2 1 0	5
...			

Table 4: Principle of catalogue entries (8 runs and first 16 run entries).

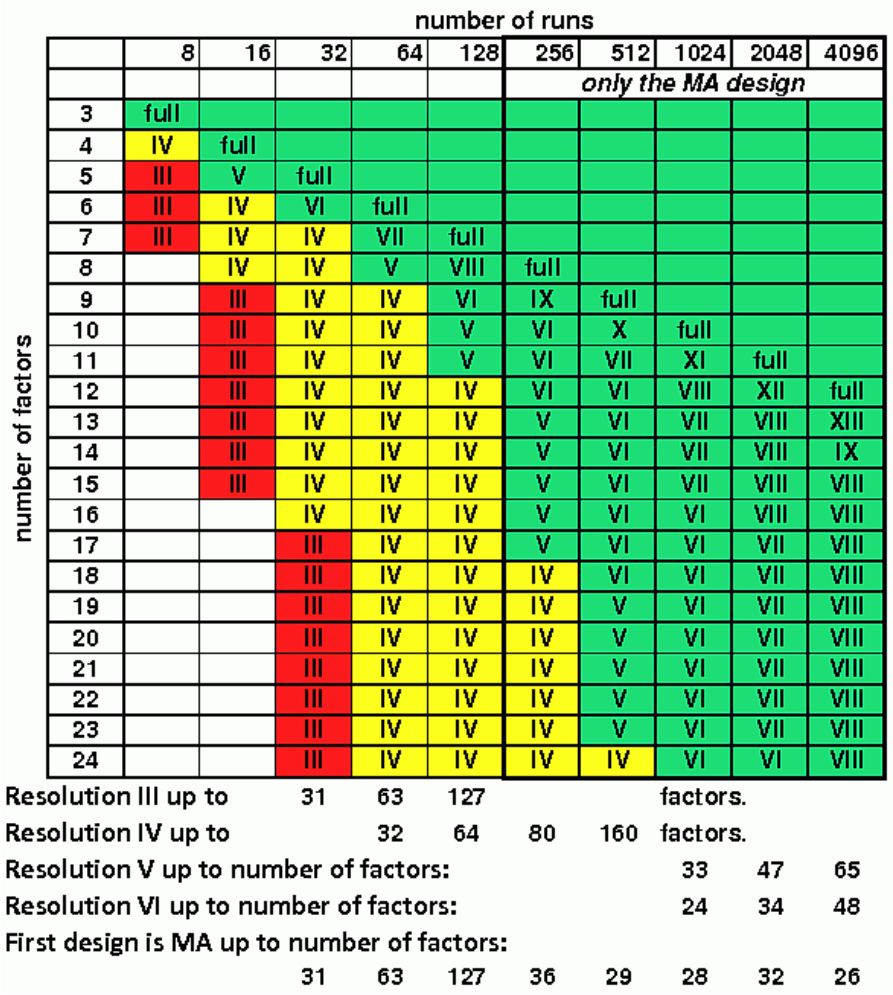
The corresponding criterion is MaxC2, and designs can also be ranked w.r.t. that criterion. However, it has been argued (Cheng, Steinberg, and Sun 1999) that this is not a good general purpose criterion, because it severely increases aliasing for the remaining 2fis, which should only be accepted with very good reason. In the spirit of this latter thinking, **FrF2** contains an algorithm for creating the minimum aberration design that can estimate a pre-specified set of 2fis clearly (Grömping 2012), which is implemented in function `FrF2`. This functionality will be detailed in Section 5.7. For brevity, designs that keep a requirement set of 2fis clear, will be called "clear designs" in the following.

3.2. Catalogues of regular fractional factorial 2-level designs

Several authors catalogued non-isomorphic regular fractional factorial 2-level designs, among them Chen, Sun, and Wu (1993), Block and Mee (2005, 2006), Mee (2009), Xu (2009) and Ryan and Bulutoglu (2010). Regular fractional factorial 2-level designs can be parsimoniously catalogued by listing their generators via Yates matrix column numbers. Table 4 shows the principle of the classical catalogue by Chen *et al.* (1993) (they started with 16 run designs).

The ordering of the catalogue is by number of runs, within that by number of factors, and within that by the MA criterion. The designs are named as m-g.pos, where m is the number of factors, g the number of generated factors (see 3.1), 2^{m-g} the number of runs, and "pos" the position number in the MA ranking. Within **FrF2**, all catalogue entries contain the information available in the Chen *et al.* (1993) catalogue, and have additionally been enhanced by so-called clear interactions graphs (CIGs, see Grömping 2012) in support of the estimability functionality of function `FrF2` (see Section 5.7).

Figure 1 shows which designs are available within **FrF2** (in a catalogue named `catlg`, which also has the class `catlg`, with more detail in C). This figure is displayed for users of the GUI package **RcmdrPlugin.DoE** on pressing an info button of the dialog for regular fractional factorial 2-level designs.



number of factors	number of runs									
	8	16	32	64	128	256	512	1024	2048	4096
						only the MA design				
3	full									
4	IV	full								
5	III	V	full							
6	III	IV	VI	full						
7	III	IV	IV	VII	full					
8		IV	IV	V	VIII	full				
9		III	IV	IV	VI	IX	full			
10		III	IV	IV	V	VI	X	full		
11		III	IV	IV	V	VI	VII	XI	full	
12		III	IV	IV	IV	VI	VI	VIII	XII	full
13		III	IV	IV	IV	V	VI	VII	VIII	XIII
14		III	IV	IV	IV	V	VI	VII	VIII	IX
15		III	IV	IV	IV	V	VI	VII	VIII	VIII
16			IV	IV	IV	V	VI	VI	VIII	VIII
17			III	IV	IV	V	VI	VI	VII	VIII
18			III	IV	IV	IV	VI	VI	VII	VIII
19			III	IV	IV	IV	V	VI	VII	VIII
20			III	IV	IV	IV	V	VI	VII	VIII
21			III	IV	IV	IV	V	VI	VII	VIII
22			III	IV	IV	IV	V	VI	VII	VIII
23			III	IV	IV	IV	V	VI	VII	VIII
24			III	IV	IV	IV	IV	VI	VI	VIII
Resolution III up to			31	63	127			factors.		
Resolution IV up to				32	64	80	160	factors.		
Resolution V up to number of factors:								33	47	65
Resolution VI up to number of factors:								24	34	48
First design is MA up to number of factors:										
			31	63	127	36	29	28	32	26

Figure 1: Designs available in `catlg`. The catalogue is complete for up to 32 runs for all resolutions and for 64 runs in resolution IV (up to 32 factors). For 128 runs with up to 24 factors, it contains a good selection from the catalogue of even/odd designs, which is separately available (**FrF2.catlg128**). (A complete catalogue of 128 run resolution IV designs with up to 24 factors was available in earlier versions of **FrF2.catlg128** and is now still available on the author's web page.)

Complete catalogues of non-isomorphic designs sorted by a quality criterion are a very helpful tool in finding the best design with certain properties – they can simply be looped from beginning to end, and the first success will yield the best possible design. This principle is behind the estimability functionality of function `FrF2` (see Section 5.7). While it often works well, the computational burden can sometimes be enormous both in terms of storage space and computing time. A recent result by Wu, Mee, and Tang (2012) has been helpful for reducing the storage space issue substantially: these authors showed that clear designs cannot be even designs (= designs with only words of even lengths). Thus, even designs can be eliminated from all catalogues for the purpose of creating clear designs. This has substantially

Run size	Max. number	Run size	Max. number
4	2	512	23
8	3	1024	33
16	5	2048	47
32	6	4096	65
64	8	8192	69
128	11	16384	92
256	17	32768	120

Table 5: Maximum number of factors in resolution V regular fractional factorial 2-level designs.

reduced the size of the 128 run catalogues in R package **FrF2.catlg128**. For the purpose of finding MA clear designs, further reduction to so-called dominating designs would be useful (introduced by Wu *et al.* 2012, who mainly concentrated on admissible designs). However, for other purposes, non-dominating designs might be interesting as well. Therefore, dominating designs have only been flagged as such in order to speed up the search algorithm.

Apart from the classical catalogues of designs, which are limited to designs with up to 4096 runs within **FrF2** and – to the authors knowledge – also elsewhere, Sanchez and Sanchez (2005) proposed a construction algorithm for resolution V designs in many factors (up to 120; the largest design has 32768 runs); this very simple algorithm is also used in **FrF2** (function `FrF2Large`). The approach does not require a large number of generators, but just one long generating vector of Yates matrix column numbers, the first m entries of which constitute a resolution V design in m factors. The approach does not give any guarantees, except that the resulting designs are resolution V.

Table 5 shows how many factors can be accomodated at resolution V for various run sizes, when using the catalogued designs for up to 4096 runs and the Sanchez and Sanchez (2005) approach for larger designs. For many experiments with physical samples, the larger run sizes are of course completely infeasible. For some computer experiments with qualitative (or hard-to-code quantitative) 2-level factors, they may, however, be interesting. The tabled information can be obtained from within R with function `nrunsV`.

3.3. Estimability of two-factor interactions

Ideally, one would often like to be able to estimate all main effects and 2fis free of aliasing. This requires a resolution V design, provided that higher order interactions can be assumed negligible. However, a resolution V design is often not feasible because of resource limitations (see Table 5 in Section 3.2). In such cases, it may be helpful to distinguish between 2fis that need to be estimated and other 2fis that are either not of interest or can even be assumed to be negligible.

Grömping (2010) discussed the distinction between assuming some 2fis to be negligible (called the "distinct" approach) and not being interested in some 2fis that are nevertheless not assumed to be negligible (called the "clear" approach). This distinction has also been made in the literature (see e.g., Wu and Wu 2002), but is not widely spread in computer software. Two notable exceptions are the longstanding SAS procedure `FACTEX` (SAS Institute Inc. 2009), where it is even possible to distinguish between effects of interest, effects not of interest but

non-negligible and negligible effects, and the recent R package **planor** (Kobilinsky *et al.* 2013) that appears to provide a similar functionality within R software. (Note, however, that neither the SAS procedure `FACTEX` nor the R package **planor** guarantee that the design they produce is minimum aberration for the requirements specified by the user.)

Clear and distinct designs

In function `FrF2`, 2fis of interest are specified in option `estimable` (see Section 5.7). The non-interesting 2fis must either be all negligible (the "distinct" approach, option `clear = FALSE`) or all allowed to be non-negligible ("clear" approach, default). Under the "distinct" approach, main effects and the 2fis requested in option `estimable` have to be on distinct columns of the Yates matrix. The "clear" approach makes the stricter requirement that even the non-interesting effects must not be allocated to columns of the Yates matrix that hold effects of interest. In the author's experience, the "clear" approach is often more appropriate than the "distinct" approach. In terms of resolution, a "clear" design usually makes sense for resolution IV only (resolution V designs are trivially "clear", resolution III designs are usually inadequate, as main effects should be considered as important as the 2fis from the requirement set). Different from the "clear" approach, a "distinct" approach may more often make sense for resolution III designs. Grömping (2010) gives various examples of the different numbers of runs and alias structures of designs resulting from both approaches. R package **FrF2** can be considered leading in terms of its ability to create minimum aberration clear designs; the principle of the algorithmic implementation is described in Grömping (2012), and also discussed in Section 5.7.

Compromise plans

Estimability requirements of a specific structure are known under the heading "compromise plans". Addelman (1962) introduced three classes of compromise plans, all of which divide the factors into two groups G1 and G2: Class 1 considers only 2fis within G1 (G1xG1) as interesting, class 2 2fis within both groups (G1xG1 and G2xG2) and class 3 2fis within G1 and 2fis between the groups (G1xG1 and G1xG2). Later, Sun (1993) introduced a fourth class for which only the 2fis between G1 and G2 are required to be estimable. Addelman discussed distinct compromise plans, Ke, Tang, and Wu (2005) discussed clear compromise plans, Grömping (2012) provided a large catalogue of minimum aberration clear compromise plans. The latter was created with function `FrF2`.

Compromise plan type estimability requirements are practically relevant; for example, a compromise plan of class 3 or class 4 may be useful in a robustness experiment, in which some control factors (grouped in G1) are investigated together with some noise factors (grouped in G2). Especially the interactions between the two groups indicate which settings for the control factors robustify a product or process w.r.t. the noise factors in G2. Function `compromise` from **FrF2** supports easy creation of such requirement sets of estimable effects (element `requirements` of the output object) and reports the minimum number of runs needed for a clear compromise plan for that requirement set (see Section 5.7).

3.4. Aspects on blocking a design

As was discussed before, the block factor is not of interest in itself, i.e., its effects are not required to be estimable. Factor effects that are confounded with the block factor are of

course not estimable. Thus, confounding of the block factor with main effects of experimental factors must be prevented. One might think that confounding of the block factor with 2fis of experimental factors should also be prevented; often, this is in fact a good approach. However, enforcing this strategy can sometimes imply unnecessary amounts of confounding among the 2fis of the experimental factors which could be avoided by allowing confounding of the block factor with 2fis of experimental factors. Section 5.4 shows an example of such a situation.

3.5. Non-regular fractional factorial 2-level designs

For regular fractional factorial 2-level designs, we have already considered the concepts of aliasing, word lengths, WLP and MA (see Section 3.1). There, aliasing is either complete or absent: For example, the design of Table 3 has two completely aliased triples of factors (A,B,D and A,C,E), each of which contributes one word of length 3 to the total of two words of length 3, whereas all other triples are clear of aliasing. For the completely aliased triples, any main effect of a factor from the triple is completely aliased with the 2fi of the other two factors; for the unaliased triples, on the other hand, the design (when ignoring all other factors) is (a replicate of) a full factorial in that triple, and the main effect of any factor in the triple is orthogonal to the 2fi of the other two factors. Because of this behavior, the WLP contains integer entries only.

For non-regular fractional factorial 2-level designs, Deng and Tang (1999) and Tang and Deng (1999) considered generalizations of the WLP and of resolution: Defining the f-dimensional J-characteristics (or J_f-characteristics) as the sums of the elementwise products of f design columns in $-1/+1$ notation, they proposed to base an assessment of a design's quality on the normalized J_f-characteristics, i.e., the absolute J_f-characteristics divided by N, the number of runs. Clearly, all normalized J_f-characteristics are 0 or 1 for regular fractional factorial 2-level designs, and the elements of WLP are sums of the respective squared normalized J-characteristics:

$$A_f = \sum_{S \text{ an } f \text{ tuple}} J_f(S)^2/N^2. \tag{1}$$

For non-regular 2-level designs, at least some (and perhaps all) normalized J_f-characteristics are between 0 and 1, and the A_f of Equation (1) constitute the generalized word length pattern (GWLP), which can also contain non-integer values (expression GWLP coined later by Xu and Wu 2001). Based on this GWLP, Tang and Deng (1999) defined minimum G_2-aberration in complete analogy to MA. Xu and Wu (2001) introduced the term "Generalized minimum aberration" (GMA) for more general designs and showed that GMA coincides with Tang and Deng's minimum G_2 aberration. Grömping (2011a) gave an accessible account on the definition of GWLP for general orthogonal arrays.

Based on the GWLP, the resolution R can be defined as the smallest f for which A_f is non-zero (i.e., for which there is at least one non-zero J_f-characteristic), in complete analogy to the definition for regular fractional factorials based on WLP. For 2-level designs, Deng and Tang (1999) introduced "Generalized resolution" (GR) as a refinement of resolution:

$$GR = R + 1 - \max_{S \text{ an } R \text{ tuple}} \frac{|J_R(S)|}{N}. \tag{2}$$

Thus, $GR = R$ for all regular fractional factorial 2-level designs, but for non-regular designs $GR > R$ is possible, and the larger GR, the closer the design to the next higher resolution. For interested readers, Deng and Tang (1999) gave a projection interpretation of GR.

Functions `lengths` and `GR` in package `DoE.base` calculate the (G)WLP and GR. These are now exemplified for the well-known 12 run Plackett-Burman design for 11 factors, which has resolution III with all normalized J_3-characteristics (and therefore of course also their maximum) equal to 1/3:

```
R> lengths(pb(12))

       2        3        4        5
 0.00000 18.33333 36.66667 29.33333

R> GR(pb(12))$GR

[1] 3.67
```

Note that the GWLP starts with length 2 in order to give indication of non-orthogonality, if needed. GMA for non-regular designs is not as useful as MA for the regular designs, as it is much more difficult to catalogue all non-isomorphic non-regular designs so that it is in most cases not possible to confirm overall optimality of an array.

Plackett-Burman designs (Plackett and Burman 1946) are the best-known non-regular fractional factorial 2-level designs. They exist, where the number of runs is a multiple of four. The resolution III 12 run array or 20 run array have been recommended for screening purposes, because they avoid complete aliasing of main effects with 2fis (because of $GR > 3$). Whenever the number of runs is a *power* of four, Plackett-Burman designs coincide with a regular fractional factorial design. This is unfortunate for screening purposes, because it implies complete aliasing among some triples of factors. Therefore, alternative designs have been developed: Box and Tyssedal (2001) recommended a 16 run design that allows estimating the main effects of up to 14 factors without any complete aliasing. Samset and Tyssedal (1999) proposed a 32 run design that is better for screening than the regular fractional factorial 2-level design obtained by the Plackett-Burman approach. Doubling (see Appendix D) allows to increase that 32 run design to 64 runs. Only the 8 run design cannot be improved upon vs. the regular fractional factorial 2-level design. Section 7.2 and Appendix D provide details about the way Plackett-Burman or related arrays are implemented in **FrF2**.

4. Examples

This section introduces two example experiments, a regular and a non-regular fractional factorial, respectively. These will be used in the sections afterwards for illustrating design creation and analysis.

4.1. A regular fractional factorial: The MI experiment

Bafna and Beall (1997) published an experiment on factors that affect the accuracy of Melt Index (MI) measurements. The MI is used for assessing the quality of a plastic melt; it

has high economic importance and is therefore regulated by a strict procedure. In their experimental setup, Bafna and Beall (1997) prepared a homogeneous plastic melt that was then measured under different conditions all of which were in compliance with the standard for the measurement procedure, or as close as was possible within the constraints of the experimental setup. The experimental goal was to distinguish between factors that have a strong or a weak effect on measurement accuracy. The idea was that specifications for the measurement process might have to be tightened for factors with a relevant effect on MI measurements at the experimental settings, while there might be opportunities for loosening a specification of the measurement process regarding a factor with no relevant effect.

Mee (2009, pp. 249) presented the data from the Bafna and Beall (1997) experiment. This 16 run experiment in six factors will be called the "MI experiment" in the sequel. It was conducted with 3 repeated measurements per run. Mee (2009) emphasized that these were repeated measurements but not replications and therefore analyzed the run-wise averages. The six experimental factors are

- the die orifice diameter in mm (2.0930 or 2.1448),
- the piston diameter in mm (9.462 or 9.500),
- the sample mass in g (4 or 8),
- the temperature in degree Celsius (188.1 or 191.1),
- the die cleanliness (dirty or clean) and
- the barrel cleanliness (dirty or clean).

The experiment itself and the observed MI values (averages or individual measurements) will be used for illustrating the use of function `FrF2` in Section 5 and the analysis features in Section 6.

4.2. A non-regular fractional factorial: shot length of a potato cannon

This example has been published on the internet (Mayfield 2007). The experiment investigates a so-called potato cannon that works according to the following principle: the cannon is powered by an air chamber set under pressure and then released by a valve which gets triggered by battery-driven electricity. The air sets a wad into motion which will move a golf ball through a barrel of a certain length into the air. The angle of the barrel can also be modified. The experimental goal is to find settings for the experimental factors such that a golf ball (or a potato or a similar object) consistently travels a far distance (the farther the better). The following eight experimental factors are investigated:

- Air volume (size of air chamber) in cubic inches (198 or 672),
- Pressure in psi (20 or 40),
- Valve (two different ones from the same manufacturer whose valves are known to be quite variable),
- Voltage (one or three 9V batteries) (9 or 27),

- Barrel length in feet (4 or 6),
- Angle in degrees (45 or 60),
- Wad type (paper or cloth),
- Ball type (white = expensive, pink = cheap).

The design was conducted as a 12 run Plackett-Burman experiment (in its Taguchi arrangement). Each run was repeated (not properly replicated) four times, and the travel distance of the golf ball (in feet) was recorded. This example will be used for illustrating design and analysis functionality in Section 7.

5. Regular fractional factorial 2-level designs with `FrF2`

Function `FrF2` implements regular fractional factorial 2-level designs, i.e., designs created according to the construction principle discussed in Section 3, in up to 4096 runs. Based on a catalogue of designs – complete for resolution III up to 32 runs and resolution IV up to 64 runs, and with only selected larger designs as pointed out in Section 3.2 – it is possible to search for the best catalogued design according to various specifications, as well as to block designs or create split plot designs.

This section provides overview information on which aspects of fractional factorial 2-level designs are implemented in **FrF2** in which way. The first section introduces the syntax of function `FrF2`, giving an overview about groups of options for various purposes. Afterwards, usage of function `FrF2` for the simple case of a fractional factorial without any randomization restrictions or specific estimability requirements is presented, including options on annotation, randomization and replication/repeated measurements. Subsequently, further aspects – blocking, split plot, estimability of certain 2fis in spite of resolution IV only – are dealt with one at a time.

5.1. Available options

The R function `FrF2` comes with many options, most of which have reasonable defaults and can be left unspecified in most situations. Table 6 summarizes and categorizes them. Their use will be illustrated in the appropriate context.

Note that some specific features cannot be combined with each other – first of all, split plotting cannot be combined with any other special feature, not even with the addition of center points. Furthermore, estimability and blocking features cannot be combined with each other.

5.2. Creating regular fractional factorial 2-level designs for simple cases

Suppose we are at the outset of planning the MI experiment; the six factors and their levels have been tentatively fixed, and the design is to be created. Complete randomization is considered possible, i.e., no blocking or split plotting is necessary. All effects are considered equally important, i.e., we want to create the MA design for the six factors; we would like to limit the experiment to 16 runs, if a reasonable design in 16 runs exists.

Option	Default setting	Also valid for `pb`	Also valid for `FrF2Large`	Section
General options				
`nruns`	`NULL`	*	*	5.2
`nfactors`	`NULL`	*	*	5.2
`factor.names`	`NULL`	*	*	5.2
`default.levels`	`c(-1, 1)`	*	*	5.2
`replications`	`1`	*	*	5.3
`repeat.only`	`FALSE`	*	*	5.3
`randomize`	`1`	*	*	5.2
`seed`	`1`	*	*	5.2
`resolution`	`NULL`			5.2
Center points				
`ncenter`	`0`	*	*	5.9
`center.distribute`	`NULL`	*	*	5.9
Explicit design specification				
`generators`	`NULL`		*	5.2
`design`	`NULL`			5.2
`select.catlg`	`catlg`			C
Estimability requirements				
`estimable`	`NULL`			5.7
`clear`	`TRUE`			5.7
`sort`	`"natural"`			5.7
`res3`	`FALSE`			5.7
`max.time`	`60`			(5.7)
`perm.start`	`NULL`			(5.7)
`perms`	`NULL`			(5.7)
`MaxC2`	`FALSE`			(5.7)
`alias.info`	`2`		*	(9)
Options for blocking				
`blocks`	`1`			5.4
`block.name`	`"Blocks"`			5.4
`bbreps`	`replications`			(5.4)
`wbreps`	`1`			(5.4)
`alias.block.2fis`	`FALSE`			5.4
Options for split plot designs				
`hard`	`NULL`			(5.6)
`check.hard`	`10`			(5.6)
`WPs`	`1`			5.5
`nfac.WP`	`0`			5.5
`WPfacs`	`NULL`			(5.5)
`check.WPs`	`10`			(5.5)

Table 6: Options for function `FrF2`.

A very simple call to function `FrF2` creates the MA design for six factors in the specified 16 runs. The summary function displays its properties, and per default prints it. For a preliminary check, it may be desirable to switch off randomization, in order to make it easier to grasp the design structure from its printout:

```
R> plan <- FrF2(16, 6, randomize = FALSE)
R> summary(plan)

Call:
FrF2(16, 6, randomize = FALSE)

Experimental design of type  FrF2
16  runs

Factor settings (scale ends):
   A  B  C  D  E  F
1 -1 -1 -1 -1 -1 -1
2  1  1  1  1  1  1

Design generating information:
$legend
[1] A=A B=B C=C D=D E=E F=F

$generators
[1] E=ABC F=ABD

Alias structure:
$fi2
[1] AB=CE=DF AC=BE    AD=BF    AE=BC    AF=BD    CD=EF    CF=DE

The design itself:
    A  B  C  D  E  F
1  -1 -1 -1 -1 -1 -1
2   1 -1 -1 -1  1  1
3  -1  1 -1 -1  1  1
4   1  1 -1 -1 -1 -1
5  -1 -1  1 -1  1 -1
6   1 -1  1 -1 -1  1
7  -1  1  1 -1 -1  1
8   1  1  1 -1  1 -1
9  -1 -1 -1  1 -1  1
10  1 -1 -1  1  1 -1
11 -1  1 -1  1  1 -1
12  1  1 -1  1 -1  1
13 -1 -1  1  1  1  1
14  1 -1  1  1 -1 -1
15 -1  1  1  1 -1 -1
```

```
16  1  1  1  1  1  1
class=design, type= FrF2
```

The same design is also created by the following request, which leaves it to the software to determine the smallest design in the required resolution for the given number of factors:

```
R> FrF2(nfactors = 6, resolution = 4, randomize = FALSE)
```

At the other extreme, if the user wants to specify the details, the same design can also be requested by explicit specification of its generators or by giving the design name from the catalog `catlg`:

```
R> FrF2(design = "6-2.1", randomize = FALSE)
R> FrF2(16, gen = c("ABC", "ABD"), randomize = FALSE)
```

The simplest design version is convenient for quickly checking possibilities. If a design has finally been selected, e.g., the above design for the MI experiment, it is usually useful to adapt some options: randomization should be switched on (this is the default), and choosing a seed ensures that exactly the same randomization order can be obtained again later. Using the `default.levels` and/or `factor.names` options prepares easy documentation of exported design files or analysis output. This is illustrated for the MI example. The first code example produces the design `plan` with levels coded as `-` and `+` and abbreviated factor names specified:

```
R> plan <- FrF2(16, 6, default.levels = c("-", "+"), factor.names = c(
+      "DieOrif", "PistDiam", "Temp", "DieClean", "SMass", "BarClean"),
+    seed = 6285)
```

A second more heavily annotated version of the design specifies the factor levels for each factor separately (see design `plan.annotated` below). Whether one prefers the first or the second version is a matter of taste. After the design itself has been created, it can be exported to html or csv format using function `export.design`, formatted as a data collection sheet for the experimenter etc. For keeping the structural design information intact, the responses – usually collected offline somewhere in a laboratory, workshop or field – have to be reimported into the design by function `add.response`. Appendix B describes the recommended way for exporting designs and re-importing response data in experimental practice. Here, for expository simplicity, a simple typed vector of responses is used:

```
R> plan.annotated <- FrF2(16, 6, factor.names = list(
+      DieOrif = c(2.093, 2.1448), PistDiam = c(9.462, 9.5),
+      Temp = c(188.1, 191.1), DieClean = c("Dirty", "Clean"),
+      SMass = c(4, 8), BarClean = c("Dirty", "Clean")),
+    seed = 6285)
R> MI <- c(35.77, 35.03, 38.5, 39.33, 35.7, 35.1, 39.27, 37, 41.07, 32.03,
+    42, 37.63, 40.2, 37, 40.1, 35.03)
R> plan.resp <- add.response(plan.annotated, MI)
R> summary(plan.resp)

Call:
```

```
FrF2(16, 6, factor.names = list(DieOrif = c(2.093, 2.1448), PistDiam =
    c(9.462, 9.5), Temp = c(188.1, 191.1), DieClean = c("Dirty", "Clean"),
    SMass = c(4, 8), BarClean = c("Dirty", "Clean")), seed = 6285)

Experimental design of type  FrF2
16  runs

Factor settings (scale ends):
  DieOrif PistDiam  Temp DieClean SMass BarClean
1  2.0930    9.462 188.1    Dirty     4    Dirty
2  2.1448    9.500 191.1    Clean     8    Clean

Responses:
[1] MI

Design generating information:
$legend
[1] A=DieOrif  B=PistDiam C=Temp     D=DieClean E=SMass    F=BarClean

$generators
[1] E=ABC F=ABD

Alias structure:
$fi2
[1] AB=CE=DF AC=BE    AD=BF    AE=BC    AF=BD    CD=EF    CF=DE

The design itself:
   DieOrif PistDiam  Temp DieClean SMass BarClean    MI
1    2.093    9.462 191.1    Dirty     8    Dirty 35.77
2    2.093      9.5 188.1    Clean     8    Dirty 35.03
3   2.1448    9.462 188.1    Clean     8    Dirty 38.50
4   2.1448    9.462 188.1    Dirty     8    Clean 39.33
5    2.093      9.5 188.1    Dirty     8    Clean 35.70
6    2.093    9.462 188.1    Clean     4    Clean 35.10
7   2.1448      9.5 188.1    Clean     4    Clean 39.27
8    2.093      9.5 191.1    Clean     4    Dirty 37.00
9   2.1448    9.462 191.1    Clean     4    Dirty 41.07
10   2.093    9.462 188.1    Dirty     4    Dirty 32.03
11  2.1448      9.5 191.1    Clean     8    Clean 42.00
12   2.093    9.462 191.1    Clean     8    Clean 37.63
13  2.1448    9.462 191.1    Dirty     4    Clean 40.20
14  2.1448      9.5 188.1    Dirty     4    Dirty 37.00
15  2.1448      9.5 191.1    Dirty     8    Dirty 40.10
16   2.093      9.5 191.1    Dirty     4    Clean 35.03
class=design, type= FrF2
```

This design will be analyzed in Section 6.

5.3. Replication and repeated measurements

The MI experiment was conducted with three repeated measurements for each run. It has already been mentioned that repeated measurements must not be treated like individual independent outcomes. The simplest permissible analysis just analyzes average measurements for each run, which is compatible with inputting the data directly as means only, as it was done in the previous section. However, more detailed analysis is possible, if all individual values are available, for example a mixed model analysis or the analysis of measurement variability as a function of the experimental factors.

For the MI experiment, the repeated measurement version of the design can be generated with the options `replication = 3` and `repeat.only = TRUE`: function `FrF2` creates three rows for each run. The resulting design object knows that these have to be treated as repeated measurements rather than proper replications. The responses are then the individual repeated measurements, given in three successive rows of the design. A function `reptowide` allows to arrange them within one row instead of underneath each other.

The above experiment created in this way looks as follows:

```
R> plan.repeat <- FrF2(16, 6, default.levels = c("-", "+"),
+    factor.names = list(DieOrif = c(2.093, 2.1448),
+      PistDiam = c(9.462, 9.5), Temp = c(188.1, 191.1),
+      DieClean = c("Dirty", "Clean"), SMass = c(4, 8),
+      BarClean = c("Dirty", "Clean")),
+    seed = 6285, replication = 3, repeat.only = TRUE)
R> MIr <- c(36.6, 35.4, 35.3, 35.8, 34.7, 34.6, 38.6, 38.1, 38.8, 38.9,
+    39.5, 39.6, 36, 36, 35.1, 35.2, 34.6, 35.5, 38.9, 39.4, 39.5,
+    36.6, 36.8, 37.6, 41.1, 40.9, 41.2, 31.9, 32.3, 31.9, 42.5,
+    41.9, 41.6, 37.8, 37.9, 37.2, 40.7, 40.9, 39, 36.6, 37.4, 37,
+    40, 39.8, 40.5, 34.8, 35.5, 34.8)
R> plan.repeat.resp <- add.response(plan.repeat, MIr)
R> summary(reptowide(plan.repeat.resp))

Call:
FrF2(16, 6, default.levels = c("-", "+"), factor.names = list(
    DieOrif = c(2.093, 2.1448), PistDiam = c(9.462, 9.5),
    Temp = c(188.1, 191.1), DieClean = c("Dirty", "Clean"), SMass = c(4, 8),
    BarClean = c("Dirty", "Clean")), seed = 6285, replication = 3,
    repeat.only = TRUE)

Experimental design of type  FrF2
16  runs

Factor settings (scale ends):
  DieOrif PistDiam  Temp DieClean SMass BarClean
1  2.0930    9.462 188.1    Dirty     4    Dirty
2  2.1448    9.500 191.1    Clean     8    Clean

Responses:
```

```
    MIr
1 MIr.1
2 MIr.2
3 MIr.3

Design generating information:
$legend
[1] A=DieOrif  B=PistDiam C=Temp     D=DieClean E=SMass    F=BarClean

$generators
[1] E=ABC F=ABD

Alias structure:
$fi2
[1] AB=CE=DF AC=BE    AD=BF    AE=BC    AF=BD    CD=EF    CF=DE

The design itself:
   DieOrif PistDiam  Temp DieClean SMass BarClean MIr.1 MIr.2 MIr.3
1    2.093    9.462 191.1    Dirty     8    Dirty  36.6  35.4  35.3
2    2.093      9.5 188.1    Clean     8    Dirty  35.8  34.7  34.6
3   2.1448    9.462 188.1    Clean     8    Dirty  38.6  38.1  38.8
4   2.1448    9.462 188.1    Dirty     8    Clean  38.9  39.5  39.6
5    2.093      9.5 188.1    Dirty     8    Clean  36.0  36.0  35.1
6    2.093    9.462 188.1    Clean     4    Clean  35.2  34.6  35.5
7   2.1448      9.5 188.1    Clean     4    Clean  38.9  39.4  39.5
8    2.093      9.5 191.1    Clean     4    Dirty  36.6  36.8  37.6
9   2.1448    9.462 191.1    Clean     4    Dirty  41.1  40.9  41.2
10   2.093    9.462 188.1    Dirty     4    Dirty  31.9  32.3  31.9
11  2.1448      9.5 191.1    Clean     8    Clean  42.5  41.9  41.6
12   2.093    9.462 191.1    Clean     8    Clean  37.8  37.9  37.2
13  2.1448    9.462 191.1    Dirty     4    Clean  40.7  40.9  39.0
14  2.1448      9.5 188.1    Dirty     4    Dirty  36.6  37.4  37.0
15  2.1448      9.5 191.1    Dirty     8    Dirty  40.0  39.8  40.5
16   2.093      9.5 191.1    Dirty     4    Clean  34.8  35.5  34.8
class=design, type= FrF2
```

This design will be analyzed in Section 6.5.

5.4. Blocked designs

The MI experiment did not require blocking. For the sake of illustration, now suppose that it can only be conducted in two blocks of eight runs each. In that case, the experiment (now again without explicit creation of repeated measurements) can be created with an additional `blocks = 2` option:

```
R> planB <- FrF2(16, 6, default.levels = c("-", "+"), factor.names = c(
+      "DieOrif", "PistDiam", "Temp", "DieClean", "SMass", "BarClean"),
+    seed = 6285, blocks = 2)
```

```
R> summary(planB)

Call:
FrF2(16, 6, default.levels = c("-", "+"), factor.names = c("DieOrif",
    "PistDiam", "Temp", "DieClean", "SMass", "BarClean"), seed = 6285,
    blocks = 2)

Experimental design of type  FrF2.blocked
16  runs
blocked design with  2  blocks of size  8

Factor settings (scale ends):
  DieOrif PistDiam Temp DieClean SMass BarClean
1       -        -    -        -     -        -
2       +        +    +        +     +        +

Design generating information:
$legend
[1] A=DieOrif  B=PistDiam C=Temp     D=DieClean E=SMass    F=BarClean

$`generators for design itself`
[1] E=ABC F=ABD

$`block generators`
[1] ACD

Alias structure:
$fi2
[1] AB=CE=DF AC=BE    AD=BF    AE=BC    AF=BD    CD=EF    CF=DE

Aliased with block main effects:
[1] none

The design itself:
  run.no run.no.std.rp Blocks DieOrif PistDiam Temp DieClean SMass BarClean
1      1         5.1.3      1       -        +    -        -     +        +
2      2        10.1.5      1       +        -    -        +     +        -
3      3         8.1.4      1       -        +    +        +     -        -
4      4         1.1.1      1       -        -    -        -     -        -
5      5        14.1.7      1       +        +    -        +     -        +
6      6        15.1.8      1       +        +    +        -     +        -
7      7        11.1.6      1       +        -    +        -     -        +
8      8         4.1.2      1       -        -    +        +     +        +
   run.no run.no.std.rp Blocks DieOrif PistDiam Temp DieClean SMass BarClean
9       9         6.2.3      2       -        +    -        +     +        -
10     10         2.2.1      2       -        -    -        +     -        +
11     11         9.2.5      2       +        -    -        -     +        +
```

```
12     12         3.2.2      2       -       -    +       -     +       -
13     13        12.2.6      2       +       -    +       +     -       -
14     14         7.2.4      2       -       +    +       -     -       +
15     15        16.2.8      2       +       +    +       +     +       +
16     16        13.2.7      2       +       +    -       -     -       -
class=design, type= FrF2.blocked
NOTE: columns run.no and run.no.std.rp are annotation, not part of the data
frame
```

The output above is annotated with block information from the `run.order` attribute of the design. The column `run.no.std.rp` contains the original run number in the non-randomized design in Yates order, the block number and the original position of the run within that block. The `rp` in `run.no.std.rp` stands for replication information; if there are replications and/or repeated measurements, this will also be reflected in further components of `run.no.std.rp`. Note that, for blocked and split plot designs, the run number in standard order refers to the run order with the first base factor changing slowest, which was also mentioned in Section 3.1, as that this is the order from which blocked or split plot designs are created. As an aside, also note that the run number in standard order in case of designs with estimable 2fis (see Section 5.7) or split plotting (see Section 5.5) can be based on an unexpected selection and ordering of base factors (this is documented in the help file for function `FrF2`).

Blocking ensures that the experimental effects can be separated from the block factor's effect. In this particular example, the design obtained by the above command appears adequate. In Section 3.4, it was mentioned that there are both advantages and disadvantages of preventing the block factor from being aliased with any 2fi. Per default, function `FrF2` does this. However, it can sometimes be better to allow aliasing of the block factor with one or very few 2fis in order to achieve less confounding among experimental effects overall. Whether or not this is the case for the experiment at hand can be investigated with the `alias.block.2fis = TRUE` option. Generally, it is recommended to also try this option, as it may occasionally yield a better design (for the above example, the design would deteriorate when using this option). For example, when allocating only five factors to 16 runs in two blocks, `alias.block.2fis = TRUE` confounds one 2fi with the block factor but has all other 2fis clear (`planB2` below), whereas a request without this option would confound six 2fis in three pairs, keeping the block factor clear from aliasing with low order experimental effects (`planB1` below). If the experiment contains any one 2fi that is not at all interesting, the allocation of `planB2` will be considered better:

```
R> planB1 <- FrF2(16, 5, default.levels = c("-", "+"), blocks = 2)
R> summary(planB1, brief = TRUE)

Call:
FrF2(16, 5, default.levels = c("-", "+"), blocks = 2)

Experimental design of type  FrF2.blocked
16  runs
blocked design with  2  blocks of size  8

Factor settings (scale ends):
```

```
  A B C D E
1 - - - - -
2 + + + + +

Design generating information:
$legend
[1] A=A B=B C=C D=D E=E

$`generators for design itself`
[1] E=ABC

$`block generators`
[1] ABD

Alias structure:
$fi2
[1] AB=CE AC=BE AE=BC

Aliased with block main effects:
[1] none

R> planB2 <- FrF2(16, 5, default.levels = c("-", "+"), blocks = 2,
+    alias.block.2fis = TRUE)
R> summary(planB2, brief = TRUE)

Call:
FrF2(16, 5, default.levels = c("-", "+"), blocks = 2, alias.block.2fis =
TRUE)

Experimental design of type  FrF2.blocked
16  runs
blocked design with  2  blocks of size  8

Factor settings (scale ends):
  A B C D E
1 - - - - -
2 + + + + +

Design generating information:
$legend
[1] A=A B=B C=C D=D E=E

$`generators for design itself`
[1] E=ABCD

$`block generators`
[1] AB
```

```
no aliasing of main effects or 2fis among experimental factors

Aliased with block main effects:
[1] AB
```

Alternatively to the automatic generation, it is also possible to specify the generators for the experimental factors themselves (option `generators`) and the generators for the block factor (give to option `blocks` instead of number of blocks). For example, design `planB2` for the five factors can also be created by the command

```
R> FrF2(16, 5, default.levels = c("-", "+"), generators = "ABCD",
+    blocks = "AB")
```

With explicit specification of block generators, the user is responsible for their alias behavior, and option `alias.block.2fis` is not needed. The online help for function `FrF2` mentions further possibilities of specifying option `blocks`, which are not covered in this article.

5.5. Split plot designs

Now, again for the MI experiment, suppose that the factors `Temp` and `SMass` can only be varied together and should not have to be changed too often; these two factors are thus made whole plot factors of a split plot design. (Note that this choice is completely arbitrary; the MI experiment does not require a split plot structure.) In that case, we would have to make sure that the experiment is run in four whole plots within which the factors `Temp` and `SMass` are not changed.

```
R> planSP <- FrF2(16, 6, default.levels = c("-", "+"), factor.names = c(
+      "DieOrif", "PistDiam", "Temp", "DieClean", "SMass", "BarClean"),
+    seed = 6285, WPs = 4, nfac.WP = 2, WPfacs = c("Temp", "SMass"),
+    design = "6-2.1")
R> MI.SP <- MI[c(5, 16, 8, 2, 3, 4, 9, 13, 6, 1, 12, 10, 7, 11, 15, 14)]
R> MI.SP <- MI[c(5, 4, 3, 2, 8, 16, 9, 13, 6, 14, 7, 10, 12, 11, 15, 1)]
R> planSP.resp <- add.response(planSP, MI.SP)
R> summary(planSP.resp)

Call:
FrF2(16, 6, default.levels = c("-", "+"), factor.names = c("DieOrif",
    "PistDiam", "Temp", "DieClean", "SMass", "BarClean"), seed = 6285,
    WPs = 4, nfac.WP = 2, WPfacs = c("Temp", "SMass"), design = "6-2.1")

Experimental design of type  FrF2.splitplot
16  runs

Factor settings (scale ends):
  Temp SMass DieOrif PistDiam DieClean BarClean
1    -     -       -        -        -        -
2    +     +       +        +        +        +
```

```
Responses:
[1] MI.SP

Design generating information:
$legend
[1] A=Temp     B=SMass    C=DieOrif  D=PistDiam E=DieClean F=BarClean

$generators
[1] B=ACD F=CDE

Alias structure:
$fi2
[1] AB=CD=EF AC=BD    AD=BC    AE=BF    AF=BE    CE=DF    CF=DE

split-plot design:  4  whole plots
                 : first  2  factors are whole plot factors

The design itself:
  run.no run.no.std.rp Temp SMass DieOrif PistDiam DieClean BarClean MI.SP
1      1         5.2.1    -     +       -        +        -        + 35.70
2      2         9.2.3    -     +       +        -        -        + 39.33
3      3        10.2.4    -     +       +        -        +        - 38.50
4      4         6.2.2    -     +       -        +        +        - 35.03
  run.no run.no.std.rp Temp SMass DieOrif PistDiam DieClean BarClean MI.SP
5      5         8.3.2    +     -       -        +        +        - 37.00
6      6         7.3.1    +     -       -        +        -        + 35.03
7      7        12.3.4    +     -       +        -        +        - 41.07
8      8        11.3.3    +     -       +        -        -        + 40.20
   run.no run.no.std.rp Temp SMass DieOrif PistDiam DieClean BarClean MI.SP
9       9         2.1.2    -     -       -        -        +        + 35.10
10     10        13.1.3    -     -       +        +        -        - 37.00
11     11        14.1.4    -     -       +        +        +        + 39.27
12     12         1.1.1    -     -       -        -        -        - 32.03
   run.no run.no.std.rp Temp SMass DieOrif PistDiam DieClean BarClean MI.SP
13     13         4.4.2    +     +       -        -        +        + 37.63
14     14        16.4.4    +     +       +        +        +        + 42.00
15     15        15.4.3    +     +       +        +        -        - 40.10
16     16         3.4.1    +     +       -        -        -        - 35.77
class=design, type= FrF2.splitplot
NOTE: columns run.no and run.no.std.rp are annotation, not part of the data
frame
```

Design creation would have been easier, if the whole plot factors had been the first factors in `factor.names`. In that case, it would have been sufficient to specify the numbers of whole plots and whole plot factors (options `WPs` and `nfac.WP`) without having to specify `WPfacs` and – more important – a specific design. The online help describes further detail, for example usage of option `check.WPs`.

In the creation of the split plot experiment above, it had to be made sure that the experiment was created such that the response values from the published MI experiment can be used for demonstrating analysis features for split plot designs later on, as response values are available for 16 level combinations of the 64 possible ones only. The 16 response values (averages used again) had to be reordered, as the split plot structure implies a randomized ordering different from the previous one. The design `planSP.resp` will be used for demonstrating the only analysis feature for split plot designs in Section 6.4.

5.6. Hard to change factors

The previous section discussed split plotting. Split plotting can also be used for accomodating hard to change factors, by making these the whole plot factors. Sometimes, researchers see the need to enforce even fewer changes than obtainable from such a split plot design with randomized whole plots. This can be achieved in function `FrF2`, using option `hard` for specifying the number of hard to change factors (these have to be the first factors specified); the function uses the slow-changing matrix given in Cheng *et al.* (1998). This option creates a split plot design with non-randomized and very systematic order of whole plots; runs within whole plots are randomized, like always. The resulting design is a multilevel split plot design: the first hard to change factor changes most slowly, the second one second most slowly etc. As long as

- the order of the runs is not influential,
- and the variability from changing hard-to-change factors is close to negligible relative to measurement variability and variability from changing easy-to-change factors,

a pragmatic researcher may consider this type of procedure as preferrable to not being able to conduct the experiment. Therefore, the package offers this type of design. For analysis, the package treats such a design as a split plot design, although its whole plot order is not randomized. It must be emphasized that the user is responsible for assessing whether the approach can be responsibly used. *Whenever feasible, a proper split plot design with the hard to change factors as whole plot factors (and resetting their levels between whole plots even if there is no level change between adjacent whole plots!) should be used instead!*

5.7. Estimability of two-factor interactions in package FrF2

The general option `resolution` is adequate whenever users simply want to treat all effects of the same order in the same way. Mainly for resolution IV designs, it is not uncommon to consider some 2fis to be more important than others, as was discussed in Section 3.3. For this situation, option `estimable` selects these more important 2fis (the requirement set), option `clear` governs whether or not a clear design is requested, and option `res3` allows the user to downgrade from the natural requirement of resolution IV to resolution III only. The other estimability options from Table 6 handle technicalities, more or less. Note that the general option `resolution` cannot be specified together with the `estimable` option.

Distinct designs

For demonstrating estimability features, let us now consider the MI experiment, assuming that we can afford 16 runs only and that we are interested in the main effects and the 2fis of

any of the first three factors (A, B and C) with any of the last three factors (D, E and F), i.e., in a class 4 compromise plan with G1 consisting of the first three factors. The requirement set can be obtained using function `compromise`:

```
R> req.set <- compromise(6, 1:3, class = 4)$requirement
R> req.set

[1] "AD" "BD" "CD" "AE" "BE" "CE" "AF" "BF" "CF"
```

The message produced by function `compromise` tells us that a *clear* design for that requirement set would require 32 runs:

```
a clear design requires at least 32 runs (resolution V)
```

As only 16 runs have been declared feasible, a clear compromise plan is not in reach. If it appears acceptable that all 2fis outside the requirement set are negligible, option `clear` can be set to `FALSE`. Function `FrF2` then searches for a design that can accomodate the main effects and the required 2fis on distinct columns of the Yates matrix:

```
R> FrF2(16, 6, estimable = req.set, clear = FALSE)

Error in mapcalc.distinct(estimable, nfac, nruns, res3 = res3, max.time =
 max.time,  : The required interactions cannot be accomodated on distinct
 columns in 16 runs with resolution IV or higher.
```

The function reports a failure, because the default is to allow resolution IV and higher designs only. If we really believe in negligibility of the non-required 2fis, we can decide to permit resolution III using the `res3` option. This leads to the following design:

```
R> plan.estim <- FrF2(16, 6, estimable = req.set, clear = FALSE, res3 = TRUE)
R> summary(plan.estim, brief = TRUE)

Call:
FrF2(16, 6, estimable = req.set, clear = FALSE, res3 = TRUE)

Experimental design of type  FrF2.estimable
16  runs

Factor settings (scale ends):
   A  B  C  D  E  F
1 -1 -1 -1 -1 -1 -1
2  1  1  1  1  1  1

Design generating information:
$legend
[1] A=A B=B C=C D=D E=E F=F
```

```
$generators
[1] C=AB  F=ADE

Alias structure:
$main
[1] A=BC B=AC C=AB

$fi2
[1] AD=EF AE=DF AF=DE
```

The output shows that the design `plan.estim` confounds main effects of factors A, B and C with the 2fi of the respective other two factors. As these 2fis have been assumed negligible, this design is acceptable under the "distinct" approach. For readers interested in the generation of the array, the `map` entry of the `design.info` attribute of the design shows that it was obtained by using the second best design for 6 factors in 16 runs, and by pulling the 5th design factor to the third position in order to make the design match the required structure (i.e., A = 1, B = 2, C = 5, D = 3, E = 4, F = 6):

```
R> design.info(plan.estim)$map

$`6-2.2`
[1] 1 2 5 3 4 6
```

Clear designs

The implementation of clear designs uses the algorithm of Grömping (2012). It heavily relies on package **igraph** (Csardi and Nepusz 2006). As a prerequisite, each catalogue entry of the catalogue `catlg` contains the CIG of the design, which is the unique graph that has an edge for each clear 2fi. Likewise, a requirement set for an experiment can be considered as a CIG, and an experiment can be accomodated within a design, if its requirement set CIG is a subgraph of the design's CIG. Internally, this subgraph relation is analyzed with function `graph.subisomorphic.vf2` from **igraph**. Manual insights into the structure of requirement set CIG and design CIG can be gained using function `CIG` from **FrF2**: Suppose (very simple example) one wants to run a 32 run experiment in 9 factors and wants to keep all interactions between two noise factors N1 and N2 on the one hand and five control factors C1 to C5 on the other hand clear, having two further environment factors E1 and E2 in the model. Then, the requirement set contains 10 2fis; factors E1 and E2 need not be included in the requirement set CIG (if included nevertheless, they are vertices without edges). For this simple situation, Figure 2 shows that the requirement set cannot be accomodated in design 9-4.1, but in 9-4.2, by assigning N1 and N2 to columns 5 and 9; the figure has been created by the code below:

```
R> par(mfrow = c(1, 3), cex = 1.1, mar = c(0, 0.4, 2, 0.4))
R> req.set <- ~ (N1 + N2) * (C1 + C2 + C3 + C4 + C5)
R> set.seed(2571)
R> CIG(req.set, static = TRUE, vertex.color = "white", vertex.size = 40,
+    vertex.label.family = "sans", vertex.label.color = "black",
+    vertex.label.cex = 1, edge.color = "black", edge.width = 1.3,
+    main = "Requirement set")
```

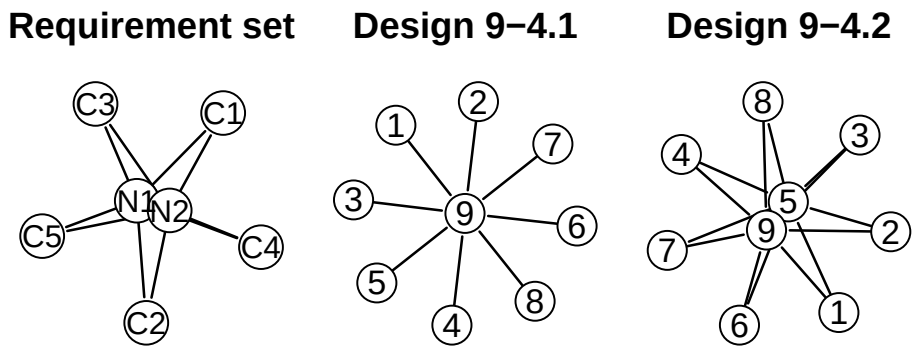


Figure 2: CIGs for requirement set and two candidate designs.

```
R> CIG("9-4.1", static = TRUE, vertex.color = "white", vertex.size = 35,
+    vertex.label.family = "sans", vertex.label.color = "black",
+    vertex.label.cex = 1.1, main = "Design 9-4.1", edge.color = "black",
+    edge.width = 1.3)
R> CIG("9-4.2", static = TRUE, vertex.color = "white", vertex.size = 35,
+    vertex.label.family = "sans", vertex.label.color = "black",
+    vertex.label.cex = 1.1, main = "Design 9-4.2", edge.color = "black",
+    edge.width = 1.3)
```

When using option `estimable`, the task of matching the requirement set CIG to the best possible design CIG is performed automatically; again, the map element of the `design.info` attribute indicates, how the requirement set was accomodated:

```
R> plan <- FrF2(32, 9,
+   factor.names = c("N1", "N2", "C1", "C2", "C3", "C4", "C5", "E1", "E2"),
+   estimable = ~ (N1 + N2) * (C1 + C2 + C3 + C4 + C5))
R> design.info(plan)$map

$`9-4.2`
[1] 5 9 1 2 3 4 6 7 8
```

As expected, the example requirement set was accommodated in design "9-4.2", assigning factors N1 and N2 to its columns 5 and 9, the other factors to the remaining columns.

Often, the search for clear designs is very fast. However, as subgraph isomorphism search is an NP-hard problem, the algorithm sometimes takes very long. Option `sort` sometimes but not always speeds up the algorithm (see manual). If the automatic search is *very* slow, a manual search of the design that the algorithm got stuck with can be helpful. After interrupting an unsuccessful search, the name of the last search design can be retrieved by the command `FrF2.currentlychecked()`. If a manual inspection of this design reveals that there is no chance of accommodating the requirement set in that design, the search can be restarted, restricting the catalogue to later designs only with the `select.catlg` option. For manual inspection, it will be helpful to omit the `static = TRUE` option from function `CIG` (see code chunk for the graphs above), which yields an interactive graph.

5.8. Large designs

Function `FrF2` is limited to designs with up to 4096 runs, regardless of the way a design is specified. Larger fractional factorial 2-level designs can be created with function `FrF2Large`. The latter function is more limited than `FrF2` in terms of design structures (no blocking, no split plot designs, no estimability requirements). The available options are those asterisked in Table 6. Function `FrF2Large` implements automatic design creation with the method by Sanchez and Sanchez (2005) that was introduced in Section 3.2. Alternatively, users can manually generate a design by specifying the generators (with slightly more restrictive entries than in function `FrF2`). Attempts to use this function for designs with up to 4096 runs return an error.

5.9. Randomization, replication and center points

Center points

Regular fractional factorial 2-level designs with quantitative factors are often used as the starting point for response surface investigations. For these, it can be quite useful to use some center points in the design. Center points can also be useful for checking for curvature in non-regular fractional factorial 2-level designs. Center points can be requested with option `ncenter` of functions `FrF2`, `FrF2Large` and `pb`. Note that their position in the design is not randomized, but can be controlled via option `center.distribute`. Per default, center points are placed at the beginning, in the middle and at the end of the design (i.e., distributed over three points). It is also possible to augment a design with center points after its creation using function `add.center`.

Note that the center points functionality does not work simultaneously with a split plot structure or specification of hard to change factors. The reason is that it is usually not a good idea to have a separate whole plot that consists of center points only, and that it is not obvious how to handle center points in a standard way in split plot designs.

Randomization and replication

Design generating functions generally block the randomization of proper replications on time, i.e., they generate a randomized sequence of all first replicates, then a randomized sequence of all second replicates, and so forth (run `FrF2(8, 4, replications = 3)` to see what this means). As the user has not a-priori specified time as a block factor, this is a mere precaution against surprises from time effects that are not unheard of; if such a time trend is found, an analysis including a replication block factor can partially account for it. However, since the user did not ask for blocking on time in the first place, the replicated design does not contain a block column, and its default analysis does not include a block factor.

If desired, the block factor that reflects the replication blocking on time can be retrieved using function `getblock`; this function will also provide separate factors for the other randomization restrictions. Users can use these factors in a custom analysis with R function `lm` or advanced analysis functions from packages.

Users who dislike the fact that replications are blocked on time or that center points are systematically placed can apply the function `rerandomize.design` to the design; this function does not randomize the replications in blocks and does randomize the position of center

points, and it also randomizes the position of blocks; in the default randomization, block order is fixed, and it is assumed that users randomize their units to the blocks. Of course, `rerandomize.design` keeps a block or split plot structure intact and keeps repeated measurements together. Users who decide to use this function have to make sure to add center points directly with design creation, as subsequent adding of center points is not possible for a re-randomized design.

6. Simple analysis tools

Simple analysis tools for regular fractional factorial 2-level designs have been discussed in Section 3.1. Their R implementation is presented here, using the MI experiment. As a prerequisite of any useful interpretation, awareness of the alias structure – obtainable from the `summary` function – is necessary.

6.1. Main effects plots

A very simple analysis visualizes the response means for the different factor levels: the main effects plot. Two versions of main effects plots are available, and which one to use is purely a matter of taste:

```
R> plot(plan.resp, cex = 1.2, cex.lab = 1.2, cex.axis = 1.2,
+    main = "Main effects plot for MI", cex.main = 2)
R> MEPlot(plan.resp, abbrev = 5, cex.xax = 1.6, cex.main = 2)
```

The main effects plot for the MI experiment (both graphs in Figure 3) shows the differences between factor levels. Clearly, controlling the die orifice diameter has the largest effect, with a difference of about 4.3 between its levels. Temperature follows suit, with a difference of about 2. The relevance of the effect sizes can usually be decided by the experimenter's gut feel, while the significance must be decided by statistical methods (see Sections 6.3 and 6.4).

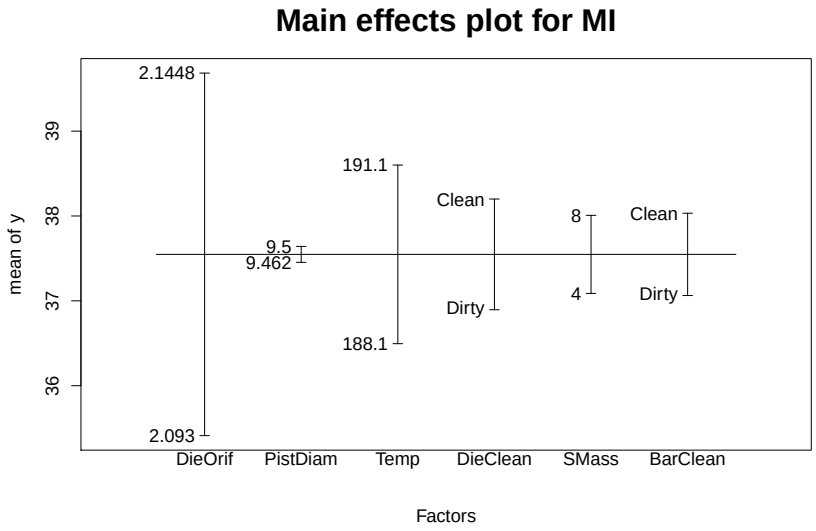
In resolution III designs, the user should be aware of aliased 2fis which can mask or inflate a main effect. This is not an issue in the resolution IV MI experiment.

6.2. Interaction plots

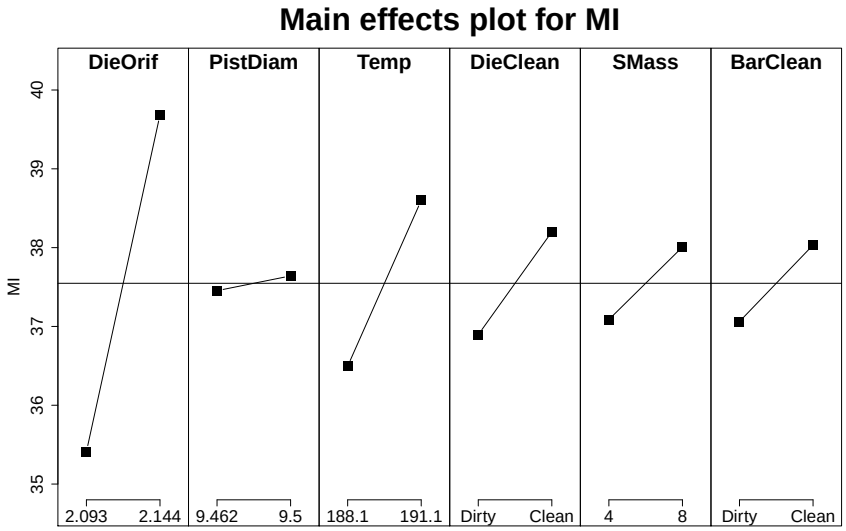
For resolution IV or higher regular fractional factorial 2-level designs, it makes sense to look at interaction plots. Function `IAPlot` with its method for class `design` objects can be used for that purpose. The graphs in Figure 4 have been created with the following code:

```
R> IAPlot(plan.resp, abbrev = 5, show.alias = TRUE, lwd = 2, cex = 2,
+    cex.xax = 1.2, cex.lab = 1.5)
R> IAPlot(plan.resp, abbrev = 5, select = 3:6, lwd = 2, cex = 2,
+    cex.xax = 1.2, cex.lab = 1.5)
```

The `show.alias = TRUE` option marks aliased interactions with the same number in order to indicate that these can only be estimated together in one sum (see top graph in Figure 4); this is very helpful for avoiding over-interpretation. For example, the summary of the design in Section 5.2 showed that the interaction between temperature and barrel cleanliness is aliased



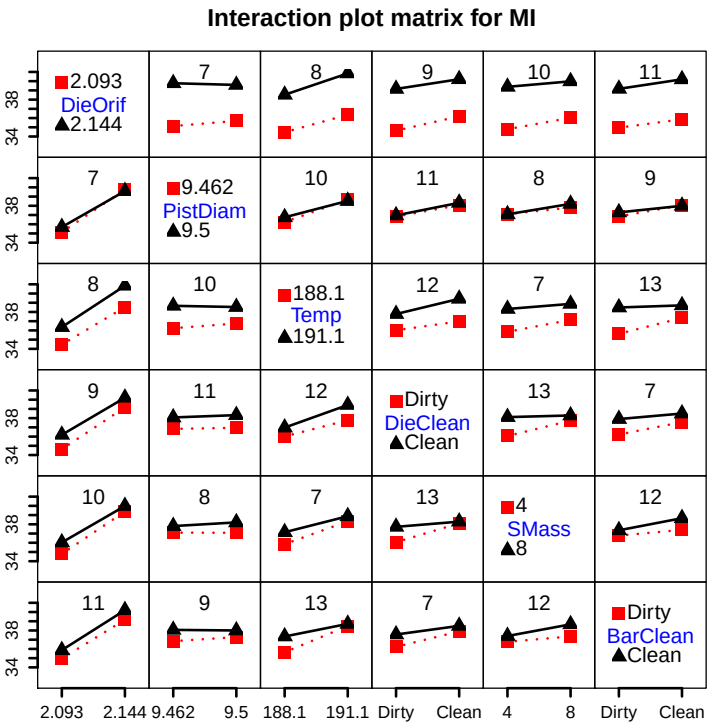
(a) `plot` method for class `design`.



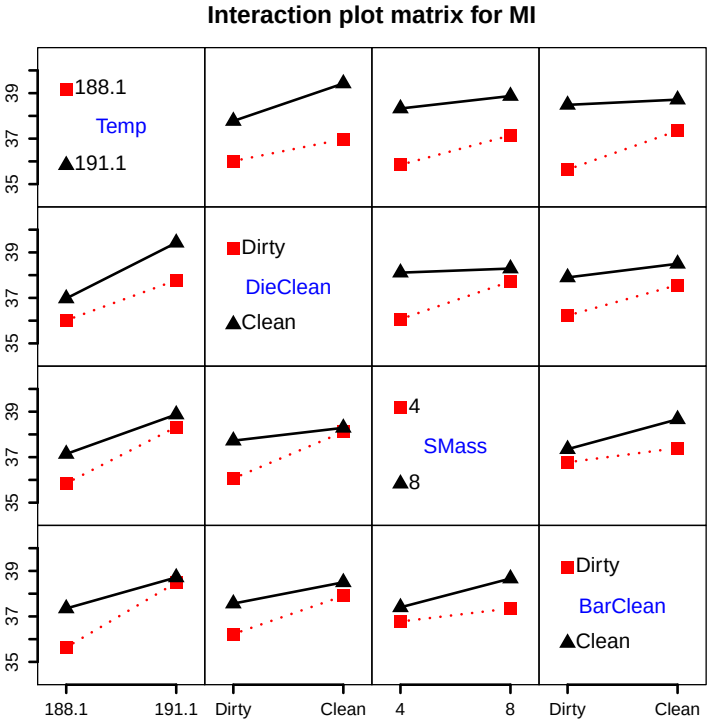
(b) Function `MEPlot`.

Figure 3: Main effects plots for the MI example.

with the interaction of die cleanliness with the sample mass (`CF=DE`); this is also visible from the figure, as these interactions are both marked with the number 13. The selection of only some factors in the bottom graph shows a larger display of some 2fis. (The selection has been based on the analysis results from the following two sections.) The interactions can be interpreted as follows: For dirty die, sample mass makes a difference, for clean die it does not OR for dirty barrels, temperature makes a difference, for clean barrels it does not OR a combination of both (OR, even, a stronger effect for one of these, and the opposite effect for the other).



(a) All interactions with alias numbering.



(b) Selected interactions.

Figure 4: Interaction plots for the MI example.

6.3. Linear model

A linear model analysis for the MI example can be run using the `lm` method for class `design` objects provided in package `DoE.base`. For regular fractional factorial designs, the default analysis models the first response with all main effects and all 2fis; in case of several responses, a different response can be specified with option `response`; the polynomial degree can be adjusted with the `degree` option.

```
R> summary(lm(plan.resp))

Number of observations used: 16
Formula:
MI ~ (DieOrif + PistDiam + Temp + DieClean + SMass + BarClean)^2

Call:
lm.default(formula = fo, data = model.frame(fo, data = formula))

Residuals:
      1       2       3       4       5       6       7       8       9
 0.1050 -0.1175  0.1175 -0.1175  0.1175  0.1050 -0.1050  0.1175 -0.1175
     10      11      12      13      14      15      16
-0.1050  0.1050 -0.1050  0.1175  0.1050 -0.1050 -0.1175

Coefficients: (8 not defined because of singularities)
                   Estimate Std. Error t value Pr(>|t|)
(Intercept)        37.54750    0.07879 476.554  4.4e-06 ***
DieOrif1            2.13625    0.07879  27.113  0.00136 **
PistDiam1           0.09375    0.07879   1.190  0.35619
Temp1               1.05250    0.07879  13.358  0.00556 **
DieClean1           0.65250    0.07879   8.282  0.01427 *
SMass1              0.46000    0.07879   5.838  0.02811 *
BarClean1           0.48500    0.07879   6.156  0.02539 *
DieOrif1:PistDiam1 -0.18500    0.07879  -2.348  0.14338
DieOrif1:Temp1      0.10625    0.07879   1.349  0.30990
DieOrif1:DieClean1 -0.12625    0.07879  -1.602  0.25025
DieOrif1:SMass1    -0.16125    0.07879  -2.047  0.17731
DieOrif1:BarClean1  0.03125    0.07879   0.397  0.72996
Temp1:DieClean1     0.17250    0.07879   2.189  0.16000
Temp1:BarClean1    -0.37000    0.07879  -4.696  0.04248 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.3152 on 2 degrees of freedom
Multiple R-squared:  0.9982,        Adjusted R-squared:  0.9863
F-statistic: 84.36 on 13 and 2 DF,  p-value: 0.01177
```

In the linear model output, when using the `lm` method for class `design` objects, all NA rows from aliased effects are suppressed, i.e., only the first occurring effect from each alias group

is included. For example, the MI experiment has six main effects and 15 2fis; the output shows only seven 2fis, which act as representatives from their alias groups. Based on 2 error *df*s, the linear model identifies five of the main effects and one interaction as significant effects. Of course, it is again important to include knowledge about the alias structure into the interpretation of results. For example, the significant 2fi of temperature with barrel cleanliness is completely aliased with that of die cleanliness with sample mass (see previous section).

The main purpose of the linear model analysis lies in the possibility of assessing significance of effects. In case of only few or even no degrees of freedom for error, it may be more appropriate to assess effect significance from effects plots (see next section). Users who prefer to look at explained variation instead of effects can use the `aov` method for class `design` objects provided in package `DoE.base` or can apply the `anova` function to the linear model result. For the designs considered in this paper with balanced orthogonal 1 *df* effects only, the results from `lm` and `aov` are equivalent in terms of significance testing and differ in scaling only (coefficient scaling versus sum of squares scaling). Users who think about their problem in terms of sensitivity analysis may prefer the sum of squares perspective.

6.4. Normal and half normal effects plots of a simple design

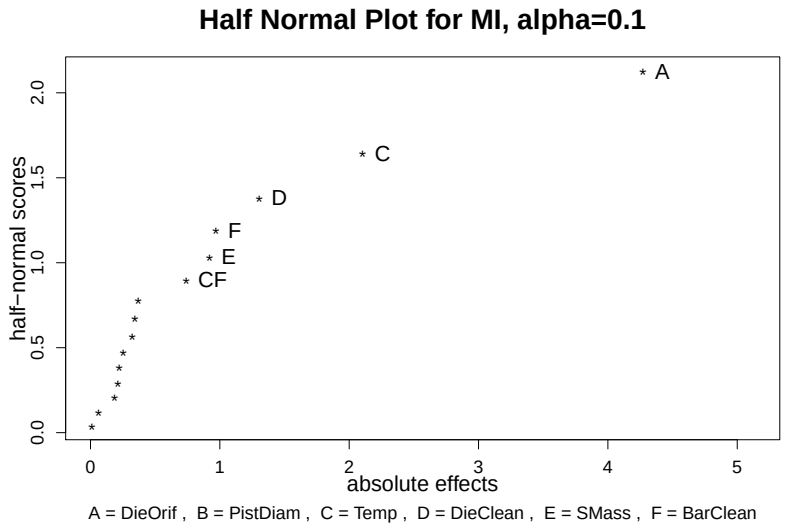
Normal and half normal effects plots can be obtained with function `DanielPlot`. Option `half = TRUE` creates a Daniel (half normal) plot, option `autolab = TRUE` (default) labels only those effects that are significant at the user-specified level `alpha` (default: 0.05) according to the method by Lenth (1989). The class `design` method of function `DanielPlot` automatically chooses the degree of interaction such that `nruns - 1` effects are included (in this case 15), which is crucial for the concept of effects plots to work.

The method of function `DanielPlot` for class `design` produces a Daniel plot for the MI experiment (top graph in Figure 5):

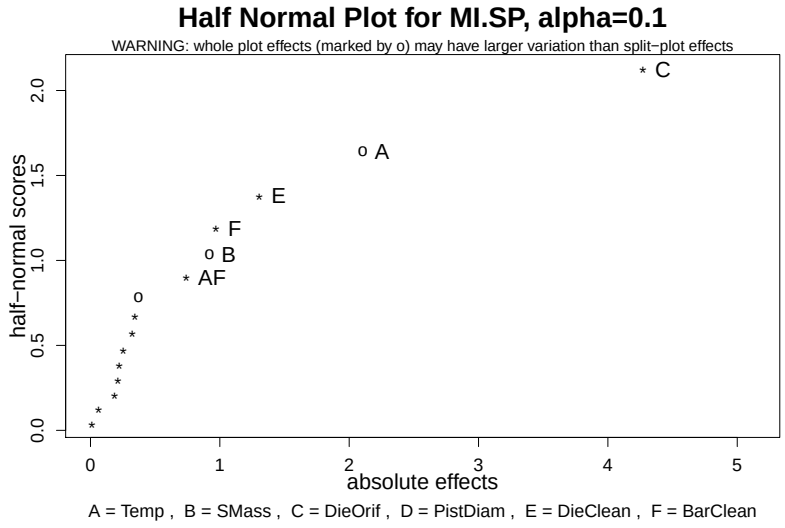
```
R> DanielPlot(plan.resp, code = TRUE, half = TRUE, alpha = 0.1,
+    cex.main = 1.8, cex.pch = 1.2, cex.lab = 1.4, cex.fac = 1.4,
+    cex.axis = 1.2)
```

As the author prefers a half normal to a full normal effects plot, option `half = TRUE` is set. Furthermore, option `code = TRUE` labels the plot points with capital letters for the factors, with a legend underneath the plot. For these data, the plot at significance level 10% shows the same significant effects as the linear model analysis at significance level 5%. Liberal values of α are often used in Daniel plots, since it is often more important to keep the relevant effects than to rule out the irrelevant ones.

This is a good place to show the only analysis feature that has so far been implemented for split plot designs: A split plot design has two types of effects, the whole plot effects with potentially higher variability and the split plot effects with potentially lower variability. Looking at these together in one plot may be misleading. Therefore, two different plot symbols are used, and users are warned. If this design had been conducted as a split plot design as postulated for the design `planSP` created in Section 5.5, the bottom graph in Figure 5 tells us that the effects marked by the symbol "o" are whole plot effects, which may be more variable than the other effects. Hence, the strong deviation of the effect of factor A from the half normal distribution line might be partially due to higher whole plot variation, whereas the



(a) Design as conducted.



(b) Pretending design was run as split plot.

Figure 5: Daniel plots for the MI example.

conclusions on significance of the other factors are solid. However, as the absolute values of the two other whole plot effects are just within the unexciting noise line, whole plot variability does not seem an issue here (which is of course not surprising, because the design was not conducted as a split plot experiment). An analogous feature is also implemented for linear model analysis: users are informed, which effects are whole plot effects and may be subject to higher variability.

6.5. Repeated measurements and replications

For designs with r proper replications, a linear model analysis is preferrable to a (half) normal

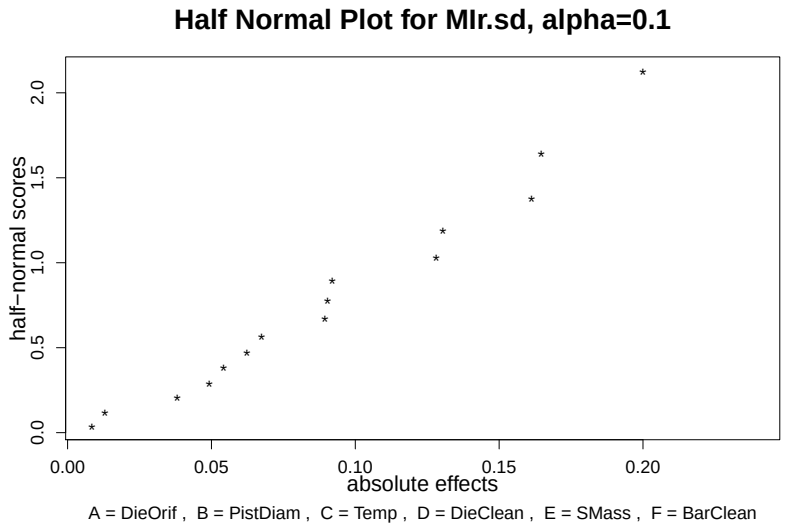


Figure 6: Daniel plot for effects on the standard deviation of the measurements.

effects plot, since there are many error degrees of freedom. Section 5.9 pointed out that randomization of proper replications is blocked on time, however without adding a block factor to the design. In the author's opinion, it is not generally necessary to account for this blocking in the analysis, and the default analysis does not do so. Users who consider a blocked analysis necessary for principle or situation-specific reasons can use function `getblock` for creating appropriate block factors that can be used for a custom analysis in R function `lm` or advanced analysis functions for mixed models. (For users who prefer an unblocked randomization of replications in the first place, Section 5.9 explained how to re-randomize the design at the design creation stage.)

Designs with r repeated measurements require special analysis, either by a mixed model approach (random effect for each run; again, function `getblock` can be used for creating a run identifier), or – much more simple and accessible to non-expert users – by analyzing averages (or other scalar functions of the repeated measurements, like the standard deviation) only. The plotting functions can handle designs with individual repeated measurements: `DanielPlot(plan.repeat.resp, half = TRUE, code = TRUE, alpha = 0.1)` produces the top plot of Figure 5 on the basis of average measurements. For analyzing the standard deviation of the measurements instead, the standard deviation can be calculated by aggregating the repeated measurements after reshaping the data frame to wide format:

```
R> plan.sd <- aggregate(reptowide(plan.repeat.resp), FUN = "sd")
```

A Daniel plot for the resulting design with the standard deviation as the response shows an almost ideal random half normal line (see Figure 6), i.e., there appears to be no influence of the experimental factors on measurement accuracy.

```
R> DanielPlot(plan.sd, half = TRUE, code = TRUE, alpha = 0.1,
+    cex.main = 1.8, cex.pch = 1.2, cex.lab = 1.4, cex.fac = 1.4,
+    cex.axis = 1.2, cex.legend = 1.2)
```

7. Non-regular fractional factorial 2-level designs in FrF2

7.1. Options of function pb

Function `pb` uses part of the options in complete analogy to those of function `FrF2` (see Table 6). There are only three additional options for special purposes: `boxtyssedal` (see the online help), `n12.taguchi` (see Section 7.3) and `oldver` (see D.1).

7.2. The implemented arrays

Function `pb` implements Plackett-Burman designs (Plackett and Burman 1946) with up to 100 runs, as introduced in Section 3.5.

Package **FrF2** contains a list with generator information for the implemented arrays (`pb.list`). For some situations, the package uses a different array than the one proposed by Plackett and Burman: the missing 92 run array is created by a Williamson construction, as reported in Hedayat, Sloane, and Stufken (1999). Furthermore, for 16, 32 and 64 runs, the alternative designs discussed in Section 3.5 are implemented in order to avoid complete aliasing of main effects and 2fis as much as possible. Table 7 provides an overview of the arrays used in function `pb` and summarizes information on their properties which are also discussed in the text below. D gives some detail on doubling, cycling blocks, and the Williamson construction, especially regarding the column order which deviates from that given in the literature and also has changed over time in **FrF2**.

Note that function `pb` always uses the first m columns of an array for a design in m factors. Thus, the order of the columns in the arrays is very important. The following considerations have driven the final default ordering of the columns: the 16 run Hadamard matrix and the arrays obtained by doubling or cyclic combination of blocks, as well as the 92 run array (i.e., the arrays for 40, 52, 56, 64, 76, 88, 92, 96 and 100 runs) contain one column, inclusion of which dramatically increases aliasing for designs with many factors: this column is completely or heavily partially (for 52, 76 and 100 runs) aliased with various 2fis. This column has therefore been moved to the last position of the array, in order to prevent heavy aliasing in screening designs, as long as not all columns are used. For the doubled arrays, the first $n/2-1$ columns together with the afore-mentioned last column yield a resolution IV design; for up to $n/2-1$ factors, the design is resolution IV per default, for exactly $n/2$ factors the option `oldver = TRUE` is needed for achieving resolution IV. The arrays created by cyclic combination of blocks yield almost resolution IV designs ($GR > 3.9$, with GR from Equation (2)) for up to $n/2-1$ factors. The aliasing properties of the arrays are summarized in Table 7.

7.3. Creation and analysis of Plackett-Burman designs

Usage of function `pb` is straightforward and works analogously to that of function `FrF2` for all standard cases. Blocking, split plot designs and estimable 2fis cannot be specified, center points can. Functions `lm`, `DanielPlot` and `MEPlot` have methods for Plackett-Burman designs, and design inspection methods can also be applied.

Usage of function `pb` is now illustrated using the potato cannon example from Section 3.5. The following commands generate the design and summarize it. The option `n12.taguchi = TRUE` makes sure that the design is generated in the Taguchi arrangement, rather than in the

Runs	Original Plackett and Burman	Construction	Max. no. of factors without complete or heavy partial aliasing with any 2fi	Max. no. of factors with (almost) resolution IV	
				default	with `oldver = TRUE`
8	yes	cycling	4	4	
12	yes	cycling	11		
16	no	Hadamard[(a)]	14	(*)	
20	yes	cycling	19		
24	yes	cycling	23		
28	yes	cycling	27		
32	no	cycling[(b)]	31	(*)	
36	yes	cycling	35		
40	yes	doubling	38	19	20
44	yes	cycling	43		
48	yes	cycling	47		
52	yes	cycling blocks	50	(25)	
56	yes	doubling	54	27	28
60	yes	cycling	59		
64	no	doubling	62	31	32
68	yes	cycling	67		
72	yes	cycling	71		
76	yes	cycling blocks	74	(37)	
80	yes	cycling	79		
84	yes	cycling	83		
88	yes	doubling	86	43	44
92	no	Williamson[(c)]	90		
96	yes	doubling	94	47	48
100	yes	cycling blocks	98	(49)	

(*) For $n/2$ factors or less, the regular design from function `FrF2` should be used.
(a) see Box and Tyssedal (2001)
(b) generating vector from Samset and Tyssedal (1999)
(c) taken from Hedayat *et al.* (1999, p.160)

Table 7: The arrays used by function `pb`.

structurally comparable arrangement proposed by Plackett and Burman (1946):

```
R> pot.cannon <- pb(12, seed = 15143,
+    factor.names = list(AirVolume = c(198, 672), Valve = c(1 ,2),
+    Barrel = c("4ft", "6ft"), Angle = c(45, 60), Pressure = c(20, 40),
+    WadType = c("paper", "cloth"), Voltage = c(9, 27),
+    BallType = c("white", "pink")), n12.taguchi = TRUE)
R> summary(pot.cannon)

Call:
pb(12, seed = 15143, factor.names = list(AirVolume = c(198, 672),
    Valve = c(1, 2), Barrel = c("4ft", "6ft"), Angle = c(45,
```

```
        60), Pressure = c(20, 40), WadType = c("paper", "cloth"),
    Voltage = c(9, 27), BallType = c("white", "pink")), n12.taguchi = TRUE)

Experimental design of type  pb
12  runs

Factor settings (scale ends):
  AirVolume Valve Barrel Angle Pressure WadType Voltage BallType e1 e2 e3
1       198     1    4ft    45       20   paper       9    white -1 -1 -1
2       672     2    6ft    60       40   cloth      27     pink  1  1  1

The design itself:
   AirVolume Valve Barrel Angle Pressure WadType Voltage BallType e1 e2 e3
1        198     2    4ft    60       40   paper      27     pink -1 -1  1
2        672     1    6ft    60       20   paper      27     pink -1  1 -1
3        672     2    4ft    45       40   paper      27    white  1  1 -1
4        198     1    4ft    45       20   cloth      27     pink  1  1  1
5        198     2    6ft    60       20   cloth      27    white  1 -1 -1
6        672     2    6ft    45       20   paper       9     pink  1 -1  1
7        198     1    4ft    45       20   paper       9    white -1 -1 -1
8        198     1    6ft    60       40   paper       9    white  1  1  1
9        198     2    6ft    45       40   cloth       9     pink -1  1 -1
10       672     2    4ft    60       20   cloth       9    white -1  1  1
11       672     1    6ft    45       40   cloth      27    white -1 -1  1
12       672     1    4ft    60       40   cloth       9     pink  1 -1 -1
class=design, type= pb
```

The summary shows a unique feature of function `pb`: if not explicitly asked for a smaller `nfactors`, the function always assigns the maximum possible number of factors, by creating additional dummy factors named `e1`, `e2` and so forth. This is done for supporting appropriate Daniel plotting: there are a total of $n - 1$ orthogonal effects in the design, and the dummy factors are among them; of course, they are not expected to have relevant effects, but they are important "no effect" points against which to compare the actual experimental factors (see Daniel plot in Figure 7). The code below adds the average responses from the four repeated measurements (`asl`) and subsequently creates the Daniel plot (`autolab = FALSE` labels all points).

```
R> asl <- c(203.771, 140.046, 424.479, 127.875, 78.667, 167.979, 85.521,
+    208, 313.813, 166.021, 466.771, 389.958)
R> pot.cannon.resp <- add.response(pot.cannon, asl)
R> DanielPlot(pot.cannon.resp, half = TRUE, autolab = FALSE, cex.main = 1.8,
+    cex.pch = 1.2, cex.lab = 1.4, cex.fac = 1.4, cex.axis = 1.2)
```

A main effects plot can be created in the same way as for `FrF2` type designs and does per default omit the dummy factors for error. Interaction plots cannot be created and usually do not make sense. (Even for the – presumably rare – cases, where resolution IV portions of a Plackett-Burmann design based on doubling are used, function `IAPlot` cannot be applied to the linear model object of such a design, because there is partial aliasing among the 2fis.)

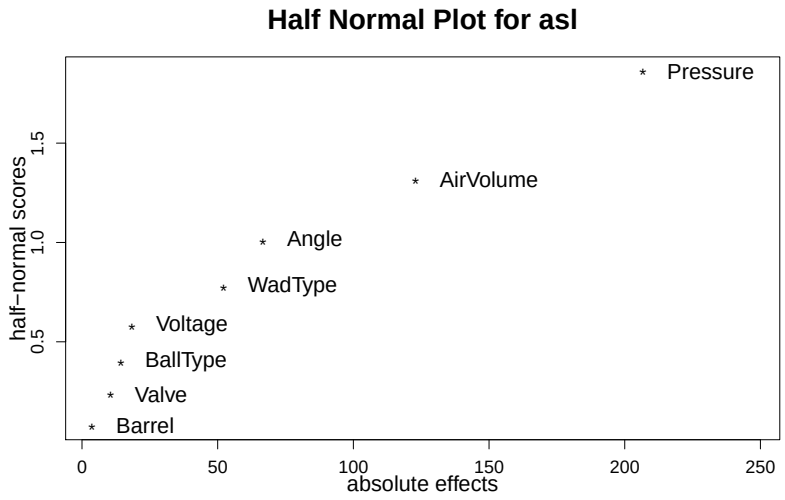


Figure 7: Daniel plot for the potato cannon experiment, all effects labelled.

For a linear model, the dummy factors for error are not needed in the formula. They are therefore automatically omitted, when using the method for class design objects of the generic `lm` from **DoE.base**. (With older versions of the package (**FrF2** before version 1.3 or **DoE.base** before version 0.23), it was necessary to manually delete the dummy factors from the formula.)

```
R> summary(lm(pot.cannon.resp))

Number of observations used: 12
Formula:
asl ~ AirVolume + Valve + Barrel + Angle + Pressure + WadType +
    Voltage + BallType

Call:
lm.default(formula = fo, data = model.frame(fo, data = formula))

Residuals:
      1       2       3       4       5       6       7       8       9
 -8.387   4.885   8.387  -6.957  10.460  -4.885   6.957  -6.957   4.885
     10      11      12
-10.460  -8.387  10.460

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  231.075      4.583  50.423 1.72e-05 ***
AirVolume1    61.467      4.583  13.413 0.000896 ***
Valve1        -5.287      4.583  -1.154 0.332219
Barrel1       -1.862      4.583  -0.406 0.711701
Angle1       -33.331      4.583  -7.273 0.005364 **
Pressure1    103.390      4.583  22.561 0.000191 ***
```

```
WadType1      26.109      4.583   5.697 0.010722 *
Voltage1       9.193      4.583   2.006 0.138514
BallType1     -7.168      4.583  -1.564 0.215736
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 15.87 on 3 degrees of freedom
Multiple R-squared:  0.9962,        Adjusted R-squared:  0.986
F-statistic: 97.78 on 8 and 3 DF,  p-value: 0.001539
```

8. Design augmentation and combination

8.1. Center points and central composite designs

A fractional factorial design can be created with center points (see Section 5.9) or can later be augmented with center points by function `add.center`. (Note that immediate inclusion of center points is preferrable, especially in cases where experimental results may depend on time.) Regular fractional factorial designs, preferrably ones that already contain center points and have at least resolution V, can later be augmented into a central composite design – a special design for response surface exploration (e.g., Montgomery 2001) – using function `ccd.augment` from **DoE.wrapper**. This feature is based on the function `rsm` from **rsm** (Lenth 2009). Note that **DoE.wrapper** cannot augment split plot designs into central composite designs.

8.2. Fold-over

If a fractional factorial design yields ambiguous results because of aliasing of main effects with 2fis, ambiguities can be resolved by the fold-over approach, which removes all or certain words of length 3. A classical fold-over requires to run another block of the same size as the original experiment. Fold-over is covered in various text books, for example Box *et al.* (2005), Mee (2009) or Montgomery (2001). In **FrF2**, function `fold.design` implements fold-over; note, however, that only standard designs can be folded (no center points, no blocked or split plot structure).

8.3. Robustness designs

Robustness experiments are often conducted using a Taguchi approach with a so-called inner and outer array (see e.g., Montgomery 2001). For the analysis, one often takes aggregate measures (e.g., mean, standard deviation or signal-to-noise ratio) over the outer array and analyzes their dependence on the factors of the inner array. It is possible to create such experiments using function `param.design` from **DoE.base**. There is some support for automatic calculation of aggregated measures, similar to the tools for designs with repeated measurements (see Section 6.5).

It has been discussed in the literature whether one should conduct robustness experiments as one large experiment with estimability requirements (as e.g., mentioned in Section 5.7) or

whether the inner-outer array approach is more useful. Like so often, the answer depends on the situation. If robustness can be achieved by exploiting interactions, the combined array is often more useful; on the other hand, if there are genuine influences of inner array factors on the variability of the outcome, possibly not even moderated by the outer array factors, an inner-outer array approach is preferable.

9. Further developments

Package `FrF2` contains all basic features and many advanced ones for fractional factorial 2-level designs. Some further features would still be desirable.

It is possible to create designs with some factors at 4 or 8 levels, based on regular 2-level fractional factorial designs. So far, such designs are not specifically supported in **FrF2**. Package **DoE.base** contains designs with 2-, 4- and 8-level factors, which can be used but do not explicitly control the alias structure, apart from keeping all main effects orthogonal to each other. Expert users can use the estimability features for obtaining suitable designs: a resolution III design with one 4-level factor can be obtained by using two 2-level factors and their interaction, keeping the interaction estimable with options `clear = FALSE` and `res3 = TRUE`; a resolution IV design with one 4-level factor is obtained in the same way, but omitting these two options; a resolution III design with one 8-level factor can be obtained by using three 2-level factors for creation of the 8-level factor, making sure that all the 2fis among these three factors are kept clear; this also ensures that the 3-factor interaction of the three factors is not aliased with any main effect. A resolution IV design with two 4-level factors requires manual intervention: in addition to keeping the 2fis of the pairs of factors for generating the 4-level factors clear, it is necessary to make sure that the four generating factors together do not occur in a word of length 5. Whether or not this is the case can be checked by setting option `alias.info = 3`. An analogous approach can also yield a resolution IV design with an 8-level factor. However, in both cases, it is not possible to automatically request the desired behavior. It would be desirable to have options for automatic creation of designs with number of levels a power of two that also handle the alias structure of the resulting design. However, with the advent of the new package **planor**, the priority on this improvement has reduced; it would only be added value if the resulting design could be guaranteed to be best in some well-defined way, or if finding a design would be much faster (which might be the case for moderate and large scenarios, at least when considering the current implementation of **planor**).

Some features are currently not combinable, for example center points with split plot designs, crossing of blocked designs, or estimability requests and blocking. The implementation of all these combinations requires substantial mathematical and programming work; it will have to be checked whether it is feasible within the current approaches to blocking, estimability and split plotting to achieve any of the combinations with acceptable effort.

There are (not so many) instances for which creation of a clear design is prohibitively slow in the current implementation that evaluates subgraph isomorphism with the VF2 algorithm by Cordella, Foggia, Sansone, and Vento (2001) as implemented in **igraph**. Recent experiences with a few of these showed that the LAD algorithm (Solnon 2010) was very fast in ruling out impossible matches, where VF2 took a long time. Once LAD has been implemented in **igraph** (it will be part of the next major release), it will replace or complement the VF2 algorithm

in **FrF2**, depending on broader experiences to be gained with LAD.

It would be desirable to enhance the automatic analysis features to also include some more advanced types, like mixed model analyzes of designs with repeated measurements or split plot designs. The recently-added function `getblock` is a first step towards that goal.

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A. Class design and functionality for it

Functions FrF2, FrF2Large and pb create an output design that is of S3 class design and thus follows a certain structure (see Section A.1) and allows application of certain inspection, modification and analysis methods and functions (see Section A.2).

A.1. Class design

An object of S3 class design is a a data frame with the three attributes desnum, run.order and design.info. All three attributes can be accessed by accessor functions with the same name (e.g., run.order(plan)).

- Attribute desnum contains a numeric version of the data frame, which may be useful for users who want to do manual matrix calculations. The package functionality itself makes little use of that attribute.
- Attribute run.order has the main purpose of always being able to switch back and forth between a standard order (Yates order, see Section 3.1) and the randomized run order.
- Attribute design.info is a list that contains important information on the design and is heavily used by the methods and functions of packages **DoE.base** and **FrF2**. This attribute will be described in some detail in A.3.

A.2. Functionality for class design objects

There are inspection methods (print, summary, plot) and analysis methods (lm, DanielPlot, MEPlot, IAPlot) for this class, as well as a subsetting method which is currently useful for reordering designs only.

Furthermore, there are functions useful for inspecting or modifying the content of a class design object (design.info, run.order, desnum, generators, aggregate.design (method for the generic aggregate), factor.names, response.names, col.remove, fix.design (method for the generic fix adapted from package **utils**), qua.design, change.contr, reptowide, reptolong, paramtowide, undesign, redesign), functions for augmenting a design with further runs or response data (add.center, add.response, ccd.augment, fold.design), and functions for combining class design objects (cross.design, param.design).

A.3. The design.info attribute

The design.info attribute has some mandatory elements that have to be present for all class design objects and many elements that are needed for some types of designs only. The author's web page contains a large table that details which types of designs need which elements of the design.info attribute (http://prof.beuth-hochschule.de/fileadmin/user/groemping/downloads/classDesignOverviewStructure.pdf). Table 8 lists the elements relevant for designs created with **FrF2**.

Element	Data type	Role
Mandatory elements		
`type`	character string	identifies the type of design
`nruns`	number	number of runs (replications not counted)
`nfactors`	number	number of factors
`factor.names`	named list	factor names and factor levels (or scale ends for quantitative factors)
`replications`	number	number of replications or repeated measurements per run
`repeat.only`	logical	if TRUE, the number given in the replications element refers to repeated measurements only
`randomize`	logical	if TRUE, run order has been randomized
`seed`	number	the seed used for randomization
`creator`	call or list of menu settings in GUI	the creation history of the object
Optional general elements		
`response.names`	vector of character strings	names of the response columns (column names from the data frame)
Elements for blocked designs (from functions `fac.design` *or* `FrF2`*)*		
`block.name`	character string	name of block variable
`nblocks`	number	number of blocks
`block.gen`	number	Yates matrix column number(s) of factor(s) used for blocking (`FrF2`) or block generator matrix (`fac.design`)
`blocksize`	number	run size of each block (replications not counted)
`bbreps`	number	number of between block replications (identical to `replications`)
`wbreps`	number	number of within block replications (these can be proper replications or repeated measurements only)
Further element for full factorial designs (function `fac.design`*)*		
`nlevels`	numeric vector	number of levels for each factor
Further elements for designs created by function `FrF2`		
`aliased`	list with character elements	information on the alias structure of the design up to degree 2 or 3 (as requested by option `alias.info`)
`FrF2.version`	character string	version of **FrF2**, with which design was created
`generators`	character vector	design generators in the format "D=ABC" etc.

Continued on next page

Continued from previous page

Element	Data type	Role
`catlg.name`	character string	name of the catalogue used for design creation
`catlg.entry`	list of length 1 of class `catlg`	the catalogue entry used for the design
`ntreat`	number	identical to nfactors, present for blocked designs for backwards compatibility
`aliased.with.blocks`	character vector	lists 2fis that are aliased with the block main effect
`base.design`	character string	element of design catalogue named in `catlg.name` that has been used for creating a blocked or split plot design
`nfac.WP`	number	number of whole plot factors
`nfac.SP`	number	number of split plot factors
`nWPs`	number	number of whole plots
`plotsize`	number	run size of each plot (replications not counted)
`res.WP`	number	resolution of the whole plot portion of the design
`map`	numeric vector with k elements	mapping of base factors so that estimability or randomization restriction requirement is fulfilled
`orig.fac.order`	numeric vector with `nfactors` elements	order of original factors from function call for split plot designs
`clear`	logical	if TRUE, the design is clear (for estimability requirement)
`res3`	logical	if TRUE, resolution III has been permitted for estimability request
Further elements common to designs created by functions `pb` *and* `FrF2`		
`quantitative`	logical vector with `nfactors` elements	`TRUE` elements indicate quantitative factors
`ncube`	number	number of cube points in a design with center points
`ncenter`	number	number of center points
`coding`	list of formulae	coding of quantitative factors (for use with package **rsm**)
Further element for designs created by function `pb`		
`ndummies`	number	number of dummy factors for error effects

Table 8: Elements of the `design.info` attribute of class `design`.

For class `design` objects created by design combination functions, some of the entry types given in the table can also be replaced by lists of several such entries. Functionality for combined designs is currently very limited.

B. Exporting designs and importing experimental data

For actual usage of an experimental design package, it is crucial that the R user (who may or may not be the experimenter) can easily customize the design for actual data collection. In many cases, data collection happens with a spreadsheet software rather than with R. Therefore, data export and import are important. Specifically, for making full use of the packages' functionality, it is necessary to preserve the class `design` information and to add adequate response information to the `design.info` attribute of the design.

This can be done using the functions `export.design` for exporting the actual design to a `csv` or `html` file. It is strongly recommended to also save an `rda` file with the current state of the experimental design R object. This R object can later be used for adding response data to it with function `add.response`.

Function `export.design` exports a design in the desired format, function `add.response` can be used for re-importing it. Details can be found in the online help. The code example below shows the general principle. Of course, settings have to be adapted to the user's computer system, e.g., the `InDec` and `OutDec` options that influence the decimal separator and separator settings.

```
R> getwd()
R> des <- FrF2(8, 4)
R> export.design(des, filename = "des", type = "all", OutDec = ",")
```

This export command writes the three files '`des.rda`', '`des.csv`' and '`des.html`' to the current R working directory (the location could have been changed by the `path` option of function `export.design`). The `OutDec = ","` option corresponds to the R `csv2` command for European `csv` settings for the author's German computer. The csv or html file can be used for collecting response data. The actual re-import of the response data into R must use a csv file (but the html file could be stored as csv after inputting data). With the same active working directory as before, the following command can re-import the data, after responses have been added:

```
R> des.resp <- add.response("des", "des.withresponses.csv",
+    rdapath = "des.rda", InDec = ",")
```

This command reads the design `des` from the `rda` file `des.rda` and adds the response values from the `csv` file to it (provided, there are no obvious mismatches between the files in which case an error message will result).

C. Class `catlg` and methods for it

The catalogue `catlg` available in **FrF2** contains an ordered list of experimental designs, as detailed in Section 3.2. Each entry is a list, for example:

```
R> catlg[["8-4.2"]]

$res
[1] 3
```

```
$nfac
[1] 8

$nruns
[1] 16

$gen
[1]  3  5  9 14

$WLP
[1] 0 0 3 7 4 0 1

$nclear.2fis
[1] 1

$clear.2fis
     [,1]
[1,]    1
[2,]    8

$all.2fis.clear
numeric(0)

$dominating
[1] TRUE
```

The entire list has the class `catlg`, for which there are a `print` method, a subsetting method, and various accessor methods (named in most cases after the list element they access). The subsetting method makes sure that the '`[`' subsetting retains the class properties. The effect of the `print` method can be observed by observing the difference of the previous output to the one shown now:

```
R> catlg["8-4.2"]

Design:  8-4.2
   16  runs,  8  factors,
   Resolution  III
   Generating columns:  3 5 9 14
   WLP (3plus):  3 7 4 0 1 ,  1  clear 2fis
```

Besides affecting the way catalogue elements are printed, the `print` method also has selection options regarding the number of runs, the number of factors or the resolution of a design. Details can be found in the online help (`?print.catlg`).

As an example for application of an accessor method, the following code provides the resolution for each of the 13 designs of Table 4:

```
R> res(catlg[1:13])
```

```
3-1.1 4-1.1 4-1.2 5-2.1 6-3.1 7-4.1 5-1.1 5-1.2 5-1.3 6-2.1 6-2.2 6-2.3
    3     4     3     3     3     3     5     4     3     4     3     3
6-2.4
    3
```

Instead of an accessor for the `gen` element, there is a `generators` method for class `catlg`, which allows to print the generators in more human-friendly form, here for all catalogued designs in 16 runs for 6 factors:

```
R> generators(catlg[10:13])

$`6-2.1`
[1] "E=ABC" "F=ABD"

$`6-2.2`
[1] "E=AB"  "F=ACD"

$`6-2.3`
[1] "E=AB" "F=CD"

$`6-2.4`
[1] "E=AB" "F=AC"
```

The catalogue `catlg` is the default catalogue used by function `FrF2`. A different catalogue can be selected with the option `select.catlg`, for example a catalogue from **FrF2.catlg128**, or a subset from `catlg` for continuing a previously successless search for a design with certain estimability requirements (omitting the designs that have already been searched and thus slowly moving forward towards success in case of large important problems). Note that **FrF2.catlg128** must be installed but need not be loaded; if one of its catalogues is requested by function `FrF2`, the function automatically loads that package and the relevant catalogue.

D. Column ordering aspects for Plackett-Burman designs

D.1. Designs based on doubling

Starting from an array D with n rows and $n/2-1$ columns, an array in $2n$ rows and $2n-1$ columns can be obtained by doubling. Doubling has some history in **FrF2**. Versions before 1.0-5 used the following arrangement:

$$\begin{pmatrix} D & -D & \mathbf{1} \\ D & D & -\mathbf{1} \end{pmatrix}.$$

The placement of the column of plus one and minus one vectors last is very beneficial, because that vector is the negative product of $n/2-1$ pairs of the $n-1$ columns of the doubled design (column 1 with column $n/2$, column 2 with column $n/2+1$ etc.). Hence, whenever this column is among the design columns, there is severe complete aliasing, so that including it last keeps

	Partially aliased 52 run triple				Completely aliased 56 run triple			
	Third factor				Third factor			
	−1		+1		−1		+1	
Second factor	−1	+1	−1	+1	−1	+1	−1	+1
First factor								
−1	1	12	12	1	14	0	0	14
+1	12	1	1	12	0	14	14	0

Table 9: Complete and severe partial aliasing.

all designs with $n-2$ or fewer factors clear of complete aliasing. With version 1.0-5, it was decided that the ordering of design columns should allow designs with few factors to benefit from the fact that up to $n/2$ factors can be accomodated at resolution IV in a doubled design. Unfortunately, the placement of the column of plus and minus one vectors was overlooked in this consideration, and hence these versions had the following structure:

$$\begin{pmatrix} \mathbf{1} & -D & D \\ \mathbf{-1} & D & D \end{pmatrix}.$$

Consequently, all doubled designs with more than $n/2$ factors were always affected by some complete aliasing. The latest version (from 1.3 onwards) moved the column of plus and minus one vectors to the very end again, i.e. doubling is now implemented as

$$\begin{pmatrix} D & D & \mathbf{1} \\ -D & D & \mathbf{-1} \end{pmatrix}.$$

Thus, design based on a doubled array is now automatically resolution IV in case of $n/2-1$ factors (only), with the benefit of avoiding complete aliasing for up to $n-2$ factors. Option `oldver` (set to `TRUE`) allows to exactly reproduce designs from version 1.0-5 (Jan 2010) to version 1.2-10 (updated Feb 2012). A user who wants to use exactly $n/2$ factors of a doubled array (e.g., 20 factors in a 40 run design) can also use this option for making the design resolution IV.

D.2. Designs based on cycling block matrices with special first row and column

Arrays created on the basis of cycling block matrices with a special first column (52, 76 and 100 runs) have a similar issue as doubled arrays with the first column chosen as the column of plus and minus one vectors: the extra first column is not completely aliased but quite heavily partially aliased with the remaining columns, and the GR of a design can be strongly increased by excluding that first column from the design. The degree of partial aliasing as compared to complete aliasing is illustrated in Table 9 for two triples of factors from the 52 run and the 56 run design: while only half of the eight possible factor level combinations occur for the completely aliased design, the partially aliased design has one occurrence each for the one half and distributes all other runs on the other half of the combinations. While slightly better than complete aliasing, severe partial aliasing should of course also be avoided wherever possible.

Furthermore, a design in $n/2$ factors that only uses the originally odd-numbered columns (i.e., columns 1, 3, 5, ...) is very close to resolution IV ($GR > 3.9$ in all cases). Thus, starting with version 1.3 of **FrF2**, function `pb` moves the orginally first column to the very end and the orginally even-numbered columns behind the other originally odd-numbered columns in order to drastically increase GR for most practically relevant designs. Option `oldver` can be used for reproducing a design from an earlier version.

D.3. The 92 run design

Finally, the 92 run array also has a similar issue to that of the just-mentioned arrays: its 69th column is involved in some triples with heavy aliasing. That column has therefore been moved to the very end in order to improve GR for designs with up to 90 factors; again, option `oldver` can be used for reproducing the earlier behavior.

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