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"Clear" and "Distinct": two approaches for regular fractional factorial designs with estimability requirements

"Clear" und "Distinct": Zwei Ansätze für reguläre fraktionierte faktorielle Versuchspläne mit Schätzbarkeits-Anforderungen (englischsprachig)

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"Clear" and "Distinct": two approaches for regular fractional factorial designs with estimability requirements

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Abstract

In many experimental situations, some two-factor interactions are more interesting than others. It is therefore useful to study designs that allow estimation of a prespecified set of two-factor interactions, the requirement set. This report compares two approaches to estimability of two-factor interactions: in the "Distinct" approach, all twofactor interactions outside the requirement set are assumed to be negligible, while the "Clear" approach does not rely on such an assumption. The literature regarding the two approaches is reviewed, and their relation is illustrated through several examples.

Key words: clear 2fis, compromise plan, design of experiment, linear graph, clear design, distinct design

1. Introduction

In industrial experimentation, the need for information competes with cost considerations. Many designed experiments are conducted based on fractional factorial 2-level plans, because these are parsimonious in the number of runs and can be adapted to be able to estimate effects of interest. With infinite resources available, an experiment with m 2-level factors could be conducted as a 2^m run full factorial plan in the *m* factors (of course, with infinite resources, the numbers of factor levels could also be increased). A regular fractional factorial 2-level plan in m factors consists of a "fraction" of the full factorial plan. Its construction usually starts from a full factorial plan in *m*-*k* so-called base factors and assigns the additional *k* so-called generated factors to certain interactions among the base factors. As a consequence of assigning additional factors to interaction effects, i.e., of running m 2-level factors in an experimental plan with only 2^{m-k} runs, it is not possible to separately estimate all effects up to the interaction of order m. Instead, the 2^m effects (global mean, factor main effects and all interaction effects up to order m) that would be estimable from a full factorial experiment, fall into 2^{m-k} sets of 2^k effects each that cannot be separately estimated, i.e. are perfectly "aliased" or "confounded" with each other.

The choice of interactions for assigning the generated factors determines the structure of the design, i.e. the aliasing pattern. If specific estimability needs are known prior to experimentation, the design can be tuned such that these can be fulfilled. Usually, one wants to be able to estimate all main effects. In addition, a selection of two-factor interactions (2fis in the sequel) is also often of interest. For example, in a robustness experiment with the purpose to find control factor settings such that the effect of some noise factors is as small as possible, interactions between control and noise factors may be of special interest. In the following, the effects that are required to be estimable will be called the "requirement set". For the aforementioned robustness

experiment, the requirement set would consist of all main effects and the 2fis between control factors and noise factors.

There are two fundamentally different approaches to guaranteeing estimability of the requirement set. In the more widely spread "Distinct" approach, it is assumed that all effects outside the requirement set are negligible, i.e. it is assumed that the nature of the model is known, except for the actual size of effects. This approach is called the "Distinct" approach, because estimability can be guaranteed by ensuring that all effects from the requirement set end up in distinct sets of aliased effects - or, equivalently, on distinct columns of the model matrix (cf. also the following section). The competing "Clear" approach does not require specific assumptions regarding the model underlying the experiment. It assumes negligibility of interactions of degree higher than 2, which is reasonable in many situations, where 2-level fractional factorial plans are used. However, no assumptions are made as to negligibility of any main effects or 2fis. According to this logic, effects from the requirement set may be confounded with interactions of degree three or higher, but must not be confounded with main effects or 2fis, in order to be estimable without bias. It is customary to call all effects "clear" that are neither confounded with main effects nor with 2fis (cf. e.g. Wu and Chen 1992). This is the reason for calling this the "Clear" approach.

The difference between situations calling for the "Clear" or the "Distinct" approach lies in the justification for using a requirement set: for the "Distinct" approach, the requirement set expresses knowledge about which effects are active in the model: all effects outside the requirement set are assumed to be negligible. To the contrary, the requirement set for the "Clear" approach expresses an *interest* in particular effects, but no knowledge regarding which effects are active. Thus, the "Distinct" approach equates the requirement set with the set of (potentially) non-negligible effects, while the "Clear" approach considers all main effects and 2 fis to be (potentially) non-negligible. Note that there is also a way in-between the two approaches: besides effects to be estimable (in the requirement set), it is possible to distinguish the remaining effects (that need not be estimable) into a set of potentially non-neglible effects and a set of effects that are assumed to be negligible. Franklin and Bailey (1977) introduced the distinction of these three types of effect, SAS software (the procedure PROC FACTEX; SAS Institute Inc. 2008) implements it by offering both an ESTIMATE and a NONNEGLIGIBLE option, implying that effects that appear in neither are assumed to be negligible. This intermediate approach is not considered in this article.

This report compares the "Distinct" and the "Clear" approach in some detail. Section 2 introduces terminology and notation for regular 2-level fractional factorial designs and their quality criteria. Section 3 reviews in detail the "Distinct" and the "Clear" approach, as treated in the literature. Section 4 provides various examples that illustrate the performance of the "Clear" approach vs. the "Distinct" approach. The report concludes with some summarizing remarks and recommendations.

2. Regular 2-level fractional factorial designs

This section briefly restates the basics of regular 2-level fractional factorial designs, in order to install a common terminology and notation. As mentioned in the introduction,

the starting point for construction of a regular 2-level fractional factorial design for m factors is a full factorial in 2^{m-k} runs for m-k base 2-level factors. Factor levels are denoted as "-1" and "+1", which conveniently leads to orthogonal columns of the model matrix for the saturated model for the full factorial design in the m-k base factors. This model matrix is shown in Table 1 for an 8 run design. The table shows the matrix in the so-called "Yates order", which is the obvious continuation of the order **1 2 12 3 13 23 123** ..., if **1**, **2**, **3** ... are the m-k base factors of the full factorial. This matrix is called the "Yates matrix" in the following. Orthogonality of each pair of effects is easily verified by checking that the scalar product of the respective model matrix columns is zero.

Table 1 shows the Yates matrix with several title rows: the first two rows represent the base factors in two customary notations, as digits or capital letters. The third row provides the Yates matrix column number, which is used in various modern design catalogues (Chen, Sun and Wu 1993; Block and Mee 2005; Xu 2009). The fourth row contains the binary representation of the column number, which can be used to determine the column effect from the column number: the digit "1" in the binary number in position *i* from the right is a check in the box next to the *i*-th factor; for example, column 6 has the binary representation 110, i.e. the 2^{nd} and 3^{rd} position from the right hold a "1", all other positions are "0"s. Hence, column 6 contains the interaction effect **23** (or **BC**, depending on notation).

	1	2	12	3	13	23	123
	Α	В	AB	С	AC	BC	ABC
col.no.	1	2	3	4	5	6	7
binary	001	010	011	100	101	110	111
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 an 8 run full factorial 2-level design

There are many different ways to assign *k* additional (generated) factors to the columns of a Yates matrix with $2^{m \cdot k}$ rows. For example, one could add a fourth factor D to column ABC in Table 1, or one could add D to column AB instead. In the former case, the main effect of factor D would coincide with the three-factor interaction of factors A, B and C, in the latter case with the 2fi AB. Usually, one would consider aliasing with higher degree interactions to be better than aliasing with lower degree interactions, i.e. one would prefer assigning D to the ABC column. The assignment rule, e.g., D=ABC, is called a generator for the design. The element wise product ABCD is the same as the product of column 7 with itself and thus yields a column of "+1"s. This implies that the four-factor interaction ABCD is aliased with the overall mean. All groups of factors whose products are a column of "+1"s, are called "words" of the design. *k* generators are needed for generating *k* factors to be added to the full factorial in *m*–*k* factors; these imply a total of 2^{k} –1 words (not counting trivial ones like

AA), since each product of two or more words is also a word. The length of the shortest word is called the resolution of the design and is denoted as a roman numeral.

Resolution III designs confound main effects with 2fis, resolution IV designs confound main effects with three-factor interactions or 2fis with each other, and resolution V designs do not confound any main effects or 2fis with each other, etc. As one is often prepared to assume negligibility of interaction effects of order three and higher, resolution V designs are generally considered adequate, if 2fis are to be estimated. However, resolution V designs are often not affordable (at least 16 runs for 5 factors, 32 runs for 6 factors, 64 runs for 7 or 8 factors, 128 runs for 9 to 11 factors, 256 runs for 12 to 17 factors). As an aside, note that there are non-regular fractional factorial plans that allow orthogonal estimation of all main effects and two-factor interactions for up to 15 factors in 128 runs or up to 19 factors in 256 runs (cf., e.g., Mee 2009, Chapter 8.2). These are not covered in this article.

Design	Runs	WLP							No. of Column numbers of	
<i>m-k</i> .no.	2 ^{<i>m-k</i>}	A ₃	A ₄	A ₅	A ₆	A ₇	A ₈	Resolution	clear 2fis	factors <i>m-k</i> +1 to <i>m</i> in Yates matrix*
4-1.1	8	0	1					IV	2110	7
4-1.2	8	1	0							3
6-2.2	16	1	1	1					6	3 13
6-2.3	16	2	0	0	1			III	9	3 12
7-3.1	16	0	7	0				IV	0	7 11 13
7-3.2	16	2	3	2					2	3 5 14
7-2.1	32	0	1	2				IV	15	7 27
9-4.1	32	0	6	8	0	0		IV	8	7 11 19 29
9-4.2	32	0	7	7	0	0		IV	15	7 11 13 30
10-5.1	32	0	10	16	0	0		IV	0	7 11 19 29 30
11-6.1	32	0	25	0	27	0	10	IV	0	7 11 13 19 21 25
10-4.1	64	0	2	8	4	0	1	IV	33	7 27 43 53
10-4.3	64	0	3	7	4	0	0	IV	30	7 11 29 51
12-6.2	64	0	8	20	14	8		IV	27	7 11 21 46 54 56
17-11.6 =	64	0	105	35	280	168		IV	31	7 11 13 14 19 21
17-11.38**										22 25 26 28 63

 Table 2: Base Designs from the CSW (1993) catalogue used in this article

* Column numbers for factors i=1, ..., m-k are 2^{i+1} , i.e. 1, 2, 4, etc.

** The design is called 17-11.6 in the CSW catalogue in the paper, but 17-11.38 in the complete enumeration of 64 run resolution IV designs as obtained from the authors (personal communication with D.X.Sun). Numbering in the paper reflects some trade-off choices by the authors regarding MA and MaxC2 criteria, numbering in the complete listing is strictly in terms of MA.

Substantial research has been conducted in order to list non-isomorphic regular fractional factorials (cf. e.g. Chen, Sun and Wu 1993, Xu 2009), where two designs are considered isomorphic, if they can be obtained from each other by switching rows or columns or levels within columns. The non-isomorphic regular fractional factorials for m factors in $2^{m\cdot k}$ runs are usually denoted as $m\cdot k$.idno with an index number "idno" denoting the different non-isomorphic versions. Designs are ordered from best to worst, i.e. lower "idno" implies better performance on some overall quality criterion, usually the minimum aberration criterion (abbreviated as MA, details cf. below). The designs used

in the examples of this article have been taken from Chen, Sun and Wu (1993; called CSW in the sequel). For the reader's convenience, they are listed in Table 2.

All columns of Table 2 are now briefly explained using the 16 run designs 7-3.1 and 7-3.2 as examples. Design 7-3.1 adds the Yates matrix columns 7 (E=ABC), 11 (F=ABD) and 13 (G=ACD) to the base factors A to D. Herewith, ABCE, ABDF and ACDG are words. As products of words are again words, there is a total of $2^3-1 = 7$ words; the additional four words can be obtained as ABCEABDF=CDEF. ABCEACDG=BDEG, ABDFACDG=BCFG, and ABCEABDFACDG=AEFG. Thus, all seven words have length 4, as shown in the word length pattern (WLP) in Table 2. The resolution of the design is of course IV, the length of the shortest word. Analogously, design 7-3.2 adds the Yates matrix columns 3 (E=AB), 5 (F=AC) and 14 (G=BCD) to the base factors A to D, which yields the words ABE, ACF, BCDG, ABEACF=BCEF, ABEBCDG=ACDEG, ACFBCDG=ABDFG and ABEACFBCDG=DEFG, with two words each of lengths 3 and 5, and three words of length 4. Because of the words of length 3, the design has of course resolution III. Table 2 also indicates the number of clear 2fis. A 2fi is clear, if it is not contained in any word of length less than 5. From the above listings of words, it is easy to see that all pairs of factors occur in a word of length 4 for design 7-3.1, i.e. there are no clear 2fis. For design 7-3.2, the two pairs AD and AG only occur together in words of length 5. Thus, the latter design has two clear 2fis, however at the usually unacceptable price of confounding main effects with 2fis instead. For practical purposes, it is useful and customary to look at the aliasing pattern among low order effects, usually main effects and 2fis, which are direct consequences of the word list. For the resolution IV design 7-3.1, the aliasing pattern for effects up to 2 is AB=CE=DF, AC=BE=DG, AD=BF=CG, AE=BC=FG, AF=BD=EG, order AG=CD=EF and BG=CF=DE, meaning that the model matrix columns coincide for each triple of effects connected by an equality sign. The aliasing pattern for the resolution III design 7-3.2 is A=BE=CF, B=AE, C=AF, E=AB, F=AC, BC=DG=EF, BD=CG, BF=CE, BG=CD, DE=FG, DF=EG.

The above-mentioned minimum aberration (MA) criterion is the most important quality criterion for regular fractional factorial 2-level designs. It ranks designs according to their resolution (the higher the better). Designs of equal resolution are ordered w.r.t. the pertinence of the most severe form of aliasing, measured by the word length pattern (shortest words are considered first; in case of ties the ranking is based on the shortest word length at which the designs differ for the first time). For example, the resolution IV design 9-4.2 is ranked behind the resolution IV design 9-4.1 because it has 7 instead of 6 words of length 4. The logic behind the minimum aberration criterion is that effects of the same degree are equally important, and effects of lower degree are more important than effects of higher degree. The MA criterion has been reported to lead to model-robust designs (Cheng, Steinberg and Sun 1999), i.e. to designs that allow good properties for obtaining useful estimates for a broad range of true models.

A competing overall criterion for resolution IV designs is MaxC2, i.e. maximization of the number of clear 2fis. For small designs, MA and MaxC2 often coincide (cf. also Wu and Wu 2002). For large designs, however, there are various situations for which MaxC2 designs are much worse than MA designs in terms of aberration (cf. e.g. Block

and Mee 2005). The author would argue that MaxC2 as an overall criterion is to be avoided. If certain 2fis are of special interest, one should strive to specifically make *these* clear, but try to do this with a design that has the best possible aberration for the purpose. The reason for this recommendation is the good model robustness of MA designs that was mentioned above.

3. Two alternative approaches for estimable 2fis

3.1. The "Distinct" approach

Under the "Distinct" approach, the suitable and even optimal fractional factorial can theoretically be determined as a D-optimal design for the model specified in the requirement set, provided the desired set of interactions can be accommodated in the specified number of runs which is a power of 2. However, algorithms for D-optimal designs do not always find the global optimum but do in many cases provide a non-orthogonal design that is worse than the D-optimal orthogonal fractional factorial. Thus, it is more satisfactory to implement a special strategy for fractional factorials. Franklin and Bailey (1977) provided an algorithm for constructing the smallest possible fractional factorial design(s) that can accommodate a certain requirement set. The most general form of their algorithm even allows the specification of some further effects outside the requirement set that are not of interest but may be non-negligible; thus, their algorithm would be usable for the "Clear" approach. As this algorithm becomes quite computer-intensive with a large number of factors, Liao and Iyer (1999) proposed a non-exhaustive stochastic alternative.

Taguchi (1988) provided linear graphs that enable the experimenter to allocate design columns so that all effects of interest are estimable, provided all other effects are negligible. Addelman (1962) coined the expression "compromise plans" for designs that have certain patterns of interactions – called classes one, two and three – to be estimable (cf. also Section 3.2). His tables can be seen as special cases of linear graphs. Wu and Chen (1992) criticized usage of Taguchi linear graphs, because they are not a complete listing of all non-isomorphic possible graphs, and their usage does not guarantee "goodness" of the design in terms of usual criteria like aberration. This criticism also applies to Addelman's compromise plans, as he provided maximum plans with no clear instructions on how to proceed if the full spectrum is not needed.

Wu and Chen (1992) proposed a graph-aided procedure for on the one hand accommodating the requirement set such that all effects of interest end up on distinct columns of the Yates matrix, but on the other hand also enforcing some global optimality criterion like minimum aberration. Their procedure starts to search the best (e.g. MA) design for a set of column allocations that permit estimation of all desired effects and sequentially proceeds to try worse designs, if the search is unsuccessful. The search is based on a complete catalogue of Taguchi-style linear graphs for each design. If allocation is impossible within the best design, the algorithm proceeds to the second best design and so forth. Although Wu and Chen mentioned computerized search, they emphasized the advantages of a manual search and did not provide a computer program, but an extensive list of graphs, which are enhanced vs. Taguchi graphs by a different line type for clear interactions. With large designs, the method

becomes infeasible due to the limitations of the human mind in processing complex graphs, and also due to the lack of catalogued non-isomorphic linear graphs.

Dey and Suen (2002) gave a projective geometric approach to constructing distinct designs. While their method has been recognized as being powerful (e.g. Wang 2007), its usage requires a strong theoretical background of the experimenter. Wang (2007) took Wu and Chen (1992) as a starting point and suggested a method that does not rely on graphs, because of the afore-mentioned complexity issues with manual treatment of graphs. Wang's method consists in successive assignment of factors to columns of the Yates matrix, starting with factors having the most interactions and crossing out all columns that are needed for factors that have already been allocated and their interactions from the requirement set. Wang mentioned that the resulting design is usually of resolution III, which already indicates that "goodness" of the design is not guaranteed in any way. If required, the method ensures resolution IV by only using the base factors and columns which are products of an odd number of those (e.g. columns 1,2,4,7,11,13,14 of the Yates matrix in 16 runs). An important issue with Wang's proposal is its inability to incorporate information from catalogues of nonisomorphic designs. For simple cases, this is not consequential, but for complicated situations, even with fast computers, the algorithm will be prohibitively resourceintensive. Recognizing the need of taking special care of more complicated cases, Wang provided special treatment for a few specific situations. However, overall, the proposed method lacks general applicability.

Ke and Tang (2003) criticized the Wu and Chen approach, because it does not at all account for confounding with effects outside the requirement set. They introduced an optimization step into the algorithm proposed by Wu and Chen (1992): Once a potential allocation of the requirement set to a design has been found, the search continues through all graphs for the current base design and chooses the one with "minimum N aberration", a newly introduced criterion. Roughly, N aberration treats 2fis from the requirement set as equally important to main effects (their two letters together are treated as one). If the current base design has the potential to accommodate (i.e., clear) all effects from the requirement set, this design is found by automated application of Ke and Tang's modified approach; thus, Ke and Tang's modification is a step towards the "Clear" approach. However, if a clear design exists, it is not necessarily based on the same base design as the distinct design. Hence, Ke and Tang's approach is mentioned in this section rather than the next.

In terms of software, many products allow creation of distinct designs through general functions for finding D-optimal designs. The resulting design is usually not guaranteed to be perfectly orthogonal. It is therefore desirable to have software that restricts the search to proper orthogonal fractional factorial designs. Among the commercial products known to the author, SAS software offers a procedure (PROC FACTEX) that satisfies this need.

3.2. The "Clear" approach

As mentioned before, the "Distinct" approach assumes that low order effects outside of the requirement set are negligible – in addition to the more realistic requirement that higher order effects are negligible. A clear design allows unbiased estimation of the

effects in the requirement set without making assumptions on negligibility of lower order effects outside the requirement set. Hence, no words of length three can exist, and no 2fis from the requirement set may occur in words of length four. This requirement is much stricter than that of the "Distinct" approach, and consequently often needs more runs than affordable. Nevertheless, there are situations for which a clear design can be found and requires fewer runs than a resolution V design, implying feasibility of very good bias properties for all effects in the requirement set.

The literature on the "Clear" approach is scarce. Wu and Chen (1991, 1992) indicated clear interactions by the line type in their catalogue of linear graphs, but did not attempt to find designs with all effects of interest clear. As outlined above, Ke and Tang (2003), although criticizing that non-negligible low order effects outside the requirement set might bias effects from the requirement set, provided a modification of the "Distinct" approach that does not guarantee that an existing clear design is found.

Ke, Tang and Wu (2005) chose the "Clear" approach, by looking for compromise plans with all 2fis clear, called "clear compromise plans" in the sequel. There are four known classes of compromise plans. For all of them, the *m* experimental factors are decomposed into the two groups G1 and G2. The requirement sets for compromise plans – regardless whether distinct or clear – contain all main effects plus the 2fis in

- (a) Class 1: G1xG1,
- (b) Class 2: G1xG1 and G2xG2,
- (c) Class 3: G1xG1 and G1xG2 or
- (d) Class 4: G1xG2.

For the "Distinct" approach, the first three classes were introduced by Addelman (1962), the fourth by Sun (1993). Ke et al. (2005) proved that there are no clear compromise plans for class 2. For the other three classes, they provided lower bounds for the number of runs for a given number of factors in G1, as well as upper bounds for the number of factors in G1 for a given number of runs. Furthermore, they provided a small catalogue of clear compromise plans in 32 and 64 runs for class 3 that can also be used for classes 1 and 4 and can in some cases be adapted to special needs by moving a factor from group G2 to group G1 or simply omitting factors. Their catalogue plays a similar role in the "Clear" approach as Taguchis linear graphs in the "Distinct" approach. It provides a simple way to obtain a clear design for special situations (compromise plans), but there is no guarantee that it is a good design. Example 1 illustrates this.

Example 1: The requirement set for a 12-factor experiment contains all 2fis among the first three factors, i.e. a class 1 compromise design with the first three factors in G1 is needed. Ke et al. (2005) recommended using their design for 17 factor class 3 compromise plans (design 17-11.6 in 64 runs, G1 contains columns 32 and 63 of the Yates matrix, the other 15 columns are in G2, cf. Table 2), moving one column from G2 over to G1 and omitting five columns from G2. Moving the first G2 column (Yates column 1) to G1 and omitting the last five G2 columns (Yates columns 21, 22, 25, 26, 28) yields a design with 18 words of length four. It has the following aliasing pattern of 2fis: AD=EH=FJ=GM=KL, AE=DH=FK=JL, AF=DJ=EK=HL, AG=DM, AH=DE=FL=JK, AJ=DF=EL=HK, AK=DL=EF=HJ, AL=DK=EJ=FH, AM=DG, EG=HM, EM=GH, FG=JM, FM=GJ, GK=LM, GL=KM. A better design can be found based on design 12-6.2 in the

complete catalogue of 64 run designs, assigning columns 11, 21 and 32 of the Yates matrix to G1, columns 1, 2, 4, 7, 8, 16, 46, 54, 56 to G2 (six words of length four only). It has the following aliased 2fis: AK=LM, AL=KM, DB=EG, DC=FH, DE=FJ=GB, DF=EJ=HC, DG=EB, DH=FC, DJ=EF, EC=HJ, EH=JC, FB=GJ, FG=JB, GA=HM, GH=AM=KL, GK=HL, GL=HK, GM=HA.

The performance improvement found in Example 1 is of practical importance, because the improved design is clear for many 2fis outside the requirement set and also has fewer alias groups of more than two 2fis. (Aliased pairs of 2fis offer a fair chance of resolving aliasing due to the principle of effect hierarchy for many possible experimental outcomes.) The design based on 12-6.2 actually has minimum aberration among all 64 run designs that can accommodate the requirement set. The algorithm for its creation follows a similar logic as the algorithm proposed by Wu and Chen (1992) and guarantees that an existing minimum aberration design is returned, provided some prerequisites are fulfilled; it will be reported elsewhere.

Most commercial software products do not cater for clear designs. Exceptions known to the author are STATISTICA (Statsoft, Inc. 2009) and SAS software (PROC FACTEX again), both of which implement the "Clear" approach. STATISTICA explicitly declares that it is not guaranteed to find all existing designs; for example, STATISTICA did find the clear design for Example 6 but not the one for Example 3 of the following section. SAS software also fails to find the clear design in some cases where it obviously exists (e.g. Examples 3 and 6 of the following section). Details on SAS PROC FACTEX can be found in Appendix 1. The open-source software package FrF2 (Grömping 2010) did create all the clear designs for the examples of the next section and is guaranteed to find clear designs of resolution IV in up to 64 runs using the above-mentioned algorithm. For the reader's convenience, the code for generating all the example designs with this software package is given in Appendix 2. The Franklin and Bailey (1977) algorithm would also be able to find clear designs, if implemented in full generality, as it allows for specification of a nonnegligible set of effects, like SAS software does. However, no implementation of the algorithm with this feature has been found - apparently, SAS software does not use this algorithm, as the Franklin and Bailey article is not among the references in the PROC FACTEX documentation.

4. Examples

The following examples compare performance of the "Clear" and the "Distinct" approach. They have been selected with a view to covering all interesting situations at least once. Table 3 summarizes the example situations. In addition, detailed descriptions are provided for each example. In these, the experimental factors are denoted by capital letters (skipping the letter "I", which is often used for denoting a column of "+1"s), while the design factors are denoted by consecutive numbers which are not to be confused with Yates matrix column numbers. For each design of resolution III or IV, the aliasing pattern among main effects and 2fis is given (all designs are resolution IV, except for Example 6, i.e. main effects are usually not involved in the aliasing patterns). For distinct designs, the effects from the requirement set are set in bold face; for clear designs, the effects from the requirement set do of course not occur within the aliasing pattern.

Example	no. of factors	requirement set		run size	base design*
2	11	all 2fis	resolution V	128	11-4.1
		among factors	clear	128	11-4.1
		A to F	distinct	32	11-6.1
3	10	all 2fis	resolution V	128	10-3.1
		among factors	clear	64	10-4.3
		A to E	distinct	32	10-5.1
4	6	AB, AF, BC,	resolution V	32	6-1.1
resolution III		CD, CF, DE	clear	16	6-2.3
permitted		and EF	distinct	16	6-2.2
resolution III		CD, CF, DE	clear	32	6-1.1
not permitted		and EF	distinct	32	6-1.1
5	10	all 2fis with	resolution V	128	10-3.1
		factors J and K	clear	64	10-4.1
			distinct	64	10-4.1
6	9	all 2fis with	resolution V	128	9-2.1
		factors H and J	clear	32	9-4.2
			distinct	32	9-4.1
7	7	all 2fis among	resolution V	64	7-1.1
		A,B,C & all 2fis	clear	64	7-1.1
		among D to G	distinct	32	7-2.1

Table 3: Overview of the example situations.

*For all resolution V designs, the base designs are the MA designs in the respective number of runs. They are not listed in Table 2.

Table 3 shows that clear and distinct designs sometimes coincide (Example 5), sometimes can be obtained in the same number of runs but based on different base designs (Example 4 with resolution III permitted, Example 6), that at other times the clear design requires resolution V (Examples 2 and 7; both clear and distinct design also need resolution V in Example 4, if resolution III is not permitted), and at yet other times the run size of a clear design is a compromise between the run sizes of a distinct design and a resolution V design (Example 3).

Example 2: Wu and Chen (1992) applied the "Distinct" approach to an experiment with 11 factors (their Example 1). The requirement set contains all pairwise interactions among the six factors A to F (i.e. a class 1 compromise plan situation). They obtained a resolution IV 32 run design that assigns all effects from the requirement set to different columns of the model matrix. An isomorphic version based on 11-6.1 can be obtained by choosing Yates matrix columns 1, 2, 4, 11, 21 and 25 for factors A to F and Yates matrix columns 8, 16, 7, 13 and 19 for the remaining 5 factors. It has the following aliased 2fis: **AB**=CJ=GD=HL, **AC**=BJ=GK=HE, **AD**=BG=JK=LF, **AE**=CH=JL=KF, **AF**=GH=DL=KE, AG=**BD**=CK=HF, AH=BL=**CE**=GF, AJ=**BC**=DK=LE, AK=CG=JD=**EF**, AL=BH=JE=**DF**, **BE**=CL=HJ, **BF**=GL=HD, BK=**CD**=GJ, **CF**=GE=HK, JF=**DE**=KL. A

resolution IV clear design does not exist, i.e. the "Clear" approach requires using the resolution V design in 128 runs.

Example 3: Consider a situation similar to the previous example, but with only 10 factors, for which all 2fis among the five factors A to E constitute the requirement set. The "Distinct" approach accommodates this situation in the resolution IV 32 run minimum aberration design 10-5.1, assigning the five interacting factors to Yates matrix columns 1, 2, 4, 8, 16, i.e. to the first five design factors. Its alias pattern for 2fis is as follows: **AB**=CF=DG=EH=JK, **AC**=BF, **AD**=BG, **AE**=BH, AF=**BC**, AG=**BD**, AH=**BE**, AJ=BK, AK=BJ, **CD**=FG, **CE**=FH, CG=DF, CH=EF, CJ=FK, CK=FJ, **DE**=GH, DH=EG, DJ=GK, DK=GJ, EJ=HK, EK=HJ. The resolution IV clear design has 64 runs using the design 10-4.3 from Table 2, assigning the five factors with 2fis to be estimable to Yates matrix columns 1, 16, 32, 29 and 51. (This design can also be obtained using Table 2 from Ke et al. 2005.) This larger design has the following alias pattern for 2fis: AF=GJ=HK, AG=FJ, AH=FK, AJ=FG, AK=FH, GH=JK, GK=HJ. A resolution V design would require 128 runs.

Example 4: Wu and Chen (their Example 2) considered 6 factors with the 2fis AB, AF, BC, CD, CF, DE and EF in the requirement set. The distinct design is based on the 16 run resolution III base design 6-2.2 (of course, main effects are aliased with 2fis outside the requirement set only), with factors A to F assigned to Yates matrix columns 1, 4, 2, 8, 3, 13. The design has the following aliasing pattern of main effects and 2fis (effects from the requirement set in bold face): **A**=CE **C**=AE **E**=AC, **AB**=DF AD=BF **AF**=BD. If resolution III is permitted, the resolution III clear design also needs 16 runs; however, it cannot be based on design 6-2.2, but on 6-2.3, which has more severe aliasing of main effects with 2fis from outside the requirement set: **A**=CE **B**=DF **C**=AE **D**=BF **E**=AC **F**=BD (allocation of factors A to F to Yates matrix columns 1, 4, 2, 8, 3, 12). Normally, the logic of the "Clear" approach would preclude usage of resolution III designs so that one would again have to resort to the resolution V design in 32 runs for the "Clear" approach for this example.

Example 5: Now, 10 factors are investigated, and all 2fis with factors J and K (and anything else) are in the requirement set, i.e. a compromise plan of class 3 is sought. A resolution IV clear design can be achieved in 64 runs, and the minimum aberration design 10-4.1 will accommodate these by allocating the last two factors to its factors 4 and 10 (Yates matrix columns 8 and 53). The aliasing pattern of 2fis in this design is given as AB=CF, AC=BF, AF=BC, DE=GH, DG=EH, DH=EG. The "Distinct" approach yields the same resolution IV design here, provided that the Ke and Tang optimization or a human brain make sure that the chance to obtain a clear design is recognized – a purely automatic search for a design with distinct columns for each effect in the requirement set is not guaranteed to exploit this opportunity. In this example, permission of a resolution III design does not reduce the number of runs needed, neither for the "Clear" nor for the "Distinct" approach. Also note that Table 2 of Ke et al. 2005 would suggest using design 10-4.3, which is worse in terms of aberration (three instead of two words of length three).

Example 6: If 9 factors are investigated, a clear design for the situation analogous to Example 5 – having all interactions with factors H and J in the requirement set – can be accommodated in 32 runs using the resolution IV design 9-4.2, assigning factors H

and J to its factors 5 and 9 (= Yates matrix columns 16 and 30; also provided in Table 2 of Ke et al. 2005). The resulting aliasing pattern among 2fis is AB=CE=DF AC=BE=DG AD=BF=CG AE=BC=FG AF=BD=EG AG=CD=EF BG=CF=DE. The "Distinct" approach would instead use the MA design 9-4.1 in natural factor order. It thus would confound some 2fis from the requirement set with 2fis outside the requirement set, with the benefit of better overall aberration. The aliasing pattern for this design would be AB=CF=DG=EH, AC=BF, AD=BG, AE=BH, AF=BC, AG=BD, AH=BE, CD=FG, CE=FH, CG=DF, CH=EF, DE=GH, DH=EG.

Example 7: Finally, 7 factors are considered, and all 2fis of the first three factors with each other and of the last four factors with each other make up the requirement set, i.e. a compromise plan of class 2 is sought. The distinct design requires 32 runs and can be conducted using the MA design in the default factor order; the aliasing pattern among 2fis is **AB**=CF, **AC**=BF, AF=**BC**. Although the number of required 2fis is lower than in Example 6, a clear design in resolution IV does not exist for this scenario according to the proof by Ke et al. (2005, Corollary 1), as this is a class 2 compromise plan. Thus, the "Clear" approach requires using the resolution V design in 64 runs.

5. Final Remarks

Both the "Distinct" approach and the "Clear" approach are methods for ensuring estimability of some 2fis if a resolution V design is not feasible. They try to accommodate effects of a prespecified requirement set such that they are on distinct columns of the model matrix or such that they are clear of aliasing with any main effects or 2fis. The "Distinct" approach runs the risk of biasing the effects in the requirement set, if low order effects outside the requirement set are non-negligible. The "Clear" approach avoids this risk (provided resolution III is not permitted), but pays the clearness of requirement set. The examples have illustrated the obvious fact that the clear design needs at least as many runs as the distinct design and at most as many runs as a resolution V design, i.e. it can be regarded as a compromise between the two. Clear designs identical or identical in run number to the distinct design do occur in practice, and situations for which there is no clear design smaller than the resolution V design are also common.

If there is a convincing reason to formulate a requirement set, the author recommends a resolution IV clear design over a distinct design whenever possible. Otherwise, the more severe aliasing among effects outside the requirement set that is a consequence of keeping effects clear is seen as a disadvantage of the clear design. Thus, in situations for which there is no natural requirement set, one should rather use the more model-robust distinct design, of course basing it on the best possible design in terms of the MA criterion.

References

Addelman, S. (1962). Symmetrical and asymmetrical fractional factorial plans. *Technometrics* 4, 47-58.
Block, R.M. and Mee, R.W. (2005). Resolution IV designs with 128 runs. *J. Quality Technology* 37, 282-293. With corrigendum 2006, *J. Quality Technology* 38, 196.

- Chen, J., Sun, D.X. and Wu, C.F.J. (1993). A catalogue of 2-level and 3-level orthogonal arrays. *International Statistical Review* **61**, 131-145.
- Cheng,C.-S. Steinberg, D.M. and Sun, D.X. (1999). Minimum aberration and model robustness for twolevel fractional factorial designs. *J. Roy. Statist. Soc.* **B 61** 85-93.
- Dey, A. and Suen, C.-Y. (2002). Optimal fractional factorial plans for main effects and specified two-factor interactions: a projective geometric approach. *Annals of Statistics* 30, 1512-1523.
- Franklin, M.F. and Bailey, R.A. (1977). Selection of defining contrasts and confounded effects in two-level experiments. *Applied Statistics* **26**, 321-326.
- Grömping, U. (2010). FrF2: Package for analysing Fractional Factorial designs with 2-level factors. R package version 1.1-1 (<u>http://cran.r-project.org/web/packages/FrF2/index.html</u>). In R Development Core Team (2010). *R: A language and environment for Statistical computing*. R Foundation for Statistical Computing, Vienna, Austria.
- Ke, W. and Tang, B. (2003). Selecting 2^{m-p} Designs Using a Minimum Aberration Criterion When Some Two-Factor Interactions Are Important. *Technometrics* 45, 352-360.
- Ke, W., Tang, B. and Wu, H. (2005). Compromise plans with clear two-factor interactions. *Statistica Sinica* 15, 709-715.
- Liao, C.T. and Iyer, H.K. (1999). A Stochastic Algorithm for Selecting of Defining Contrasts in Two-Level Experiments. *Biometrical Journal* **41**, 671-678.
- Mee, R.W. (2009). A comprehensive guide to factorial two-level experimentation. Springer, Berlin.
- R Development Core Team (2010). R: A language and environment for Statistical computing. R Foundation for Statistical Computing, Vienna, Austria. (<u>http://www.R-project.org</u>)
- SAS Institute, Inc. (2008). SAS/QC® 9.2 User's Guide. Cary, NC: SAS Institute Inc.
- StatSoft, Inc. (2009). STATISTICA (data analysis software system), version 9.0. [Computer software]. (<u>www.statsoft.com</u>)
- Sun, D.X. (1993). Estimation capacity and related topics in experimental designs. Ph.D. Dissertation, University of Waterloo, Waterloo.
- Taguchi, G. (1988). *Systems of experimental design* (2 volumes, editor for english edition, Don Clausing). Quality Resources & American Supplier Institute, Dearborn, Michigan.
- Wang, P.C. (2007). Planning experiments when some specified interactions are investigated. *Computational Statistics and Data Analysis* **51**, 4143-4151.
- Wu, C.F.J., Chen, Y. (1992). A graph-aided method for planning two-level experiments when certain interactions are important. *Technometrics* 34, 162–175.
- Wu, H. and Wu, C.F.J. (2002). Clear two-factor interactions and minimum aberration. Annals of Statistics 30, 1496-1511.
- Xu, H. (2009). Algorithmic Construction of Efficient Fractional Factorial Designs With Large Run Sizes. *Technometrics* 51, 262–277.

Appendix 1

SAS software (SAS/QC®, PROC FACTEX) accommodates both the "Clear" and the "Distinct" approach and even an approach inbetween: within the MODEL statement, an ESTIMATE option allows specification of the effects of interest, while the option NONNEGLIGIBLE allows the specification of further effects that are not of interest themselves but are suspected to be active and must not confound the effects of interest. The "Distinct" approach is implemented by specifying only the ESTIMATE option, the "Clear" approach is implemented by specifying all 2fis that are not of interest in the NONNEGLIGIBLE option, and anything inbetween is possible. For the commercial software SAS, the algorithm is not publicly available.

The following example shows the syntax for requesting the smallest design that accommodates the requirements of Example 6 of the Examples section:

For this example, SAS does not find the smallest possible design in 32 runs (cf. Example 6) but returns a design in 64 runs instead. SAS also fails to find the smallest clear design for Example 3 but does find the smallest clear design for Example 5.

Appendix 2

The **R** package **FrF2** (Grömping 2010) is a freely available open source software published in the programming environment **R** (R development core team 2010), which accommodates both the "Clear" and the "Distinct" approach, but does not allow separate specification of a nonnegligible set of effects. **FrF2** finds the 32 run design for Example 6 (which SAS did not find, cf. previous appendix), and is generally guaranteed to find the smallest possible resolution IV design in up to 64 runs. When permitting resolution III designs, this guarantee holds for up to 32 runs only.

All code in this appendix requires **R** package **FrF2** to be installed and loaded. The following brief code creates the clear design for Example 6 of Section 4 and can be compared to the SAS code of the previous appendix:

The code below generates all example designs of this report, with suffix D for the "Distinct" approach, suffic "C" for the "Clear" approach. Wherever possible, the syntax uses function compromise for compromise plans. This function generates the requirement set and – for distinct designs – the helpful matrix perms.full that can be used in the perms option of function FrF2 for limiting the search time needed by the algorithm for the "Distinct" approach.

```
## function that extracts design and Yates column information from
## automatically-generated designs with estimability requirements
Yates.cols <- function(design){</pre>
    des <- names(design.info(design)$map)</pre>
    k <- eval(parse(text=strsplit(des,".",fixed=TRUE)[[1]][1]))</pre>
    aus <- list(des=c(2^(0:(k-1)),</pre>
                catlg[des][[1]]$gen)[design.info(design)$map[[1]]])
    names(aus) <- des</pre>
    aus
}
## Example 1
## Design automatically created by FrF2
Ex1 <- FrF2(estimable=formula("~(A+B+C)^2"), nfactors=12, nruns=64,
              clear=TRUE)
Yates.cols(Ex1)
summary(Ex1)
## Ke et al. version, based on 17-6.1
Ex1.worse <-
FrF2(factor.names=c("A","D","E","F","G","B","C","H","J","K","L","M"),
       gen=c(63, 7, 11, 13, 14, 19), nruns=64)
## Yates.cols does not work on this design,
##
        only on automatically-generated ones
## use aliases function instead of summary,
## because summary would confuse by using the capital letters
##
       A to M in order of appearance,
##
       with A the code for "A", B the code for "D", C the code for "E"
##
       and so forth
aliases(lm(rnorm(64)~(.)^2,Ex1.worse))
## Example 2
## distinct design, usage of perms option makes run times manageable
comp <- compromise(11, 1:6, class=1, msg=FALSE)</pre>
Ex2.D <- FrF2(estimable=comp$requirement, nfactors=11,</pre>
    perms=comp$perms.full, clear=FALSE)
 Yates.cols(Ex2.D)
 summary(Ex2.D, brief=TRUE)
```

```
## clear design
## nruns=128, because the automatic run size 32 and nruns=64
##
              do not yield a clear design
Ex2.C <- FrF2(estimable=comp$requirement, nruns=128,</pre>
            nfactors=11, clear=TRUE)
 summary(Ex2.C)
## Example 3
## distinct design, usage of perms option makes run times manageable
comp <- compromise(10, 1:5, class=1, msg=FALSE)</pre>
Ex3.D <- FrF2(estimable=comp$requirement, nfactors=10,
   perms=comp$perms.full, clear=FALSE)
 Yates.cols(Ex3.D)
 summary(Ex3.D, brief=TRUE)
## clear design
## nruns=64, because the automatic run size 32
##
             does not yield a clear design
Ex3.C <- FrF2(estimable=comp$requirement, nfactors=10, nruns=64,
              clear=TRUE)
 Yates.cols(Ex3.C)
 summary(Ex3.C)
## Example 4
## distinct design
## only possible in resolution III
Ex4.D <-
FrF2(estimable=formula("~(A+B+C+D+E+F)+A:B+A:F+B:C+C:D+C:F+D:E+E:F"),
   nfactors=6, res3=TRUE, clear=FALSE)
 Yates.cols(Ex4.D)
 summary(Ex4.D, brief=TRUE)
## clear design
## only possible in resolution III
Ex4.C < -
FrF2(estimable=formula("~(A+B+C+D+E+F)+A:B+A:F+B:C+C:D+C:F+D:E+E:F"),
    nfactors=6, res3=TRUE, clear=TRUE)
 Yates.cols(Ex4.C)
 summary(Ex4.C, brief=TRUE)
## next larger design is of resolution V
summary(
FrF2(estimable=formula("~(A+B+C+D+E+F)+A:B+A:F+B:C+C:D+C:F+D:E+E:F"),
   nfactors=6, nruns=32, clear=TRUE) )
```

```
## Example 5
## distinct design, usage of perms option makes run times manageable
## nruns=64, because the automatic run size 32
##
             does not yield a distinct design
##
             (would not even when permitting resolution III)
comp <- compromise(10, 9:10, class=3, msg=FALSE)</pre>
Ex5.D <- FrF2(estimable=comp$requirement, nfactors=10, nruns=64,</pre>
    perms=comp$perms.full,clear=FALSE)
 Yates.cols(Ex5.D)
 summary(Ex5.D)
## clear design
## nruns=64, because the automatic run size 32
             does not yield a distinct design
##
Ex5.C <- FrF2(estimable=comp$requirement,</pre>
    nfactors=10, nruns=64, clear=TRUE)
 Yates.cols(Ex5.C)
 summary(Ex5.C)
## Example 6
## distinct design, usage of perms option makes run times manageable
comp <- compromise(9, 8:9, class=3, msg=FALSE)</pre>
Ex6.D <- FrF2(estimable=comp$requirement, nfactors=9,</pre>
    perms=comp$perms.full,clear=FALSE)
 Yates.cols(Ex6.D)
 summary(Ex6.D, brief=TRUE)
## clear design
Ex6.C <- FrF2(estimable=comp$requirement, nfactors=9, clear=TRUE)</pre>
 Yates.cols(Ex6.C)
 summary(Ex6.C, brief=TRUE)
## Example 7
## distinct design, usage of perms option makes run times manageable
comp <- compromise(7, 1:3, class=2, msg=FALSE)</pre>
Ex7.D <- FrF2(estimable=comp$requirement, nfactors=7, nruns=32,
   perms=comp$perms.full,clear=FALSE)
 Yates.cols(Ex7.D)
 summary(Ex7.D)
## clear design
## the following call yields an error,
## as a resolution IV clear design is not possible here
Ex7.C <- FrF2(estimable=comp$requirement, nfactors=7, nruns=32,
   clear=TRUE)
```