A Note on Dominating Fractional Factorial Two-Level Designs With Clear Two-Factor Interactions

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Abstract

This note builds on results from Wu, Mee and Tang‘s (2012) article (henceforth WMT) on admissible fractional factorial two-level designs, specifically concentrating on the “dominating designs” that have been introduced but not further pursued in WMT. WMT’s work has been used for increasing the efficiency of the author’s graph-based algorithm for creation of minimum aberration designs that keep a requirement set of two-factor interactions clear (Grömping 2012, implemented in free open source software): That algorithm originally searched aberration-sorted complete catalogues of non-isomorphic resolution IV designs; according to WMT’s proposal, it suffices to search the dominating designs. For implementing this reduction of search space, aberration-sorted catalogues of dominating resolution IV regular fractional factorial two-level designs with up to 128 runs were created; this was achieved with the help of a recent subgraph isomorphism algorithm (Solnon 2010) that proved to be particularly efficient for this search task. The supplementary material provides the code used for identifying the dominating designs and ASCII files with the design generators for all resolution IV and higher dominating designs in 64 and 128 runs.

1. INTRODUCTION

This note serves the purpose of improving an algorithm for creating a minimum aberration (MA) design that can estimate a pre-specified requirement set of two-factor interactions (2fis) clear of aliasing with any main effects or other 2fis (short: MA clear design): an existing algorithm by Grömping (2012) has been improved by incorporating recent results from Wu, Mee and Tang (2012; henceforth WMT). Specifically, catalogues of dominating designs in the sense of WMT (2012) have been created, and the search space of the algorithm has been restricted to these dominating designs. Based on WMT's results, this more efficient version of the algorithm is still guaranteed to yield the MA clear design, if one exists.

In the following, basic terminology regarding fractional factorial two-level designs (like resolution, aberration or word length) is assumed known; if needed, explanations can be found in WMT or, e.g., in Mee (2009). WMT considered creation of resolution IV fractional factorial two-level designs for situations where main effects and certain two-factor interactions (2fis) are requested to be estimable clear of potentially active further 2fis, while interactions of more than two factors are assumed to be negligible. The 2fis to be estimable clearly are called the requirement set. In this note, designs that keep a requirement set of 2fis clear are called "clear designs"; so-called "clear compromise plans" (cf. e.g. Ke, Tang and Wu 2005) refer to clear designs for which the requirement set has a specific form: the experimental factors are divided into two groups G1 and G2, and the requirement set consists of all 2fis within G1 and between G1 and G2 (class 3, G1xG1 and G1xG2) or of G1xG1 only (class 1) or of G1xG2 only (class 4). The need for clear compromise plans may, e.g., arise in robustness studies, for which interactions between control and noise factors are of particular interest. Ke et al. (2005) proved that resolution IV class 2 (G1xG1 and G2xG2) clear designs do not exist.

2. ADMISSIBLE AND DOMINATING DESIGNS

WMT introduced the notions of admissibility and dominance for resolution IV regular fractional factorial two-level designs, using graphs that represent the factors as vertices and each clear 2fi as an edge between the respective vertices. Grömping (2012) refers to these same graphs as "clear interactions graphs" (CIGs) to distinguish them from the more widely known linear graphs usually attributed to Genichi Taguchi. Two definitions and one result of WMT are briefly re-stated here for further reference: A design d is *inadmissible* if its CIG is isomorphic to a proper subgraph of any other design's CIG, i.e. to a graph contained in the other design's CIG and missing at least one edge. A design is *dominating* if no other design dominates it, where a design d_2 dominates a design d_1, if (a) d_2 has *less* aberration than d_1 and the CIG of d_1 is a subgraph of the CIG of d_2 or (b) both designs have the same aberration and the CIG of d_1 is a *proper* subgraph of the CIG of d_2. An even design d_e (i.e., a design d_e with only even length words) can neither be admissible nor dominating, as there is always an even/odd design with less aberration the CIG of which includes the CIG of d_e as a subgraph (cf. WMT's Lemma 2; the proof works for all designs that have zero words of length 5). Note that admissible designs can be dominated: for example, the 128 run 16-factor designs with generator columns 7 120 11 19 25 28 45 77 110 or 7 120 11 19 25 26 45 77 118 have isomorphic CIGs and are both admissible; the former has 17 words of length 4 (isomorphic to 16-9.1413 of Xu 2009), the latter 19 (isomorphic to 16-9.2469 of Xu 2009); thus, the former dominates the latter.

If no assumptions on the nature of the linear model for the response are made, it is best to use the MA design, because it is model-robust (cf. Cheng, Steinberg and Sun 1999); this was also stated by WMT. The wish to keep a requirement set clear comes from a specific interest in particular 2fis. It is desirable to strive for designs that have MA among the clear designs, i.e. for MA clear designs, in order to maximize model robustness for the 2fis outside of the requirement set.

WMT mainly focused on admissible designs: They provided lists of all admissible designs for up to 128 runs ordered by number of clear 2fis, and proposed to construct clear designs by searching the admissible designs for an appropriate one that can accommodate the requirement set clearly. As was also noted by WMT, a search of the admissible designs cannot guarantee that an MA clear design is created. WMT outlined plans for creation of a software that can create MA clear designs along two possible lines: EITHER search the admissible designs first and then check for existence of a design with less aberration in a second step (called two-stage approach below), OR search dominating designs. WMTs proposal based on dominating designs has far more appeal to me than the two-stage approach; this view will be justified later.

3. AN ALGORITHM FOR CREATING MA CLEAR DESIGNS

The free open-source R package FrF2 (Grömping 2013a) already creates MA clear designs: it uses a CIG-based algorithm described in Grömping (2012), which searches all non-isomorphic regular fractional factorial two-level designs, ordered by aberration from best to worst, using the subgraph isomorphism algorithm by Cordella at al. (2001) as implemented in R package igraph (Csardi and Nepusz 2006). Of course, a search of such a sorted catalogue from beginning to end ensures finding the MA clear design, if a clear design exists. (The idea parallels that of Wu and Chen (1992), who advocated an informal graph-based algorithm for finding designs that keep a requirement set estimable under the assumption that all 2fis outside the requirement set are negligible based on the usual linear graphs instead of the CIGs.) Grömping's (2012) approach is feasible, because the unique CIG for each design can be stored within the design catalogues to be searched. Catalogues for R package FrF2 have been taken from Chen, Sun and Wu 1993 (up to 32 runs), a personal communication with Don Sun (64 runs) and Xu 2009 (128 runs). For up to 64 runs, these have the same generators as those given in WMT; the catalogue by Xu uses different (isomorphic) generators. The search for the MA clear design is then a search for the first design CIG that contains the requirement set CIG as a subgraph. Pre-filtering by simple criteria – too few edges in the design's CIG as compared to the requirement set CIG, or not enough vertices with high enough degrees (degree of a vertex=number of edges connected to the vertex) – drastically reduces search time by excluding many designs before actual subgraph isomorphism checks have to be run. As a proof of concept for the algorithm, and of value in itself, Grömping (2012) provided a catalogue of smallest MA clear compromise plans, which is complete for up to 128 runs and 24 factors and contains some additional 256 run clear compromise plans. For some situations, the smallest MA clear compromise plans coincide with plans given in Ke, Tang and Wu (2005), for others they have better aberration.

4. REDUCTION OF THE SEARCH SPACE TO DOMINATING DESIGNS

The algorithm of Grömping (2012) benefits from WMT's results, because the search space can be reduced from all non-isomorphic resolution IV designs to a much smaller subset. Where dominating designs have been determined (see next paragraph and Table 1), these can be used. Even without a catalogue of dominating designs, elimination of the even designs – which cannot be MA clear designs according to WMT – drastically reduces the search space. Some of these improvements have already been implemented in R packages FrF2 (Grömping 2013a) and FrF2.catlg128 (Grömping 2013b, which separately provides 128 run catalogues because of their size); especially in the latter case, this decrease in catalogue size was very useful, because it helps avoid R performance problems.

4.1 IDENTIFICATION OF THE DOMINATING DESIGNS

The search for dominating designs conducted for this note proceeded as follows: for each number of runs and factors, the complete catalogue of non-isomorphic even/odd resolution IV designs – sorted by the MA criterion with arbitrary order in case of ties – was searched from beginning to end; each later design was

Table 1: Numbers of even/odd designs, dominating designs and admissible graphs

	64 runs					128 runs				
factors	$N_{e/o}$	N_{dom}	$N_{adm.graph}$	r_{dom}	r_{adm}	$N_{e/o}$	N_{dom}	$N_{adm.graph}$	r_{dom}	r_{adm}
12	22	10	9	1	1	179	1	1	1	1
13	24	9	6	1	2	486	3	3	1	1
14	20	8	5	1	2	1.239	15	15	1	1
15	15	7	4	3	5	2.926	123	99	1	1
16	11	5	1	2	45	6.208	623	584	1	1
17	10	3	1	2	38	11.787	2.060	1.835	1	1
18						19.466	4.062	3.295	1	2
19						27.994	5.762	4.355	1	2
20						35.192	5.853	3.808	1	2
21						39.201	4.277	2.310	1	2
22						38.847	2.704	1.240	1	8
23						34.868	1.533	582	1	29
24						28.133	788	281	2	61
25						20.569	408	121	4	918
26						13.498	212	77	2	1.063
27						8.075	139	55	7	9
28						4.284	82	26	18	1.157
29						2.149	48	9	63	1.588
30						976	26	5	44	955
31						433	17	4	37	104
32						197	10	1	25	197
33						101	7	1	14	101

N count; e/o: even/odd designs; dom: dominating designs; adm.graph: admissible graphs
r: rank in terms of overall MA for the best dominating (r_{dom}) or the best admissible (r_{adm}) design
Note: for up to 25 factors, the rank is confirmed to refer to overall MA (subject to arbitrary sorting in case of ties in the WLP); for 26 and more factors, the even designs were not considered; it seems likely (but has not been checked) that there are no even designs among the first few thousand MA designs.

added to the dominating designs if its CIG could not be accommodated in an earlier dominating design's CIG. Thus, in case of several designs with structurally identical CIGs and the same WLP, only one of these has entered the dominating designs, even though all of them fulfill the WMT definition. In the same spirit, the admissible designs have been reduced to the admissible graphs, each of which is represented by the MA design with this graph, with arbitrary allocation in case of identical WLPs. Of course, all MA designs with admissible CIGs are among the dominating designs. Table 1 shows that there are many inadmissible dominating designs, especially in case of many factors; for example, for 25 factors in 128 runs, there are 121 admissible graphs, and 287 additional dominating designs. WMT already mentioned that overall MA designs are admissible for up to 12 factors in 64 runs and up to 17 factors in 128 runs, which is reflected in the r_{adm} columns of Table 1. The table reveals that, with many factors, the MA admissible design usually has much worse aberration than the MA dominating design, and that the proportion of inadmissible dominating designs is higher than two thirds in many cases for large numbers of factors.

4.2 BENEFIT FROM USING DOMINATING INSTEAD OF ADMISSIBLE DESIGNS

From WMT (last paragraph of Section 3), one might gain the impression that the advantage of considering inadmissible dominating designs in addition to admissible designs is relevant for small requirement sets only. The large requirement set (A,B,C,D,E,F) x (G,H,J,K,L,M,N,O,P) for a 15 factor experiment in 128 runs is a counter example against that impression: Figure 1 shows the CIGs of the MA dominating design 15-8.78 and the MA admissible design 15-8.1221 that accommodate this requirement set. The inadmissible design 15-8.78 (left-hand side CIG) has 9 words of length 4 and assigns experimental factors A,B,C,D,E,F to design columns 1, 5, 6, 8, 11, 14; with only two exceptions (one triple, one quadruple), the 2fis outside of the requirement set are aliased at most in pairs. The best admissible design 15-8.1221 (right-hand side CIG) has 14 words of length 4 and assigns A,B,C,D,E,F to any six of 1, 2, 5, 7, 8, 9, 10, which implies much more severe aliasing among some of the remaining 2fis (28 2fis are aliased in seven quadruples). Thus, the inadmissible dominating design 15-8.78 is notably better than design 15-8.1221 in terms of model robustness.

15–8.78: 31,103,43,49,78,45,62,105 **15–8.1221: 31,103,43,85,44,89,113,125**

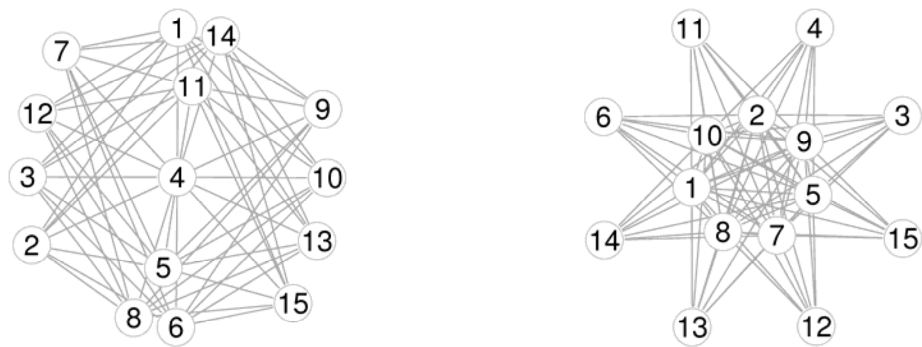

Figure 1: CIGs for two 128 run designs with 15 factors that accommodate the requirement set (A,B,C,D,E,F)x(G,H,J,K,L,M,N,O,P)
Left-hand side: Inadmissible dominating design d_1=15-8.78 with $W_4(d_1)$=9, C=62,
clear 2fis in WMT notation *(4);(1,5,6,8,11,14)x(2,3,7,9,10,12,13,15).
Right-hand side: Best admissible design d_2=15-8.1221, $W_4(d_2)$=14, C=77,
clear 2fis in WMT notation *(1,2,5,7,8,9,10).

In spite of all of the pre-filtering, subgraph isomorphism search remains an NP-hard problem. Even when only searching for an appropriate isomorphism mapping within the successful design, search time can be excessive. For example, Grömping (2012) reported an instance, where an individual search was aborted unsuccessfully after more than 48 hours. The two-stage approach proposed in WMT reduces the number of searches to be conducted for cases where a clear design does not exist (for these, stage 1 is sufficient). For all other cases, except where the admissible design identified in stage 1 is also the first design to be searched in stage 2, a direct approach using only stage 2 of the two-stage approach (based on an aberration-sorted catalogue of all even/odd or ideally all dominating designs) is preferable, because it avoids the extra subgraph isomorphism searches introduced by stage 1.

4.3 SUBGRAPH ISOMORPHISM ALGORITHM SEARCH FOR CIGS

The search for the dominating designs inspired improvements to the subgraph isomorphism search approach proposed in Grömping's (2012): As reported there, the performance of the Cordella et al. (2001)

VF2 algorithm may strongly depend on factor order. Pre-sorting of graph vertices w.r.t. their degree (high degrees first both in experiment CIG and candidate design CIG) was found to substantially improve search speed for some situations. However, even with pre-sorted vertices, there were instances for which the VF2 algorithm took a very long time for ruling out or confirming subgraph isomorphism; especially the 128 runs/21 factors search contained very tough cases. The relatively new LAD algorithm (Solnon 2010) turned out to be much faster than VF2 for such cases, and reasonably fast in general: after initial efforts of identifying the dominating designs with the VF2 algorithm (success for all but 19 to 21 factors in 128 runs within a few weeks, no success for 21 factors in 128 runs even after two months), this work was repeated from scratch with the LAD algorithm and was accomplished within a few days even for the 21 factors case. Thus, the LAD algorithm appears to be much more suitable than the VF2 algorithm for subgraph isomorphism searches within design CIGs.

Following Wu and Chen (1992), Grömping (2012) suggested attempting manual evaluations of CIGs, where a computer search fails for resource reasons. Such an approach has been successful for some 256 run clear compromise plans and is supported by the graphing function `CIG` within R package FrF2 that can create interactive (movable vertices) visualizations of the CIGs. Nevertheless, in many practically relevant cases, the automated search algorithm implemented in R package FrF2 will also find MA clear designs reasonably quickly without user intervention, even though the improvements outlined above have not all been implemented there.

5 FINAL REMARKS

I would like to encourage readers interested in clear designs to check out the R package FrF2 which aims to be state-of-the-art for fractional factorial two-level designs in general, and particularly for clear designs. For users who want to avoid command line programming, the functionality can also be accessed, although with reduced scope, by a free open source graphical user interface (R-package RcmdrPlugin.DoE, Grömping 2011 and 2013c). Feedback and suggestions for the software are very welcome.

SUPPLEMENTARY MATERIALS

Dominating designs in 64 and 128 runs: A zip-archive contains Table 1 (pdf-file), text files with the generators for the 64-run and 128-run resolution IV dominating designs, two files with R programs that were used in the search for the dominating designs, and a pdf-file with instructions how to obtain a development version for package igraph with the LAD algorithm implemented. A Readme file (pdf) in the archive provides more detail on the content.

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