2021

Augmenting Definitive Screening Designs

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AUGMENTING DEFINITIVE SCREENING DESIGNS

Dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Statistics at Virginia Commonwealth University.

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May 12, 2021

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Acknowledgments

The writer of this paper strongly feels indebted to those who provided assistance and encouragement with this work. My biggest appreciation goes to Dr. David J. Edwards, my advisor, your invaluable suggestions that helped to enhance my performance, your profound sense of caring for your students, and your willingness to be available at any time will be remembered for a long time. I would like to thank my thesis committee members: Dr. D'Arcy P. Mays, Dr. Brooke Marshall, Dr. Angela Reynolds, and Dr. Jenise L. Swall, for all of their guidance through this process; your discussion, ideas, and feedback have been absolutely invaluable. Finally, I will thank my parents for their love and support throughout my life. Thank you both for giving me the strength to reach for the stars and chase my dreams.

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Abstract

AUGMENTING DEFINITIVE SCREENING DESIGNS

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Design of experiments is used to study the relationship between one or more response variables and several factors whose levels are varied. Response surface methodology (RSM) employs the design of experiment techniques to decide if changes in design variables can enhance or optimize a process. They are usually analyzed by fitting a second-order polynomial model. Some standard and classical response surface designs are 3^k Factorial Designs, Central Composite Designs (CCDs), and Box-Behnken Designs (BBDs). They can all be used to fit a second-order polynomial model efficiently and allow for some testing of the model's lack of fit. When performing multiple experiments is not feasible due to time, budget, or other constraints, recent literature suggests using a single experimental design capable of performing both factor screening and surface response exploration. Definitive Screening Designs (DSDs) are well-known experimental designs with three levels. They are also named second-order screening designs, and they can estimate a second-order model in any subsets of three factors. However, when the design has more than three active factors, only the linear main effects and perhaps the largest second-order term can be identified by a DSD. Also, they may have trouble identifying active pure quadratic effects when two-factor interactions are present. In this dissertation, We propose several methods for augmenting definitive screening designs for improving estimability and efficiency. Improved sensitivity and specificity are also highlighted.

There are three contributions to this research. The first is constructing and evaluating augmented DSDs based on fold-over and column permutations. The second is constructing and evaluating augmented DSDs with points from the next inner orbit. The third is constructing and evaluating augmented DSDs with a uniform design. These methods are shown to improve the estimation of 2nd-order models in more than just three factors. In addition, these methodologies indicate better precision for pure quadratic effects while keeping the number of experimental runs competitive.

CHAPTER 1

INTRODUCTION

1.1 Background and Motivation

In an experiment, we change one or more variables (or factors) in order to study the effect on one or more responses. The design of experiments is a method to obtain data that can be analyzed to reach an objective conclusion. Design of experiments starts with determining the objectives of an experiment and selecting the factors for the study. A good experimental design can be useful to optimize the response for a given number of variables. The choice of an experimental design depends on the objective and the number of factors of the experiment. If we have many factors and little knowledge about them, the primary goal of the experiment might be to distinguish the few significant factors from many less important factors. In this case, screening designs should be used. In other situations, the experimental design may be used to estimate an interaction and quadratic effects; we want to investigate the shape of a response surface and would use response surface designs (Piepel and Cornell 1994). In the special case where we have factors that are proportions of a mixture, and we want to know what proportions of the factors maximize or minimize a response, then we need to use a mixture design. Response Surface Designs (RSDs), proposed by Box and Wilson 1951, are used when the active factors have been identified to optimize the response.

When the relationships between the active factors and response variable(s) are first being studied, screening experiments are used to determine the few active factors from the many factors. The number of runs in a screening design is based on the number of factors. In general, we widely use the resolution III and IV fractional factorial designs for early-stage screening; however, they have many drawbacks. The resolution III fractional factorial designs have main effects confounded with one or more two-factor interaction. If a confounded effect happens to be an active term, then the experimental results and interpretation can have substantial ambiguity. If we want to resolve this problem, we have to perform another experiment. For the resolution IV fractional factorial design, we may want to check for the presence of a few active two-factor interactions. Similar to the resolution III design, if a two-way interaction is identified as active, you may not be able to identify which of the interactions in the set of confounded two-way interactions are active. Another drawback of traditional screening designs, such as fractional factorials and Plackett-Burman designs (Plackett and Burman 1946), is that their factors have only two levels. This means these designs have no capability for capturing curvature due to quadratic effects.

In this research, we propose augmented designs based on Definitive Screening Designs (DSDs) proposed by Jones and Nachtsheim 2011. DSDs are a relatively new class of screening design consisting of three levels per factor that permit estimation of main effects, which are unbiased by second-order effects. DSDs have a simple construction based on conference matrices (Xiao, Lin, and Bai 2012). DSDs for an even number of factors only need $(2k + 1)$ runs, where k is the number of factors. In addition to the small sample size, these designs have other good properties, which will be discussed in the next section. When the number of factors is odd, Jones and Nachtsheim 2011 suggest deleting the last column of the conference matrix.

DSDs also have drawbacks. These designs only allow for the efficient estimation of the full quadratic model in any subset of three factors. If we have more than three factors in the full quadratic model and want to include all the second-order terms in the model, this design cannot estimate each term in the model. Our goal is to find an augmentation approach where DSDs can project onto a large number of factors and estimate a 2nd order model. Therefore, we propose an approach for dealing with this challenge, which is to augment DSDs to increase the ability to estimate second-order models as efficiently as possible. This can be advantageous compared to using other designs for second-order models with large run sizes. For k factors, a second-order model is

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j + \epsilon. \tag{1.1}$$

Because conference matrices do not exist when k is odd, so odd factors' DSDs cannot be directly constructed from conference matrices. Starting from six factors, the design has the capacity to estimate all possible full quadratic models with three or fewer factors with high G efficiency (Kiefer and Wolfowitz 1959). Zhou and Xu 2017 proposed augmenting a DSD with composite designs based on two-level orthogonal array (They are using the DSCD acronym to stand for it, definitive screening composite design). While this assists the estimation of bi-linear interactions, the two-level array is ineffective for improving the estimation of the pure quadratic terms. Liu, Mee, and Zhou 2019 proposed augmenting a DSD with axial runs (DSDA) for improving pure quadratic estimation. This paper introduced DSDAs for 6 to 12 factors is showed projections on 3, 4, and 5 factors. This can improve the quadratic estimation, but in some cases, it is not efficient for estimating interaction terms. Vazquez, Goos, and Schoen 2020 developed an augmented DSD based on dropping columns (The paper is using the DSDp acronym to refer to a DSD obtained by dropping one or more columns from a DSDs as a projected DSD). They introduced a classification criterion to identify the best sets of k columns to drop from the DSD. The primary weakness of DSDs is for estimation of the pure quadratic terms. If many two-factor interactions and pure quadratic effects are active, the standard DSD may not have sufficient degrees of freedom to separate the correlation between interactions of two factors and pure quadratic effects. As a result, when used as a single experimental experiment, DSDs are prone to Type-II errors, most notably for active pure-quadratic effects. When the noise level is large, the DSDs performance suffers in identifying active two-factor interactions. It also has trouble identifying active pure quadratic effects when two factor interactions are present. Estimation of full second-order models requires augmentation of DSDs. The augmentation of the DSDs could reduce the correlation between a factor's second order effects and improve precision for estimation. Even though some augmented designs did contribute to solving this problem, none of them resolve all issues. Furthermore, a comprehensive comparison of augmentation strategies for DSDs lacks in the literature. The goal of this research is to propose and evaluate augmentation strategies for DSDs to identify active effects at the screening stage and improve the efficiency of the estimates of those effects, especially improving the estimation of the pure quadratic terms. Also, we desire estimation of the second-order response surface model with three or more factors.

1.2 Research Objective

There are three aims for my research. The first is constructing and evaluating augmented DSDs based on fold-over and column permutations. The second is constructing and evaluating augmented DSDs with points from the next inner orbits to get better efficiency for the quadratic terms. The third is constructing and evaluating augmented DSDs with a uniform design to get better efficiency for the quadratic terms. The goal of this proposed research is to develop methodology that will estimate second-order models with more than three factors. In addition, another goal is that the number of experimental runs remains competitive with DSDs. Therefore, it is important to compare the number of runs in the augmented DSDs to other commonly used designs.

1.3 Overview

This dissertation remainder is organized as follows: Chapter II provides a comprehensive analysis of the literature on experimental design, including response surface designs, screening designs, definitive screening designs, and a few augmenting definitive screening designs techniques. Chapters III, IV, and V are our new augmented definitive screening designs based on some new methodologies. Each contains a summary of the research applicable to that chapter in the literature. Each chapter's original contribution is as follows: the augmented definitive screening design in Chapter III is based on fold-over and permutation of some columns from the definitive screening design. In a simulation study, when both two-factor interactions and pure-quadratic effects are present, the new augmented Definitive Screening Designs (DSD+) are able to increase the detection rate of second-order effects. Chapter IV describes an augmented definitive screening design based on subset designs. It shows the most powerful ability to obtain better precision for pure quadratic estimates and increase the ability to estimate more than three factors in a full quadratic model. Chapter V describes an augmented definitive screening design based on uniform designs. And finally, Chapter VI summarizes all the importance of studying definitive screening design and provides suggestions for future work.

CHAPTER 2

LITERATURE REVIEW

2.1 Screening Experiments

An experimental test is organized using experimental design, a statistical method. The changes in the output response in a system are detected by analyzing the input variables that change (Montgomery 2017). The design methods can be different based on the objective of the experiment. The objectives can be screening, modeling, and optimizing. Screening means finding the important factors, and modeling means fitting the best model to the response variable and optimizing means finding the maximum or minimum (the optimal) value of the response. First-order polynomial models are commonly used in screening experiments, while second-order polynomial models are usually used in modeling and optimization.

For two independent factors, the first-order polynomial or main effects model is

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon. \tag{2.1}$$

where X_1 and X_2 are the design factors, y is the response, the $\beta' s$ are unknown estimable parameters, and ϵ is a random error term in the system. Most of the time, an interaction term is usually added to the first-order model:

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \epsilon. \tag{2.2}$$

where the β_{12} represents the interaction effect between the design factors X_1 and X_2.

The two-factor second-order polynomial model is

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_{12} X_1 X_2 + \beta_{11} X_1^2 + \beta_{22} X_2^2 + \epsilon. \tag{2.3}$$

Second-order models are used for investigations of the response surface (Montgomery 2017). A general form can be written as Equation 1.1.

Even when the experimental goal is to eventually fit a response surface model (an RSM analysis), the first experiment is often a screening design when there are many factors to consider. Screening designs intend to find a few significant factors from a list of many potential ones. They usually assume a linear response function or linear function plus interactions and study the factors at two levels. Screening designs are typically of resolution III, which permits one to explore the effects of many factors with an efficient number of runs. Some notable screening designs are full and fractional 2-level factorial designs, Plackett-Burman(PB) designs, and supersaturated designs. Only the full factorial design can identify all interactions, whereas other designs can only identify the main effect and possibly some interactions. We will talk about some other designs that are capable of identifying some or all two-factor interaction effects later in this chapter.

2.1.1 Fractional Factorial Designs

"A factorial experiment in which only an adequately chosen fraction of the treatment combinations required for the complete factorial experiment is selected to be run" (Feder 1984). Generally, we select a fraction, for example, $\frac{1}{2}$, $\frac{1}{4}$ etc. of the full factorial. The following example will illustrate how to choose an appropriate fraction of a full factorial design to suit our purpose. For 2-level experiments, properly selected fractional factorial designs have the desirable properties of being both balanced and orthogonal. The 2^{k-p} fractional factorial design consist of a subset of the

2^k factorial design. The 2^{k-p} fractional factorial designs consists of k factors at just two levels each, similar to the 2^k factorial design. The value p specifies the degree of fractionation of the design, calculated by $1/2^p$. For instance, a 2^{6-3} design (see Table 1) is a $\frac{1}{2^3} = 1/8$th fraction of the 2^6 design. As such, the 2^{6-3} design contains 8 runs or 1/8th of the 64 runs for a 2^6 design.

Run	A	B	C	D=AB	E=AC	F=BC
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

Table 1.: A 2^{6-3} Fractional Factorial Design

As shown in Table 1, the first 3 independent columns are generated by a 2^3 design. The remaining 3 columns can be generated as interactions of the first 3 columns (Wu and Hamada 2011). As such, the value of 3 specifies the number of independent design generators that are necessary. Since column interactions have determined the design generators, the estimates of the 3 factor effect are aliased, meaning that it is not possible to measure the factor impacts on the response separately from factor interactions. This design's generators are D = AB, E = AC, and F = BC. Since D = AB, the effects of A and B influence the estimation of factor D's impact on the response. The 2^{6-3} design in Table 1 is of Resolution III because the main effects are aliased with two-way interactions.

Resolution defines the degree to which, in a fractional factorial design, estimated main effects are confounded with estimated interactions. The smallest resolution often considered in practice is III. The most prevalent resolutions are III, IV, and V. The confounding characteristics of these design resolutions are:

- Res III: Main effects are confounded or aliased with two-factor interactions, and two-factor interactions are aliased with each other.

- Res IV: No main effects are aliased with two-factor interactions, but two-factor interactions are aliased with each other.

- Res V: No main effect or two-factor interaction is correlated with other main effect or two-factor interaction, but maybe aliased with three factor interactions.

The design resolution can tell us the level of confounding in the design. Usually, one employs the design with the highest resolution possible while also meeting the required design run size consideration. This means that a resolution IV design is better than a resolution III model because we have a less extreme confounding pattern; higher order interactions are generally considered to be far less significant than low-order interactions. Different designs can also have the same resolution but have different confounding or aliasing structure while maintaining the overall characteristics mentioned above.

2.1.2 Plackett- Burman Designs and other Orthogonal Arrays

Plackett and Burman 1946 represented the construction of very economical designs with run sizes a multiple of four (rather than a power of 2). For example, the PB design can be used for an experiment containing up to 11 variables in 12 runs. When only main effects are of concern, Plackett-Burman designs are very successful screening designs. These designs do not have a defining relation and possess a more complex aliasing structure. With the 2^{k-p}_{III} designs, any main factor x_i is either orthogonal to $x_i x_j$ or equivalent to plus or minus $x_i x_j$ in the main effect column. The two-factor interaction column $x_i x_j$ is associated with every x_k for Plackett-Burman designs (for k not equal to i or j). However, for economically detecting large main effects, these designs are very useful, assuming that all interactions are marginal compared to the few relevant main effects.

2.1.3 Foldover Technique for augmenting designs

The fold-over technique or fold-over design, is talked by Li 2014. In order to increase the resolution of 2^{k-p}_{III} and Plackett-Burman designs, a mirror-image fold-over (or foldover) design is used to increase the size of fractional factorial designs. It is obtained by reversing the signs of all the initial design columns. The initial design runs are paired with the fold-over design runs, and this combination can then be used to estimate all primary effects without any bias from two-factor interaction. This is referred to as breaking the relation of aliasing between main effects and interactions of two variables. A mirror-image fold-over design is usually a way to build a resolution IV design from a resolution III design. The mirror-image fold-over (in which all column signs are reversed) is just one of the many potential follow-up fractions that can be used to supplement a fractional factorial design. When the original fraction is of resolution III, this is a popular choice. Alternative fold-over designs, on the other hand, can also be used to break up those alias patterns.

2.2 Response Surface Experiments

Response surface designs are used when we believe the response surface has significant curvature. Each factor requires at least three levels to estimate the curvature. Response surface designs are often referred to as second-order designs. To deal with response curvature, the experimenter can choose a 3^k or 3^{k-p} fractional factorial. Some other efficient options are the Central Composite Designs (CCDs, Box and Wilson 1951), and Box-Behnken Design (BBD, Box and Behnken 1960). Response surface methodology (RSM) aims at enhancing "the exploration of a region of design variables in one or more responses" (Myers, Khuri, and Carter 1989). The goal for RSM is to determine how changes in design variables can provide process improvement or optimization. RSM typically has two stages: factor screening and response surface exploration.

2.2.1 Central Composite Designs

Central composite designs were introduced by Box and Wilson 1951. It will allow estimation of curvature are contained a two-level factorial or fractional factorial design with center points that is augmented with a group of axial points. If the distance between the center of the design space and the factorial point for each factor is ± 1 unit, the distance between the center of the design space and the axial point is $|\alpha| > 1$. The precise value of α depends on certain characteristics needed for the layout and on the number of variables involved. Similarly, the number of center point runs also depends on certain characteristics required for the design. As there are variations in the design, a central composite design often has twice as many axial points as factors. For each factor in the design, the axial points reflect new extreme values (low and high). The addition of center points provides details on the system's overall curvature when the 2^k or 2_V^{k-p} design proves to be a poor representation of the system response, while axial points are added to allow a second-order response model to be fitted.

2.2.2 Box-Behnken Designs

In that it does not have an embedded factorial or fractional factorial design, the Box-Behnken design (Box and Behnken 1960) is an independent second-order design. In this design, the treatment combinations are at the midpoints of edges of the process space and at the center. Such designs are rotatable (or near rotatable), and each element needs only 3 levels. The designs have limited capability for orthogonal blocking compared to the central composite designs.

2.2.3 Orthogonal Array Composite Designs

Xu, Jaynes, and Ding 2014 introduced a new class of composite designs called orthogonal-array composite designs (OACDs). This design has an orthogonal array of N runs, k columns, s levels, and strength t, denoted by $OA(N, s^k, t)$. An OACD is made up of a two-level factorial configuration, a three-level orthogonal arrangement, and a few center points. As is the case for CCDs, an OACD may be used in a single or concurrent experiment. The additional points from a three-level OA in an OACD include details about linear and quadratic terms as well as bi-linear terms; in comparison, the axial points in a CCD are used to approximate linear and quadratic terms but do not include information about bi-linear terms. As a consequence, an OACD is frequently more efficient at estimating parameters, especially bi-linear terms, than a CCD. The capacity to recognize significant bi-linear terms is critical for such experiments, such as combinatory medication experiments involving a large number of medications encountered in operation. Let d be a k-factor composite design that consists of (i) a two-level design d_1 with n_1 runs, (ii) a three-level design d_2 with n_2 runs, and (iii) n_0 center points. The total number of runs of d is $N = n_1 + n_2 + n_0$. For $k = 4, ..., 12$, Xu, Jaynes, and Ding 2014 constructed

OACDs by choosing the smallest $OA(n_1, 2^k, 4)$ as d_1 and the smallest three-level OA as d_2. Specifically, they chose a full factorial 2^k for $k = 4$, or a regular 2^{k-p} design with resolution at least V for k = 5–11, and the third column of Table 2 gives the p generators. For k = 12, use an $OA(128, 215, 4)$ since the smallest regular resolution V design for 12 factors has 256 runs. For the three-level OA, use the first k columns of "oa.9.4.3.2.txt," "oa.18.7.3.2.txt," and "oa.27.13.3.2.txt" from Sloane's website http://neilsloane.com/oadir/(Zhou and Xu 2017). A detailed structure is given for composing the OACD in each number of factor level in Table 2.

k	d_1	Generators	d_2
6	2^{6-1}_{VI}	F = ABCDE	OA(18,3^6)
7	2^{7-1}_{VII}	G = ABCDEF	OA(18,3^7)
8	2^{8-2}_{V}	G = ABCDE, H= ABCF	OA(27,3^8)
9	2^{9-2}_{V}	H = ABCDE, J = ABCFG	OA(27,3^9)
10	2^{10-3}_{V}	H = ABCDE, J = ABCFG, K= ABDF	OA(27,3^{10})
11	2^{11-4}_{V}	H = ABCDE, J = ABCFG, K= ABDF, L=ACEG	OA(27,3^{11})
12		OA(128,2^{12}, 4)	OA(27,3^{12})

Table 2.: Orthogonal Array Composite Designs

2.3 Definitive Screening Designs

Definitive screening designs (DSDs) are a new class of small three level designs introduced by Jones and Nachtsheim 2011. They can investigate k factors with only $2k + 1$ runs. The DSDs consist of k fold-over pairs for k factors and a single center point. Each run, excluding the center-point, has exactly one point at its center and all others at the extremes(± 1). DSDs have a simple construction based on conference matrices by Xiao, Lin, and Bai 2012. For k even factors, a $k \times k$ matrix, initials C, is defined as a conference matrix which satisfies $C'C = (k-1)I_{k\times k}$, with $C_{ii} = 0$ (i=1,2,3. . . , k) and $C_{ij} \in -1, 1$, $(i \neq j, i, j = 1, 2, \ldots, k)$ (Goethals and Seidel 1967). The DSDs for an even number of factors only need $(2k+1)$ runs, where k is the number of factors. In addition to the small sample size, these designs have other good properties, which will be discussed next. Because conference matrices do not exist when k is odd, DSDs cannot be constructed from conference matrices. As an alternative, Xiao, Lin, and Bai 2012 suggest deleting the last column of the conference matrix. Then the design will have the same number of runs for $(k-1)$ factors as for k factors, and the main effects are completely independent of the two-factor interactions. Therefore, the estimates of the main effects are not biased. The two-factor interactions are also not completely confounded with other two-factor interactions, and any number of linear and quadratic main effect terms are estimable. The quadratic effects are orthogonal to the main effects and not completely confounded with the interaction effects. Starting from 6 factors, the design has the capacity to estimate all possible full quadratic models with three or fewer factors. The DSD is different from other regular screening designs because it has three levels for each factor and able to estimate quadratic terms. The construction of a DSD using conference matrices is shown below:

$$D = \begin{pmatrix} C \\ -C \\ 0 \end{pmatrix} \tag{2.4}$$

where 0 is a $1 \times m$ zero vector. This design structure has all the properties as those proposed by Jones and Nachtsheim 2011. Their desirable properties are:

1. The number of runs required is only one more than twice the number of variables.

2. The main effects are completely independent of two-factor interactions, unlike resolution III designs. As a consequence, the presence of active two-factor interactions does not bias estimates of main effects, regardless of whether the interactions are included in the model.

3. Two-factor interactions, unlike resolution IV designs, are not entirely confused with other interactions of two factors, although they can be correlated.

4. All quadratic effects are estimable in models.

5. Quadratic effects are orthogonal to main effects and not completely confused with interaction effects (although correlated).

6. With 6 to 12 factors, the models are able to estimate all possible full quadratic models involving three or fewer factors with very high efficiency.

Table 3 shows an example of a 10 factor Definitive screening design.

Definitive Screening Design						
Fold-Over Pair	Run(i)	Factor Levels				
		$X_{i,1}$	X_{i_2}	X_{i_3}	$\dots$	$X_{i,10}$
1	1	0	±1	±1	$\dots$	±1
	2	0	∓1	∓1	$\dots$	∓1
2	3	±1	0	±1	$\dots$	±1
	4	∓1	0	∓1	$\dots$	∓1
3	5	±1	±1	0	$\dots$	±1
	6	∓1	∓1	0	$\dots$	∓1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
10	19	±1	±1	±1	$\dots$	0
	20	∓1	∓1	∓1	$\dots$	0
Center point	21	0	0	0	$\dots$	0

Table 3.: Ten factors DSD Design Matrix

2.4 Previous Work on Augmenting Definitive Screening Designs

2.4.1 Definitive Screening Designs with Axial Runs

If there are many active interactions and pure quadratic terms in the model, the confounding issue will be a problem to estimate the 2nd-order model. Liu, Mee, and Zhou 2019 proposed augmenting a DSD with axial runs (DSDA) to solve the above problem. For improving the quadratic estimation and decoupling the correlation between two factor interaction and pure quadratic, they add a $2 \times k$ of projection factors axial pairs plus one center-point replicate (k is the number of factors). Table 4 shows an example with six factors DSDA. They added thirteen runs (six pairs of axial points plus one center-point) with $|\alpha| = 1$. Their augmentation can reduce aliasing

DSD + Axial Runs						
Run(i)	Factor Levels					
	$X_{i,1}$	X_{i_2}	X_{i_3}	X_{i_4}	X_{i_5}	$X_{i,6}$
1	0	1	1	1	1	1
2	0	-1	-1	-1	-1	-1
3	1	0	-1	1	1	-1
4	-1	0	1	-1	-1	1
5	1	-1	0	-1	1	1
6	-1	1	0	1	-1	-1
7	1	1	-1	0	-1	1
8	-1	-1	1	0	1	-1
9	1	1	1	-1	0	-1
10	-1	-1	-1	1	0	1
11	1	-1	1	1	-1	0
12	-1	1	-1	-1	1	0
13	0	0	0	0	0	0
14	1	0	0	0	0	0
15	-1	0	0	0	0	0
16	0	1	0	0	0	0
17	0	-1	0	0	0	0
18	0	0	1	0	0	0
19	0	0	-1	0	0	0
20	0	0	0	1	0	0
21	0	0	0	-1	0	0
22	0	0	0	0	1	0
23	0	0	0	0	-1	0
24	0	0	0	0	0	1
25	0	0	0	0	0	-1
26	0	0	0	0	0	0

Table 4.: DSD with Axial Runs for six Factors

from omitted second-order terms for the factors.

2.4.2 Definitive Screening Design Composite Designs

Since the primary weakness of DSDs is for estimation of the pure quadratic terms. Zhou and Xu 2017 proposed augmenting a DSD with a two-level orthogonal array for improving the estimation of the interaction terms (Their paper is using DSCD acronym to stand for it, definitive screening composite design). This two-level orthogonal array is an $OA(n_1, 2^k, 4)$, the linear, quadratic, and bi-linear terms are orthogonal to each other, and two-level OA will provide more information on linear and quadratic terms. But the two-level array is ineffective for improving the estimation of the pure quadratic terms. By integrating a two-level factorial design with a three-level DS design and some center points, they were able to build a DSCD. They generated DSCDs for $k = 4$–12 using three-level DS designs from Jones and Nachtsheim 2011, with the two-level portion chosen as in Table 2 and $n_0 = 0$ for all designs.

2.4.3 Definitive Screening Designs Obtained by Dropping Columns

Vazquez, Goos, and Schoen 2020 developed an augmented DSDs design based on dropping columns (The paper is using DSDp acronym to refer to a DSD obtained by dropping one or more columns from a DSDs as a projected DSD). The purpose of this work was to identify the screening design with the lowest expected cost for the complete experiment, measured by the total number of runs used, the number of correctly identified active effects at the screening stage, and the efficiency of the estimates of these effects. The paper demonstrated how dropping k columns from a DSD with $n = m + k$ columns will result in an m-factor design with superior aliasing properties than an $m-$factor DSD, thus increasing the likelihood that the

DSDp can detect the active effects. For example, if the researcher wanted a seven-factor design, it can drop three columns from the 10-factor DSD in Table 3, and thus use a 21-run design instead of a 17-run design. This method one main contribution is that it identifies the best sets of k columns to drop from DSDs. To classify the DSDp obtained by dropping different sets of columns, they considered the maximal absolute correlation and the number of squared correlations between pairs of two-factor interaction effects contrast vectors involving three or four factors. Table 5 shows the overall best sets of 1–4 columns to drop from each $(m + k)$-factor DSDs. There are often several overall best sets of columns that result in DSDp that are equally good.

# factors in DSDs (m+k)	# columns dropped (k)			
	1	2	3	4
6	Any	Any	Any	Any
8	Any	Any	Any	Last four
10	Any	Any	Any	6,8,9 and 10
12	Any	Any	Any	7,8,10 and 12

Table 5.: Overall best sets of k columns to drop from an (m + k)-factor DSDs

CHAPTER 3

AUGMENTING DEFINITIVE SCREENING DESIGNS USING FOLDOVER TECHNIQUE

3.1 Approach

In this chapter, the concept for our augmenting strategy is based on the fact that we are using conference matrices to create DSDs. If we have k columns in the conference matrix, C, and select one or more columns from matrix C to fold over, we will produce a new conference matrix C'. For example, one can try to fold over two columns from C, so we have $\binom{k}{2}$ new conference matrices. By continuing this strategy, we can also create $\binom{k}{3}, \binom{k}{4}, \ldots \binom{k}{k-1}, \binom{k}{k}$ different conference matrices. When folding over the columns we chose, other columns are kept fixed. After creating the new conference matrix C'(after fold over), we then permute the columns from C'. So, k factors (k columns) will give $k!$ choices of permutation. After each permutation we have a new matrix called C^2. Next, we combine C^2 and $-C^2$ with the original DSD. That is,

$$Augmented\ DSD = \begin{pmatrix} C \\ -C \\ 0 \\ C^2 \\ -C^2 \\ 0 \end{pmatrix} \tag{3.1}$$

Note that our augmented DSD has $4k + 2$ runs. To determine the best foldover permutation, two criteria are used. One is projection information capacity (PIC), proposed by Loeppky 2004. Given an $n \times m$ design, let f be the class of models containing k main effects and their second-order terms. Then the PIC is

$$d_k = \frac{\sum_f ((det(X'X/n))^{1/p}}{\binom{m}{k}} \tag{3.2}$$

where p is the number of parameters (i.e.$p = 1 + k + \binom{k}{2}$), k is the number of factors, and X is the model matrix. We seek to maximize PIC.

The second criterion is projection estimation capacity (PEC), proposed by Loeppky, Sitter, and Tang 2007. The PEC is defined as follows: given D, an $n \times m$ design, let ρ_k(D) be the number of estimable models containing k main effects and their second-order terms.

$$p_k(D) = \frac{\rho_k(D)}{\binom{m}{k}} \tag{3.3}$$

and call (p_1,p_2,...,p_k) the PEC sequence of D. It is desirable to have each element in the PEC sequence be as large as possible. We now compare these augmentation strategies with alternative designs. Table 6 provides a run size comparison for different designs.

DSD stands for Definitive Screening Design, **DSDFO** stands for DSD augmented with fold-over, **CCD** stands for Central Composite Design with the axial points at α =1, **DSCD** stands for Definitive Screening composite designs, **DSDA** stands for DSD augmented with axial runs, **DSDp** stands for Definitive Screening Designs obtained by Dropping Columns, and **OACD** stands for orthogonal-array composite design. Figure 1 shows in the 3 factors, DSDFO has the highest PIC value compared with other options. For 4 factor projections, DSDFO has the highest PIC

The number of runs for each design							
Design Name	Number of Factors						
	6	7	8	9	10	11	12
OACD	50	82	91	155	155	155	155
DSCD	45	79	81	147	149	151	153
CCD	44	78	80	146	148	150	280
DSDA	26	30	34	38	42	46	50
DSDFO	26	30	34	38	42	46	50
DSDp	26	NA	34	NA	42	NA	50
DSD	13	15	17	19	21	23	25

Table 6.: Run Size Comparison

values compared with other options after 9 factors. For 5 factor projections, DSDFO has a similar performance as the CCD for 10 or more factors. Figure 2 shows that DSDFO performs well with respect to 3 and 4 factor projections. For 5-6 factor projections, PEC performance is competitive despite the smaller run sizes for a large value of k. Since DSDFO has a significant advantage over most of the designs in the run size, DSDFO can be a good choice when the experimenter conceives an experimental design.

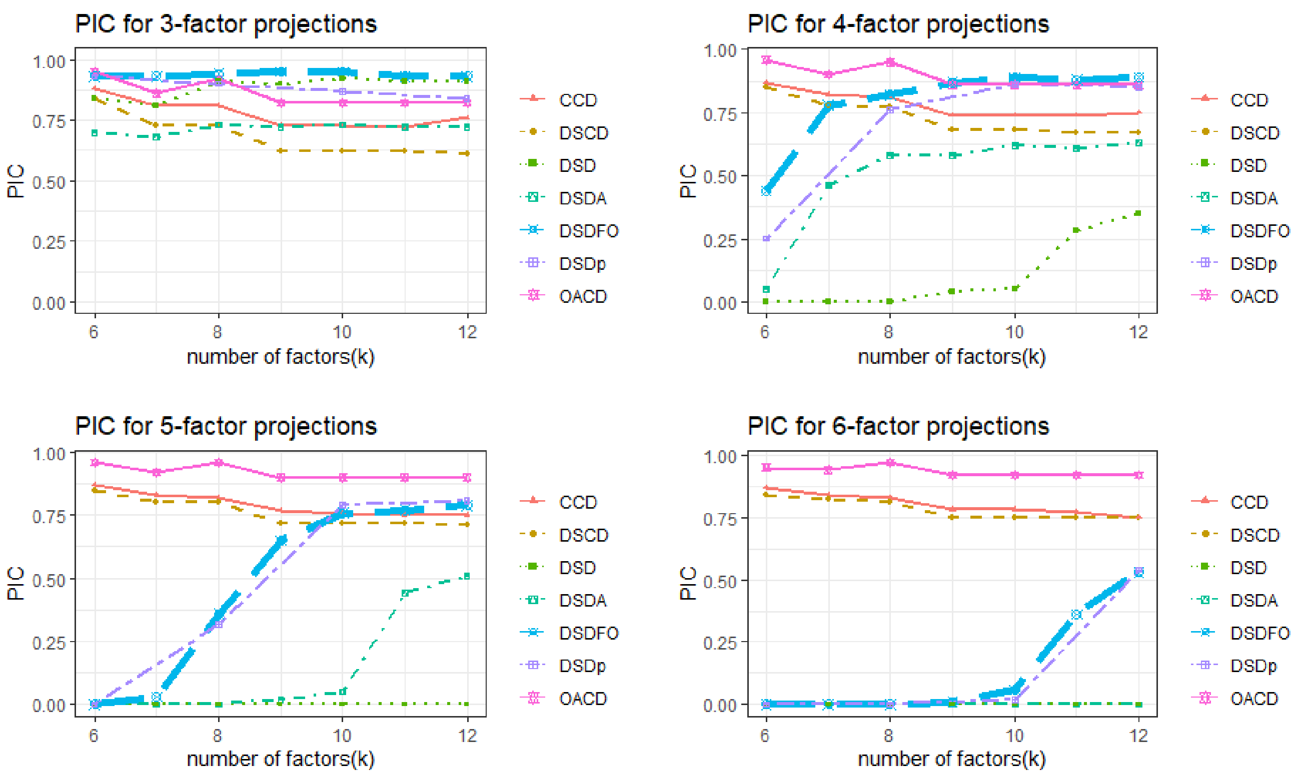

Fig. 1.: DSDFO PIC Comparison for 3-6 factor projections

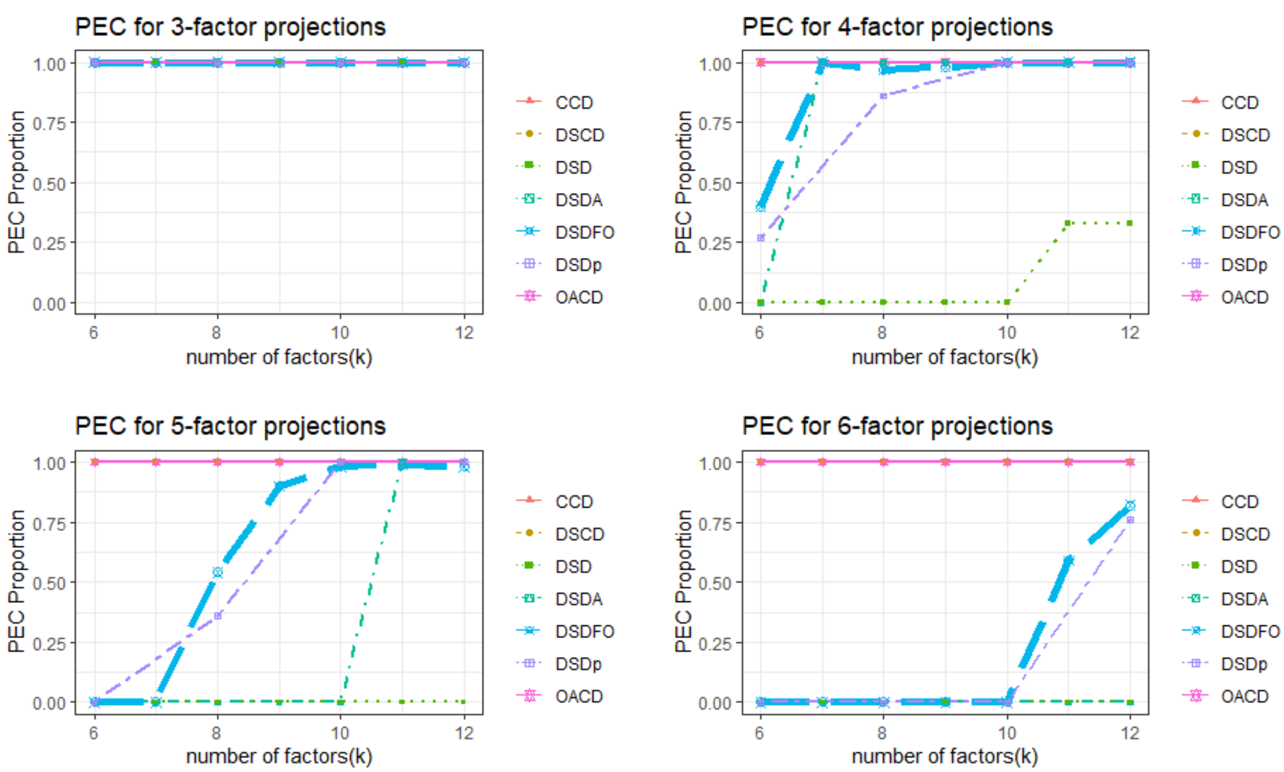

Fig. 2.: DSDFO PEC Comparison for 3-6 factor projections

3.2 Variance Analysis

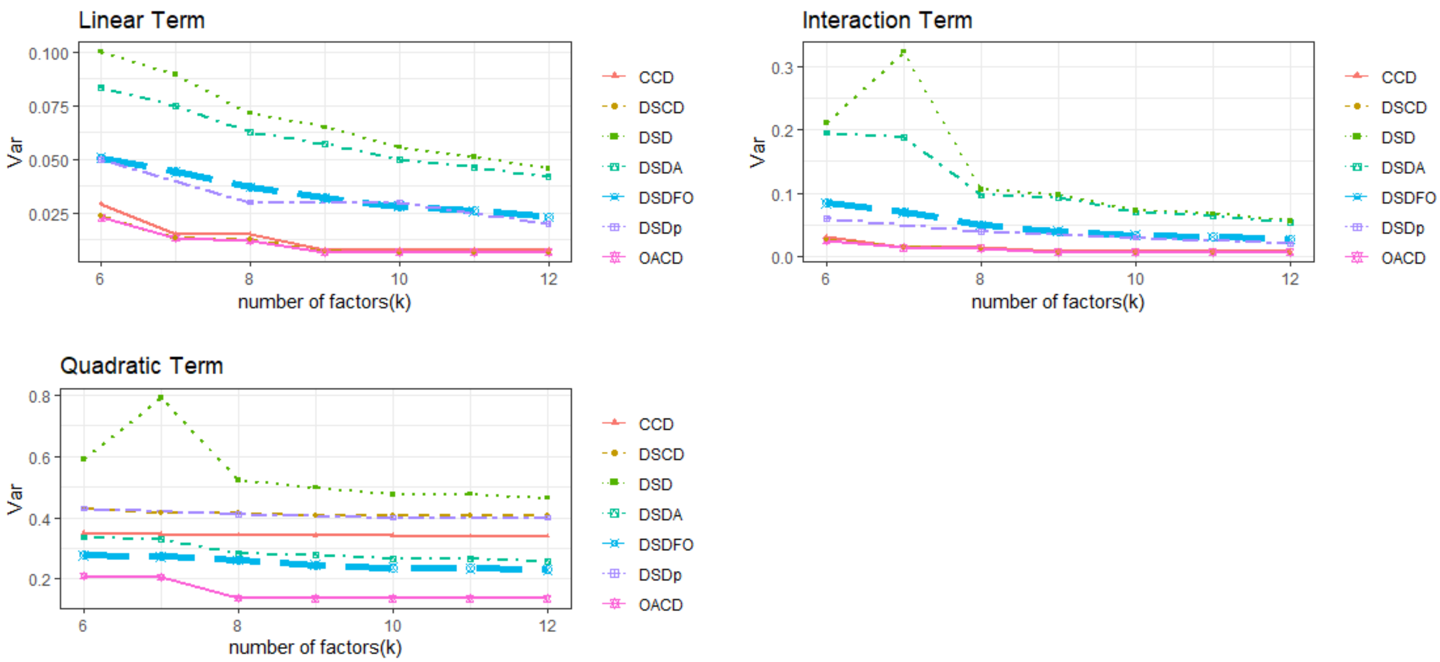

Fig. 3.: DSDFO Variance Estimation Plots

Figure 3 shows a comparison of variance of estimation. Assuming independent observations with error σ^2, the linear, interaction, and quadratic estimators would have variances calculated from $\sigma^2(X'X)^{-1}$. In our comparison, we set σ^2 to be 1. For the linear and interaction terms, DSDFO shows a much smaller variance than DSDA and DSD, and compared with other designs (with a large number of runs), the interaction term variance of DSDFO is competitive. For the quadratic term variance comparison, the DSDFO showed the second smallest variance among all these six designs. In other words, the efficiencies in estimating the pure quadratic coefficients are quite good.

3.3 D-efficiency Comparison

For any k-factor design, the D-efficiency is defined by:

$$D_{eff} = \frac{1}{n}\Big(\frac{|X'X|}{MaxD_x}\Big)^{1/p} \tag{3.4}$$

$$MaxD_x = u^k v^{\frac{k(k-1)}{2}}(u-v)^{k-1}(u+(k-1)v-kv^2) \tag{3.5}$$

where

$$u = \frac{k+3}{4(k+1)(k+2)^2}((2k^2+3k+7)+(k-1)(4k^2+12k+17)^{1/2}) \tag{3.6}$$

$$v = \frac{k+3}{8(k+1)(k+2)^3}((4k^3+8k^2+11k-5)+(2k^2+k+3)(4k^2+12k+17)^{1/2}). \tag{3.7}$$

Since DSD and augmented DSD cannot estimate the second-order model in all factors, we calculated the D-efficiency using projection onto 3 factors. Thus, we compute the average D-efficiency across all 3 factor projections. In other words, our design matrix X will be all three factor model matrices chosen from k factors. The D-optimal criterion is seeking to maximize $|X'X|$, the determinant of the information matrix. The model matrix X includes the intercept, linear, interaction, and quadratic terms. Except for the whole model D-efficiency, We also compared designs in terms of the precision for estimating a subset of the model parameters. For s, a subset of factors of a design d,

$$D_{s,eff} = \frac{1}{n}\Big(\frac{|X'X|}{|X'_{(s)}X_{(s)}|}\Big)^{1/|s|} \tag{3.8}$$

where $X_{(s)}$ are the sub-matrices of X corresponding to the parameters not in s, respectively, and $|s|$ is the number of parameters in s. So the efficiency for each term can be calculated as D_L(linear), D_B(interaction), and D_Q(quadratic), respectively.

$$D_{L,eff}(d) = D_L(d), D_{B,eff}(d) = D_B(d), D_{Q,eff}(d) = D_Q(d) \tag{3.9}$$

(Since Zhou and Xu 2017 illustrate the D_Q optimal design has a D_Q value of 1/4, so in here $D_{Q,eff}(d) = 4D_Q(d)$). The D-efficiency of the DSD is poor for estimating two-factor interactions, so we want to examine the ability of DSDFO to estimate models with interactions and quadratic terms.

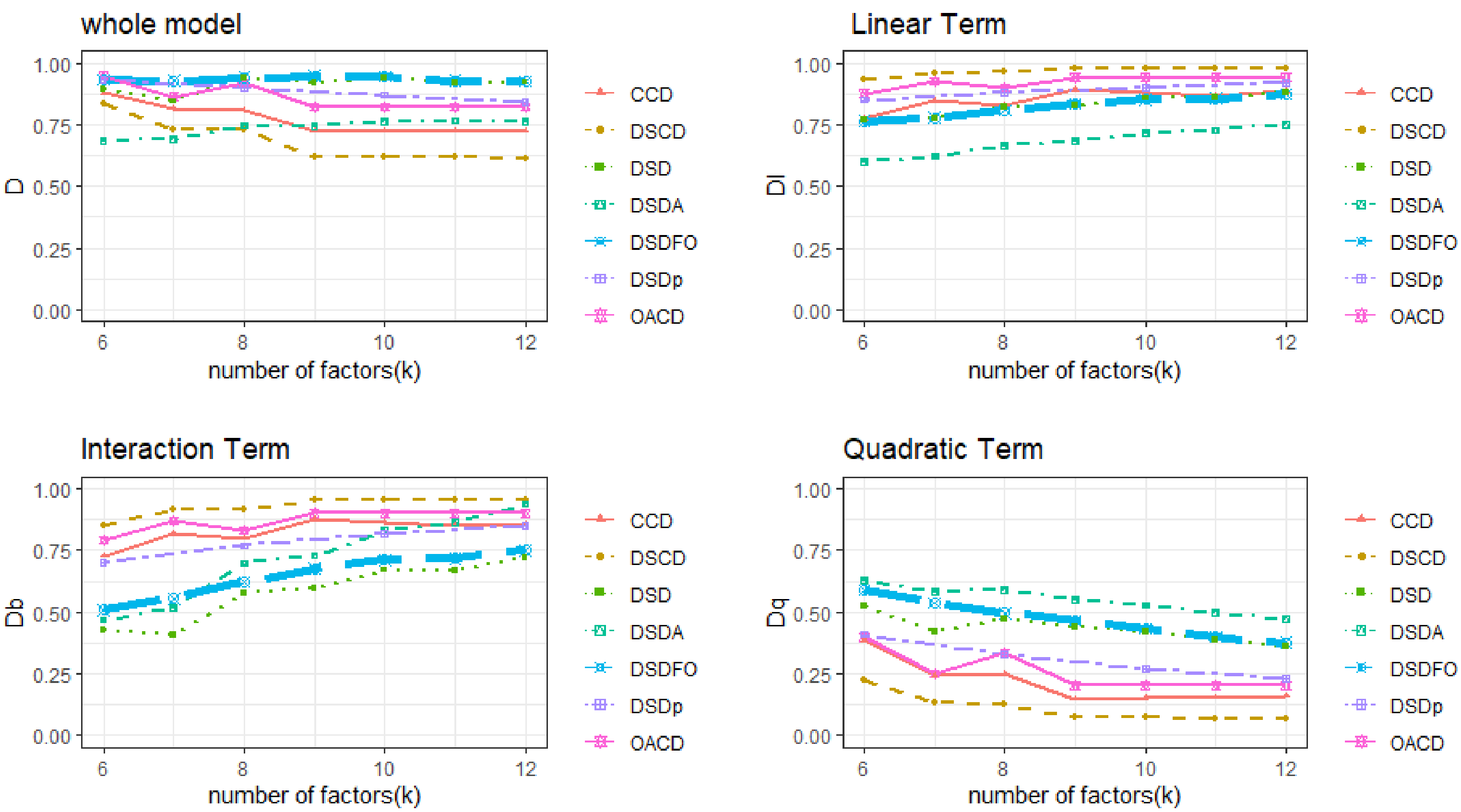

Fig. 4.: DSDFO D Efficiency Plots

For $k = 4, 5, \ldots, 12$, we compare DSDFO with DSDA, DSCD, OACDs, DSDp and CCDs. Figure 4 shows that DSCDs have the largest $D_{L,eff}$(D-linear Efficiency), but DSDFO also has reasonable $D_{L,eff}$ given their run size. For the interaction D-efficiencies comparison, DSDFO only outperforms the DSD. For the quadratic D-efficiencies comparison, DSDFO and DSDA both indicate reasonable high efficiencies. For the whole model D-efficiencies comparison, it is obvious that DSDFO gives the highest efficiencies. This illustrates that DSDFO can estimate the full quadratic model well.

3.4 Sensitivity and Specificity Analysis

We want to assess the performance of the DSDFO in terms of power and specificity rates compared with traditional DSD and other new augmenting definitive screening designs introduced in the literature review. Recall the following: (**DSDA**-Definitive Screening Designs with Axial Runs, **DSCD**-Definitive Screening Design Composite Designs, **DSDp**-Definitive Screening Designs Obtained by Dropping Columns).

The definition for power analysis and specificity analysis are: (1) Power is the ratio of the number of selected active effects over the total number of truly active effects. (2) Specificity is the ratio of the number of inactive effects not selected from the fitted model over the number of inactive effects from the true model. Below simulation protocol idea is from Errore et al. 2017.

1. We considered the number of factors, k, equal to $4, 6, 8, 10$ and 12.

2. The active effects followed either unrestricted or strong heredity (explaining in the next paragraph).

3. The model selection method used was forward step-wise selection based on the minimum AICc (Cavanaugh 1997) and Lasso (Tibshirani 1996).

4. To generate a response vector, we fit a model with all active effects and an error term.

5. The number of active main effects varied from (i) 2 to k when only main effects were active, (ii) 2 to $k-2$ for an unrestricted model having second-order effects, and (iii) 4 to $k-2$ for second-order models with strong heredity.

6. We defined the proportion of active second-order effects p_{so}. We had three levels for this scenario: 0 (only for first order models), 0.5, and 1.0.

7. We computed the signal-to-noise ratio (SN) of the active effects, with SN desired as $|\beta|/\sigma$ and $SN = 1$.

8. We calculated the power and specificity as previously described.

For clarity, we describe the setup for one simulation study. Suppose the number of factors in the design is eight, and there are four active main effects. These four active main effects are randomly selected from the eight factors. Let the proportion of second-order effects be $p_{so} = 0.5$, so the number of second-order effects is two. Note, the type of second-order effects could be a mix of interaction and quadratic terms. If the model type is unrestricted, the two active second-order effects are randomly chosen from among the $\binom{8}{2} = 28$ interaction terms and 8 possible quadratic terms. If the model type is strong heredity, then the two active effects are chosen from among $\binom{4}{2} = 6$ interaction terms and 4 allowable quadratic terms.

3.4.1 Scenario 1 : Unrestricted Models with Active Second-Order Effects

Figure 5, Figure 6, and Figure 7's top two plots show the power analysis results for a total of 10 factors with 2, 4, 6, and 8 active factors in the design and for two different model selection methods. Based on these results, the DSDFO and DSDp have much better sensitivity than the traditional DSD. Therefore, these designs also

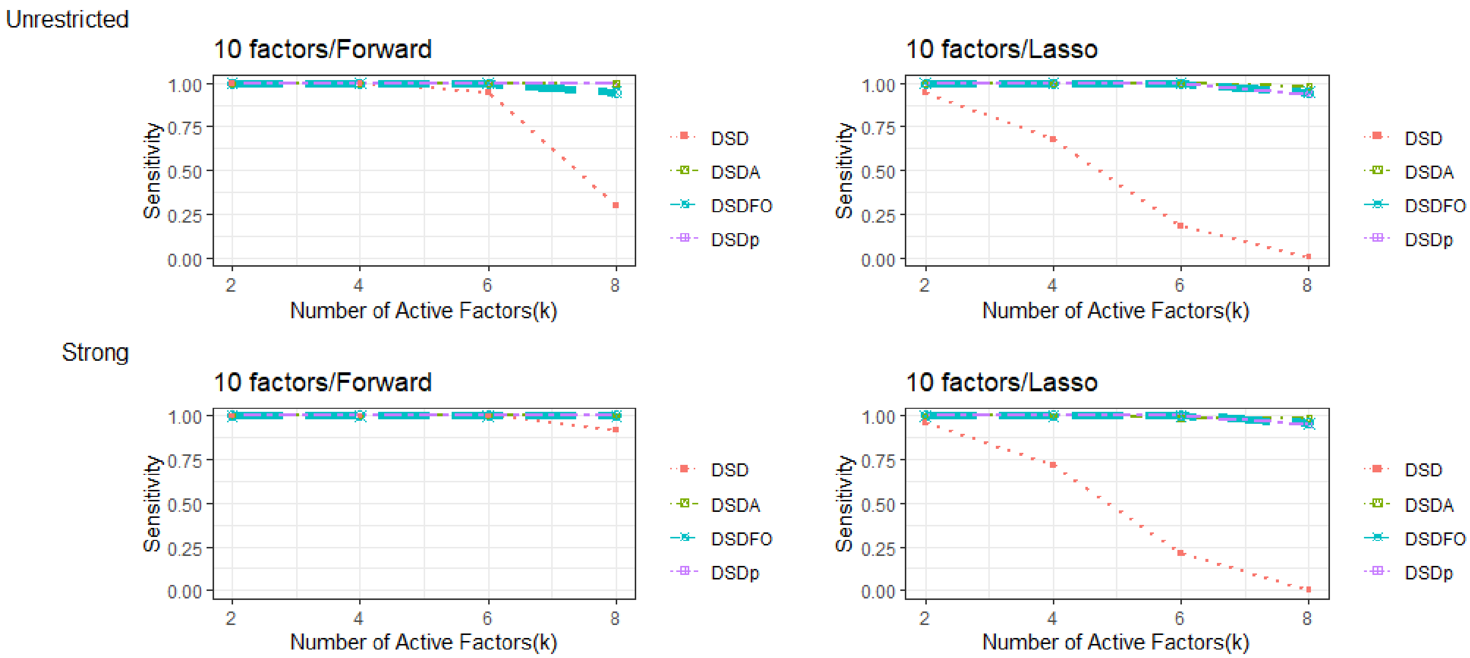

Fig. 5.: DSDFO Power Analysis of Main-Effects

have a better chance of finding the truly active effects, especially when the number of truly active factors is increasing. Figure 8, Figure 9, and Figure 10's top two graphs are the plots for comparing the specificity of the unrestricted models. The traditional DSD did well in terms of specificity. In general, the DSDFO and DSDp performed similarly to the DSD. Although the DSDFO and DSDp had lower specificity when compared to the DSD in most cases, they still performed well because specificity was close to 90% for these designs. (All designs perform well with regard to specificity).

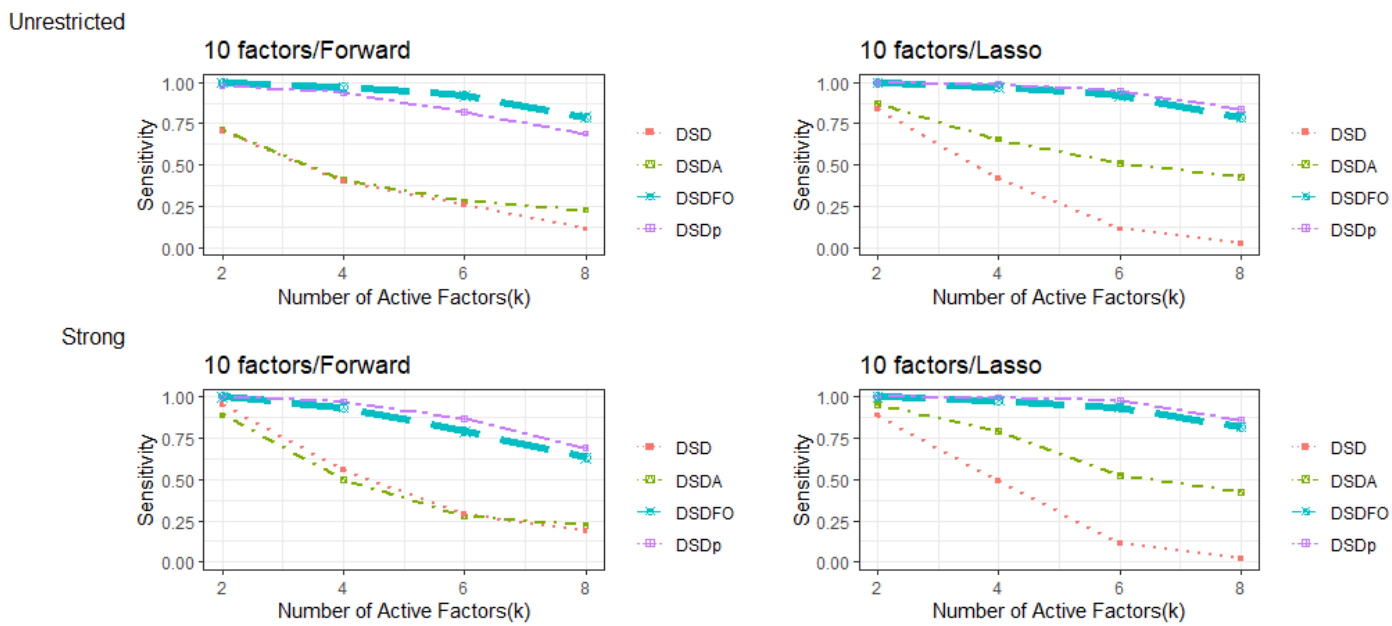

Fig. 6.: DSDFO Power Analysis of Interaction-Effects

3.4.2 Scenario 2 : Strong Heredity Models with Active Second-Order Effects

Figure 5, Figure 6, and Figure 7's bottom two plots show the results when the models are following strong heredity. There are 10 factors with 2, 4, 6, and 8 active factors in the design with two different model selection methods. The DSDFO and DSDp have much better sensitivity than the traditional DSD. They have almost 100% sensitivity to detect the main effects. The DSDFO and DSDp also have much better sensitivity than the other two designs for interaction effects; as the number of factors increases, the differences get larger. DSDFO had the best performance on quadratic effects, it was almost 5% better than DSDp and clearly better than DSD. So DSDFO has a higher probability of finding the active effects, especially when the number of

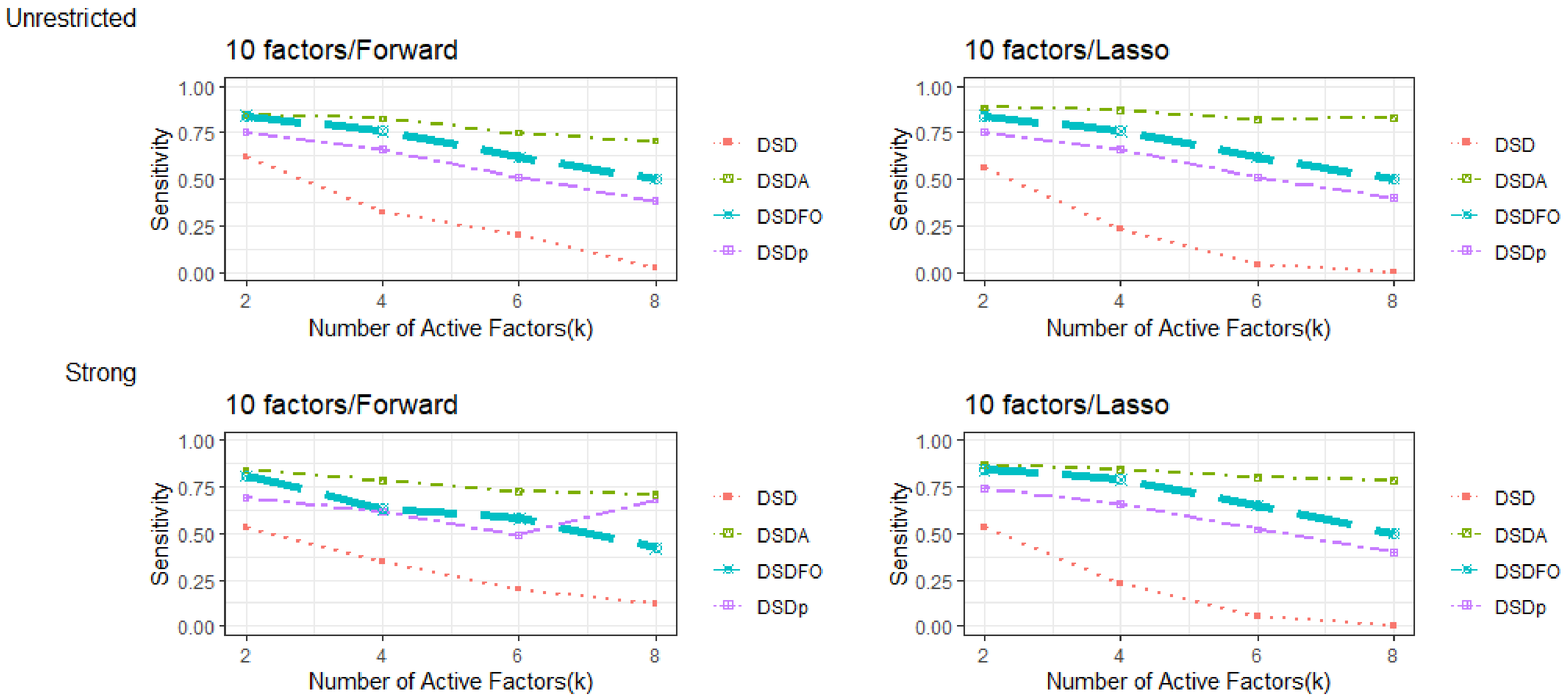

Fig. 7.: DSDFO Power Analysis of Quadratic-Effects.

active factors are increasing. Figure 8, Figure 9, and Figure 10 's bottom two graphs are the plots for comparing specificity of the strong heredity models. The traditional DSD did well in terms of specificity. In general, the DSDFO and DSDp performed similarly to the DSD. Although the DSDFO and DSDp had lower specificity when compared to the DSD in most cases, they still performed well because specificity was close to 90% for these designs. (All designs perform well with regard to specificity).

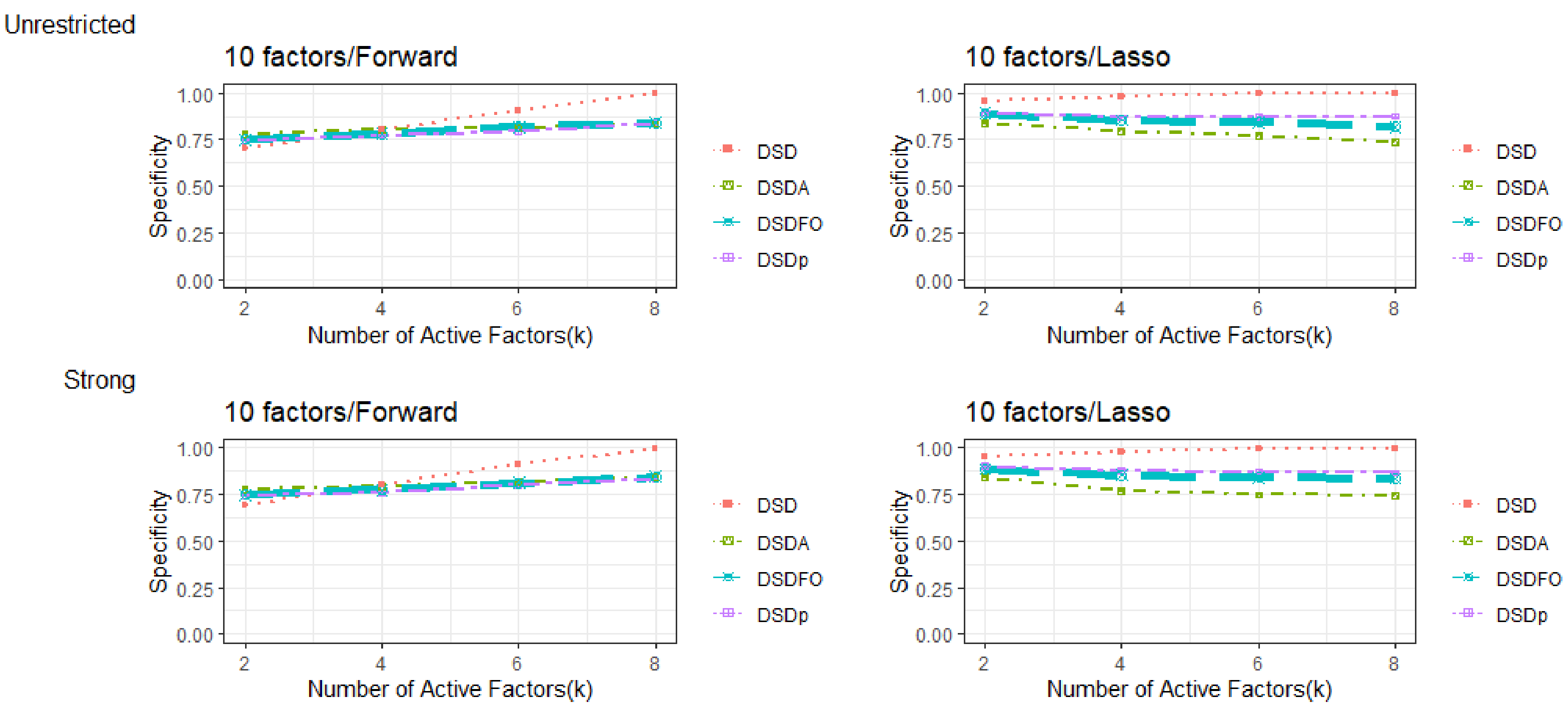

Fig. 8.: DSDFO Specificity of Main-Effects

Fig. 9.: DSDFO Specificity of Interaction-Effects

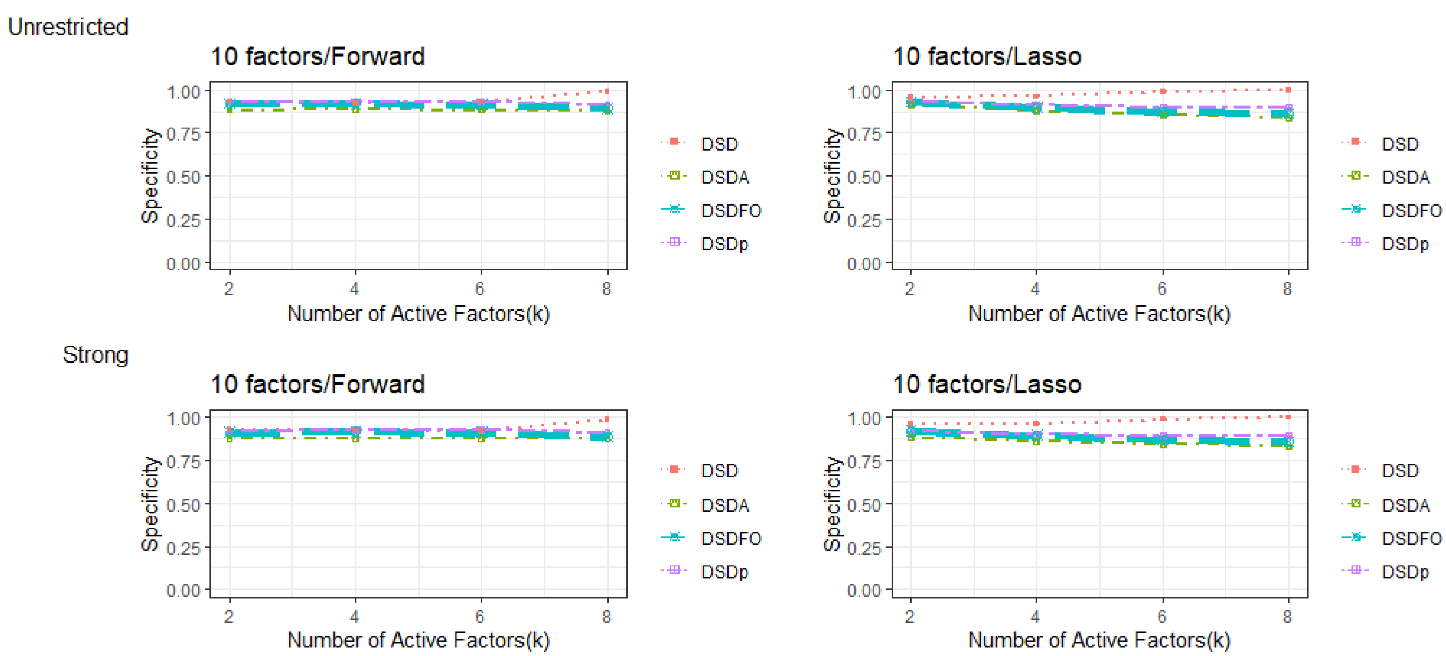

Fig. 10.: DSDFO Specificity of Quadratic-Effects.

3.5 Case Comparison

Two cases were used to compare DSDFO with DSD; these two cases represent two different combinations of model heredity (strong and weak). Strong heredity means that if a model has a two-factor interaction, then the model's constituent main effects are included. In contrast, weak heredity only allows one of the two major effects to be used in the model. Jones and Nachtsheim 2011 suggest performing a forward step-wise regression when considering all terms in a second-order model. We also add another lasso regression method to check the ability to identify the active terms. We checked three results for each model: the identified correct active terms, incorrectly identified terms (Type I Error), and not identified terms (Type II Error).

Model I is a strong heredity model:

$$y_i = 2X_1 - 1.5X_5 + 2X_7 - 3{X_1}^2 + 2.5{X_5}^2 - 4{X_7}^2 + 4X_1X_5 + 3.5X_1X_7 - 5X_5X_7 + \epsilon_i \tag{3.10}$$

In Table 7, when the DSDFO is using the Lasso regression method, it can exactly find the active terms and high order terms. However, when using the forward step-wise, DSDFO did not identify X_1^2 and X_5^2. Comparing to DSDs, DSDFO finds more active terms than DSDs. DSDFO and DSDs both have incorrectly identified some of the interaction terms. DSD only identified all the linear terms and one interaction term. It missed all quadratic terms and other interaction terms in the forward step-wise regression method. As the lasso method, DSD missed all active terms.

Model II is a weak heredity model:

$$y_i = 2X_1 + 2X_5 - 1.5{X_1}^2 + 2.5{X_5}^2 - 3.5X_1X_5 + 4X_1X_7 - 5X_5X_7 + \epsilon_i \tag{3.11}$$

From Table 8, we see that DSDFO still can find all the active terms except missing one quadratic term when using the lasso method. But DSD also only can identify all the linear terms and one interaction term. It missed all quadratic terms and other interaction terms in the forward step-wise regression method. And for the lasso method, DSD missed all active quadratic terms.

Model I				
	DSD		DSDFO	
	Forward Step-wise	Lasso	Forward Step-wise	Lasso
Identified	X_1, X_5, X_7, X_1X_5	NA	$X_1, X_5, X_7, X_1X_5, X_1X_7$ X_5X_7, X_7^2	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$
Type I Errors	$X_9, X_{10}, {X_8}^2, X_4X_{10}, X_2X_{10}$ $X_6X_8, X_3X_5, X_4X_5, X_7X_8$	X_4X_{10}	$X_2X_5, X_2X_{10}, X_4X_7$ $X_5X_6, X_7X_{10}, X_{10}^2$	$X_2X_4, X_2X_8, X_2X_9, X_2X_{10}$ $X_4X_{10}, X_6X_8, X_3^2, X_9^2$
Type II Errors	X_1^2, X_5^2, X_7^2 X_1X_7, X_5X_7	$X_1, X_5, X_7, X_1^2, X_5^2, X_7^2$ X_1X_5, X_1X_7, X_5X_7	X_1^2, X_5^2	NA

Table 7.: DSDFO Strong Heredity Model Results

Model II				
	DSD		DSDFO	
	Forward Step-wise	Lasso	Forward Step-wise	Lasso
Identified	X_1, X_5, X_1^2	$X_1, X_5, X_1X_5, X_1X_7, X_5X_7$	X_1, X_5, X_1X_5, X_5X_7 X_1X_7, X_1^2, X_5^2	$X_1, X_5, X_1X_5, X_1X_7, X_5X_7$ X_5^2
Type I Errors	$X_4X_8, X_8X_{10}, X_2X_9$ $X_7X_8, X_3X_{10}, X_{10}$	$X_1X_9, X_2X_{10}, X_4X_6, X_4X_8$	X_7, X_9, X_2X_9 X_5X_8	$X_1X_6, X_2X_{10}, X_3X_7$ X_7X_{10}, X_{10}^2
Type II Errors	X_5^2, X_1X_5, X_1X_7 X_5X_7	X_1^2, X_5^2	NA	X_1^2

Table 8.: DSDFO Weak Heredity Model Results

3.6 Summary and conclusions

DSD can be used to identify the main effects and some second-order terms. However, when we have many effects, DSD may cause an under-fit model. DSD also does not allow for the efficient estimation of the full quadratic model in any more than three factors. DSDFO can provide better precision for pure quadratic estimates, and at the same time, it can identify more interaction terms. Also, DSDFO increases the ability to evaluate more than three factors in a full quadratic model. DSDFO demonstrates quite good efficiencies in estimating the pure quadratic coefficients than other designs. DSDFO also shows a competitive result as DSDA in power analysis of quadratic effects and DSDp in power analysis of interaction effects.

CHAPTER 4

AUGMENTING DEFINITIVE SCREENING DESIGNS USING SUBSET DESIGNS

4.1 Subset Designs

The subset design proposed by Gilmour 2006 uses a two-level factorial design in subsets of the factors, with the other factors being held at their middle level. In this case, we consider the levels coded to -1, 0, and 1. Let S_r, with $r = 1, 2, \ldots, q$, be the subset of the 3^q factorial design points that lie on the hyper-sphere of radius $r^{1/2}$ about the center point, S_0. Thus, S_r contains all points which have r factors at ± 1 and the remaining $q - r$ factors at 0. A combination of S_r subsets can also be represented by $c_{r1}S_{r1} + c_{r2}S_{r2} + ...$, where c_r is the number of times the subset S_r is replicated. Gordon, Murray, and Todd 1994 used this idea for four and five factors. The Box-Behnken design is also a special case of subset design. Box-Behnken designs have treatment combinations at the midpoints of the experimental space's edges and require at least three continuous factors. Table 9 shows all available S_r for choosing a design for three factors. For projections onto two factors: each point of type $(\pm 1, \pm 1)$ appears two times in the subset S_3, each point of $(\pm 1, 0)$ or $(0, \pm 1)$ appears two times, and each point of $(\pm 1, \pm 1)$ appears one time in the subset S_2. For subset S_1, each point of $(\pm 1, 0)$ or $(0, \pm 1)$ appears one time, and $(0, 0)$ appears two times. Finally, for subset S_0, the point $(0, 0)$ appears one time. A subset design can project onto a number of replicates of the full 2^2 factorial design. An example of subset design for three factors is in Table 10 (c_2S_2, $c_2 = 1$). In addition, it will be a Box-Behnken design if an additional center run is added to it.

S_3	S_2	S_1	S_0
-1-1-1	-1-1 0	-1 0 0	0 0 0
-1-1 1	-1 1 0	1 0 0	
-1 1-1	1-1 0	0 -1 0	
-1 1 1	1 1 0	0 1 0	
1 -1 -1	-1 0 -1	0 0 -1	
1 -1 1	-1 0 1	0 0 1	
1 1 -1	1 0 -1		
1 1 1	1 0 1		
	0 -1 -1		
	0 -1 1		
	0 1 -1		
	0 1 1		

Table 9.: Subsets for three factors

Subset design can be useful for model selection, especially when the quadratic effects are small (Gilmour 2006). The projection of the design when non-significant factors are removed is an important criterion to consider for second-order polynomial models.

Subset Design			
	Factor Levels		
	X_1	X_2	X_3
1	-1	-1	0
2	+1	-1	0
3	-1	+1	0
4	+1	+1	0
5	-1	0	-1
6	+1	0	-1
7	-1	0	+1
8	+1	0	+1
9	0	-1	-1
10	0	+1	-1
11	0	-1	+1
12	0	+1	+1

Table 10.: One of Subset Design With Three Factors

4.2 Augmenting DSDs with Subset Designs

Table 11 again shows a general structure of DSDs. In general, if we have k factors in the design model, DSDs are a $S_{k-1}+S_0$ subset design. Based on the definition of S_r, the next level subset design after S_{k-1} will be S_{k-2}. So following the DSD(S_{k-1}), we will augment it with a S_{k-2} subset design. For example, if we want to create a four-factor augmented DSD, a fully detailed design structure appears in Table 12.

As k increases, the design space's volume increases quickly based on the next-order inner orbit design combinations. Using all of S_{k-2} for augmentation is not practical in many applications. Therefore, there is a need for an optimization al-

Definitive Screening Design						
Fold-Over Pair	Run(i)	Factor Levels				
		$X_{i,1}$	X_{i_2}	X_{i_3}	$\dots$	$X_{i,k}$
1	1	0	±1	±1	$\dots$	±1
	2	0	∓1	∓1	$\dots$	∓1
2	3	±1	0	±1	$\dots$	±1
	4	∓1	0	∓1	$\dots$	∓1
3	5	±1	±1	0	$\dots$	±1
	6	∓1	∓1	0	$\dots$	∓1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
k	2k-1	±1	±1	±1	$\dots$	0
	2k	∓1	∓1	∓1	$\dots$	0
Center point	2k+1	0	0	0	$\dots$	0

Table 11.: DSD Design Matrix

gorithm to choose the optimal subset. D-optimality is a widespread criterion for choosing the best design. For a second-order polynomial model matrix X, it can be achieved by maximizing the determinate of $X'X$. However, when $n < P$, $X'X$ will be singular. DuMouchel and Jones 1994 presented a Bayesian D-optimality criterion that can solve this problem. Supposing a linear model $y = X\beta + \epsilon$ with $\epsilon \sim N(0, \sigma^2 I_n)$, the prior distribution of the parameters is $\beta|\sigma^2 \sim N(\beta_0, \sigma^2 R^{-1})$, where β_0 is intercept and R is a prior covariance matrix, and the conditional distribution of y given β is $y|\beta, \sigma^2 \sim N(X\beta, \sigma^2 I)$. The posterior distribution for β given y is then $\beta|y \sim N(b, \sigma^2(X'X + R)^{-1})$, where $b = (X'X + R)^{-1}(X'y + R\beta_0)$. Since the posterior variance is $\sigma^2(X'X + R)^{-1}$, the Bayesian D-optimal designs maximize $|X'X + R|$. DuMouchel and Jones 1994 incorporate prior information and model

Augmented Definitive Screening Design					
		Factor Levels			
		X_1	X_2	X_3	X_4
	1	0	1	1	1
	2	0	-1	-1	-1
	3	1	0	-1	1
DSD(S_3)	4	-1	0	1	-1
	5	1	-1	0	-1
	6	-1	1	0	1
	7	1	1	-1	0
	8	-1	-1	1	0
	9	0	0	0	0
	10,11	-1	±1	0	0
S_2	12,13	1	±1	0	0
	14,15	-1	0	±1	0
	16,17	1	0	±1	0
	18	0	0	0	0

Table 12.: Example Augmented DSDs With Four Factors

uncertainty into the regression parameters by splitting model terms into two sets: one set contains terms assumed to be active called primary terms (P_1), the other set contains terms that may or may not be active (P_2). P_1 primary terms are given a prior distribution with an arbitrary prior mean and prior variance tending towards infinity. For the potential terms P_2, they are given a prior mean zero and finite variance $\sigma^2\tau^2$ since they are not supposed to have large effects; τ represents the expected effect of a factor relative to residual standard error (DuMouchel and Jones 1994). We use the SAS proc optex to select a design; the prior precision values' inverses can be interpreted as prior variances for the linear parameters corresponding to each effect. Then the matrix R is set to $R = K/\tau^2$, where

$$K = \begin{pmatrix} \mathbf{0}_{p_1\times p_1} & \mathbf{0}_{p_1\times p_2} \\ \mathbf{0}_{p_2\times p_1} & \mathbf{I}_{p_2\times p_2} \end{pmatrix}. \tag{4.1}$$

Since this addition of the prior information can make the information matrix invertible, the total number of $P = P_1 + P_2$ could be greater than the number of runs, n. If there are many active interactions and pure quadratic terms, the confounding issue will make the estimation poor. An initial DSD may only identify the linear main effects and perhaps some large second-order terms. So we will consider all main effects and quadratic effects as primary terms and interaction effects as potential terms. In the proc optex function, we selected our candidate points from S_{m-2} subset design points. Here we considered two instances with different run sizes. One is the size of a DSD, and the second is half the run size of a DSD. We will talk about the cost and benefit tradeoffs and compare them later. We set the precision value for main and quadratic effects to 0, meaning there is no prior information for the main effects and quadratic effects. We performed a sensitivity analysis to decide on the prior precision (from 5 runs to 20 runs). In the end, we chose $\tau = 1$. Suppose we have n_1 runs for the DSD corresponding to the X_1 model matrix and let X_2 be another model matrix subset from S_{k-2} with n_2 rows. For getting the optimal design, we need to maximize $|X'X|$ of the model matrix X, which consists of X_1 and X_2, set $X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}$. So $X'X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}' \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = X_1'X_1 + X_2'X_2$, we are looking to maximize $|X_1'X_1 + X_2'X_2|$ and create an augmented D-optimal design using the row-exchange algorithm (Broughton et al. 2010). The row-exchange algorithm is an iterative search algorithm and operates by incrementally changing an initial design matrix, X, to increase $|X^T X + R|$ at each step. There is randomness built into the selection of the initial design and into the choice of the incremental changes. This algorithm will return a locally D-optimal design. At each step, the row-exchange algorithm exchanges an entire row of X with a row from a design matrix to another design matrix, C, containing a candidate set of feasible factor levels. We applied a projection estimation capacity (PEC) criterion (Loeppky, Sitter, and Tang 2007) and projection information capacity (PIC) (Loeppky 2004) to check the new augmented design properties. Recall the following: Table 13 provides a run size comparison for different designs.

The number of runs for each design							
Design Name	Number of Factors						
	6	7	8	9	10	11	12
OACD	50	82	91	155	155	155	155
DSCD	45	79	81	147	149	151	153
CCD	44	78	80	146	148	150	280
DSDA	26	30	34	38	42	46	50
DSDFO	26	30	34	38	42	46	50
DSDSD	26	30	34	38	42	46	50
DSDp	26	NA	34	NA	42	NA	50
DSD	13	15	17	19	21	23	25

Table 13.: Run Size Comparison

In Figure 11 and Figure 12, DSD stands for definitive screening design, DSDFO stands for DSD augmented with fold-over, CCD stands for central composite design with the axial points at $|\alpha| = 1$, DSCD stands for DSD augmented with compos-

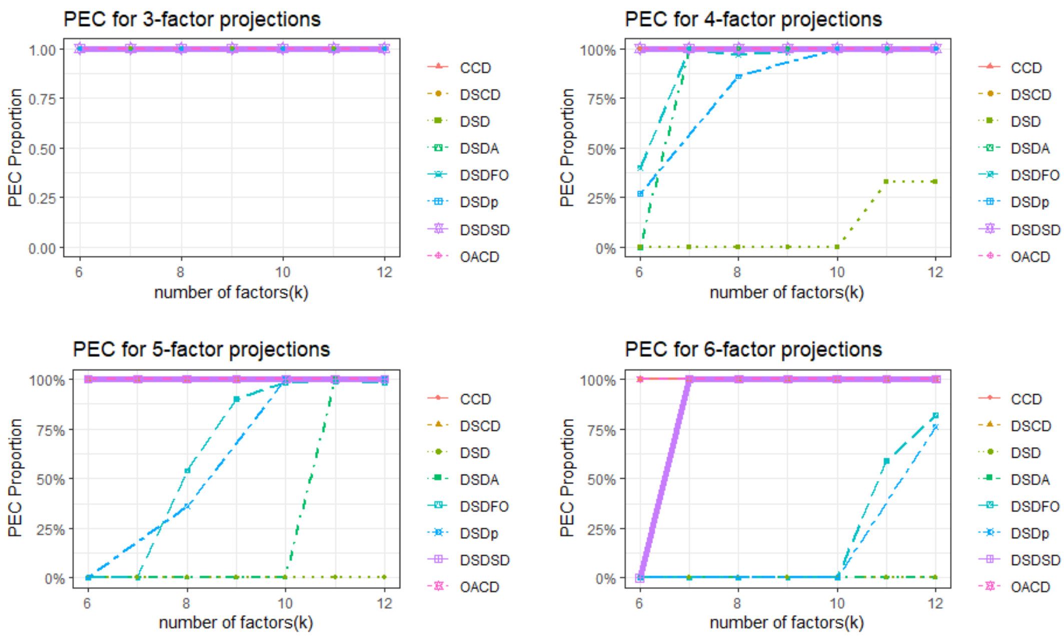

Fig. 11.: DSDSD PEC Comparison for 3-6 factor projections

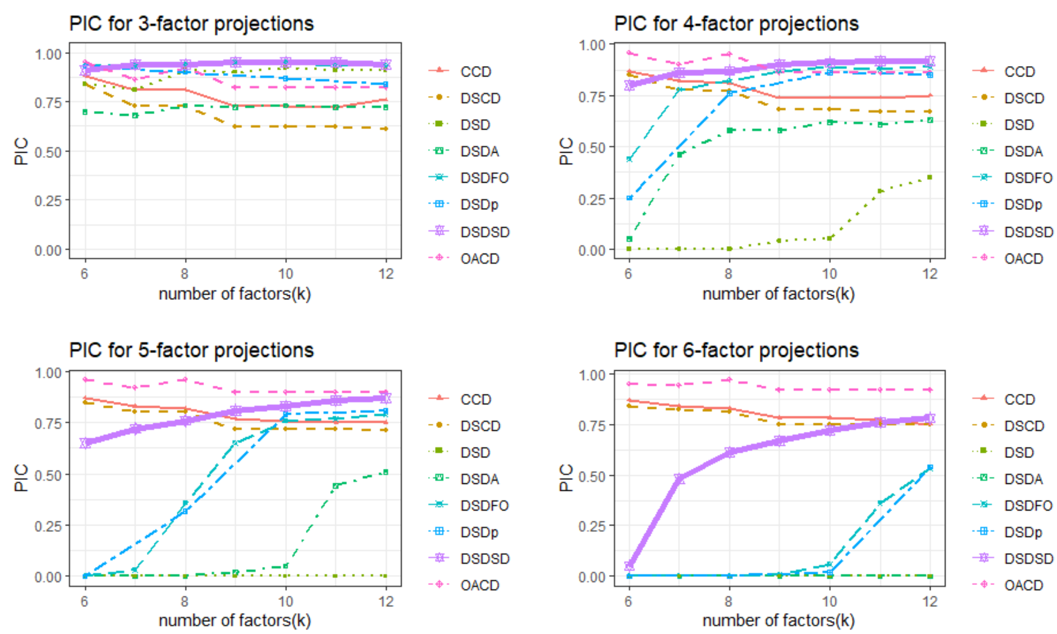

Fig. 12.: DSDSD PIC Comparison for 3-6 factor projections

ite designs, DSDA stands for DSD augmented with axial runs, OACD stands for orthogonal-array composite design, DSDp stands for Definitive Screening Designs obtained by Dropping Columns and our new augmented DSD with subset design is named as DSD+SD (DSDSD). Figure 11 shows DSD+SD PEC can estimate all 3-5 factors main effects with their associated two-level interactions. For 6 factors' main effects with its associated two-level interactions, DSD+SD can estimate them when DSD+SD has more than seven factors. Figure 12 shows in the 3 and 4 factor projections, DSD+SD is competitive with other designs. For 5 and 6 factor projections, DSD+SD clearly outperforms DSD and DSDFO. A comparison of augmentation run sizes will be introduced in the Appendix section.

4.3 Variance Analysis

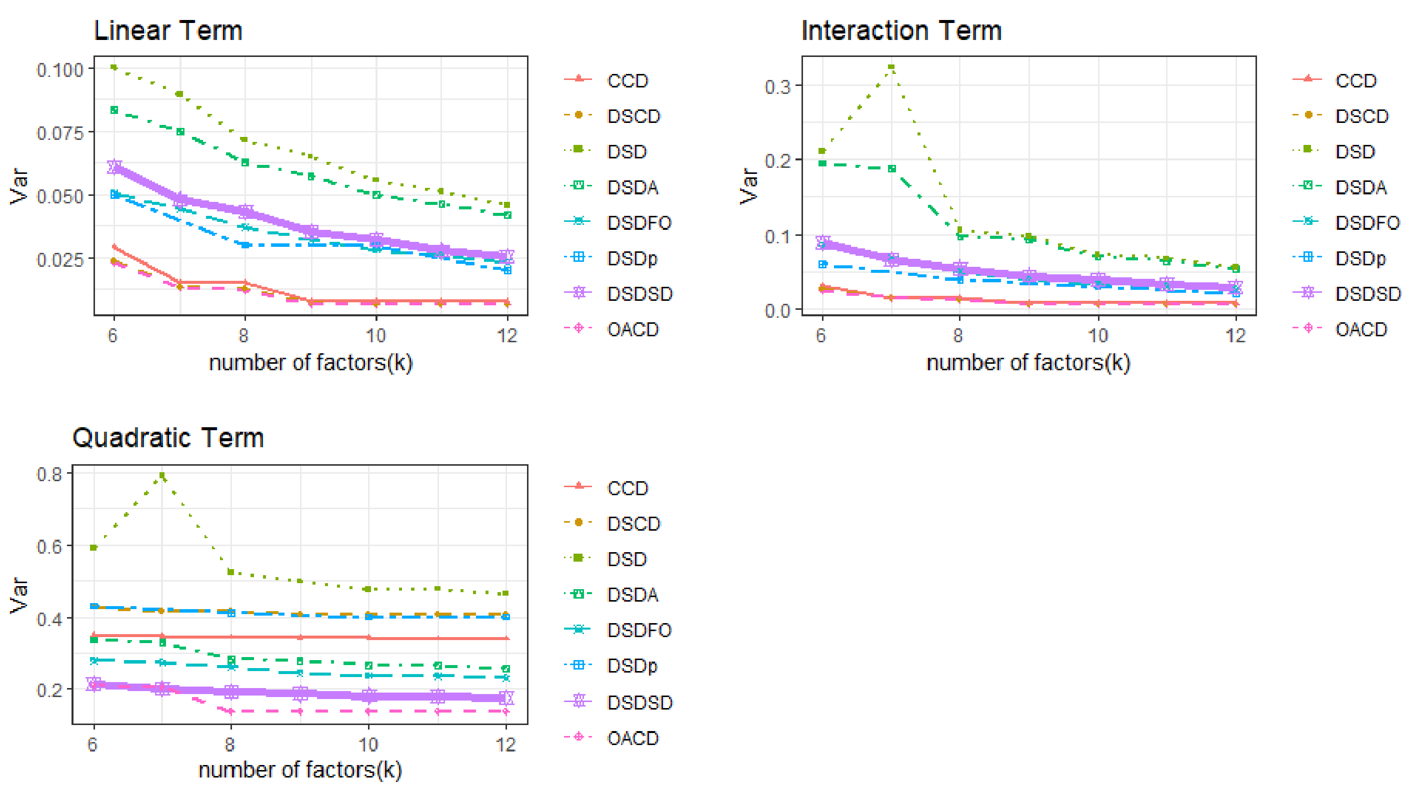

Fig. 13.: DSDSD Variance Estimation Plots

Figure 13 shows the variance comparison in the same screening designs. Assuming independent observations with error σ^2, the linear, interaction, and quadratic estimators would have variances calculated from $\sigma^2(X'X)^{-1}$. In our comparison, we set up σ^2 is equal to 1. We can see that the DSD shows a high variance of estimation for interaction and quadratic terms compared with DSD+SD. DSD+SD has a smaller variance in quadratic terms compared with others. DSD+SD shows to have the best cost-performance ratio.

4.4 D-efficiency Comparisons

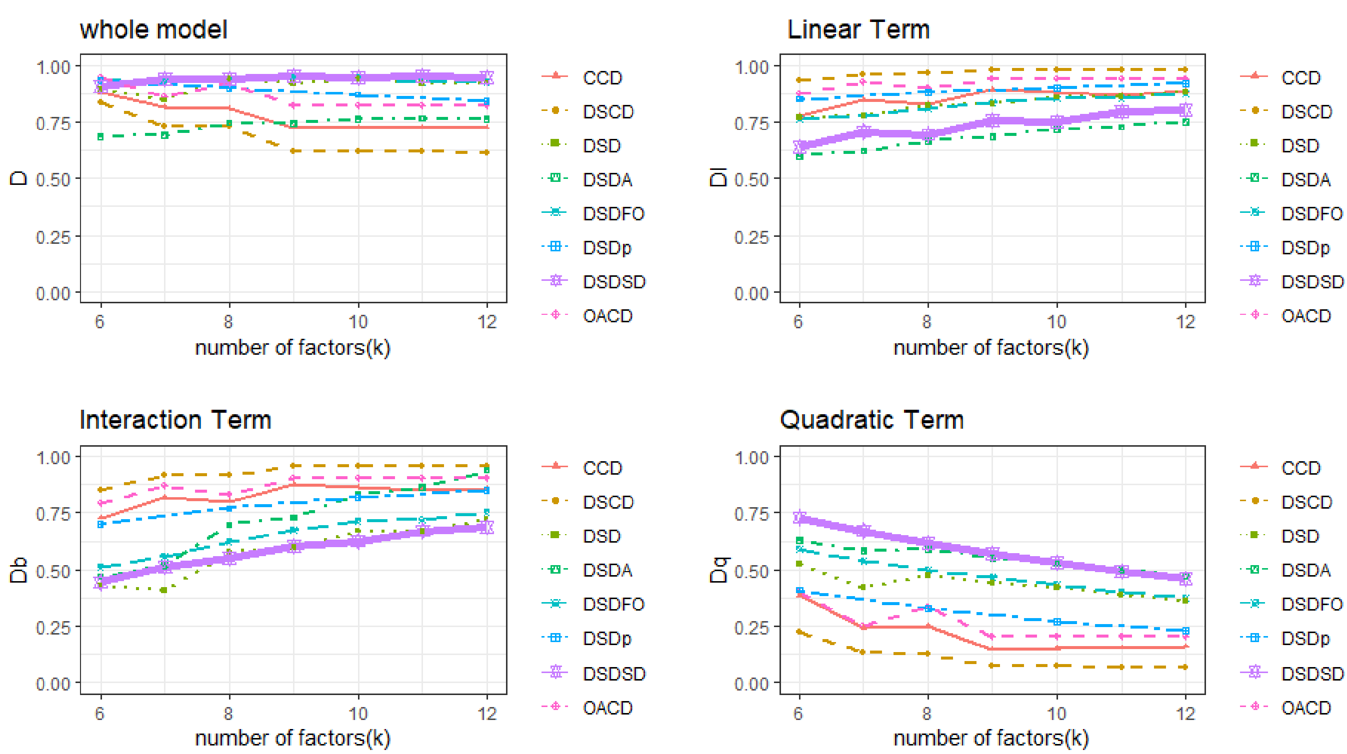

Fig. 14.: DSDSD D Efficiency Plots

Figure 14 shows the D efficiency comparison. On the top left, DSD+SD has a high D Efficiency (above 90%) for whole model calculation even as the number of factors increases. On the top right, our DSD+SD's linear term shows an increasing trend as the number of factors increases. DSCD and OACD show good linear term efficiency. However, due to their numbers of runs and our focus on the high-order terms, DSD+SD still shows a reasonable D efficiency. On the bottom left, DSD+SD's interaction term is also showing an increasing trend in the plot. The DSD+SD shows the highest D-efficiency value over all the screening designs for quadratic terms on the bottom right.

4.5 Sensitivity and Specificity Analysis

We want to assess the performance of the DSD+SD in terms of sensitivity and specificity rates compared with traditional DSD and some other augmented DSD strategies like DSDp, DSDA, and DSDFO. We constructed the same simulation study as in Chapter 3 with all possible combinations of the factors. We calculated the number of selected active effects over the total number of active effects to perform a power analysis.

4.5.1 Scenario 1: Unrestricted Models with Active Second-Order Effects

Figure 15, Figure 16, and Figure 17's top two plots show the sensitivity analysis results for a total of 10 factors with 2, 4, 6, and 8 active factors in the design and two different model selection methods. Based on these results, for the linear and interaction terms, all augmented DSDs except the traditional DSDs have a strong power to identify the active terms. For the quadratic terms, DSD+SD has the most powerful ability to detect corrected active quadratic terms using forward model selection even when there are many active terms in the model and shows competitive results to DSDA when using lasso model selection. And their performance in quadratic terms is better than other options. Finally, DSD+SD has much better sensitivity than the

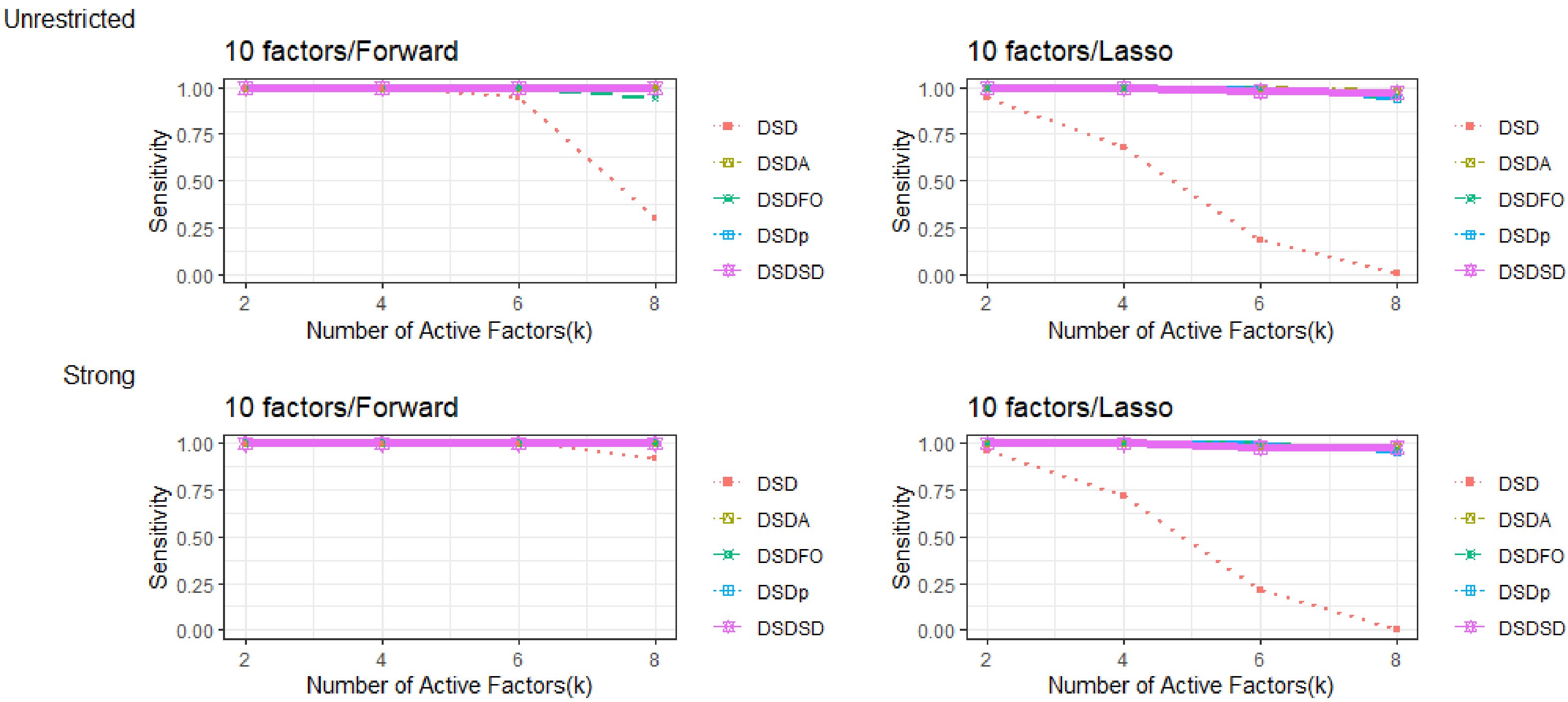

Fig. 15.: DSD+SD Linear Term Sensitivity

traditional DSD. Therefore, these designs also have a better chance of finding the truly active effects, especially when the number of truly active factors increases.

Figure 18, Figure 19, and Figure 20's top two graphs are the plots for comparing the unrestricted models' specificity. The traditional DSD did well in terms of specificity. In general, the DSD+SD performed similarly to the DSD. It performed well because specificity was close to 90% for these designs. All designs perform well with regard to specificity.

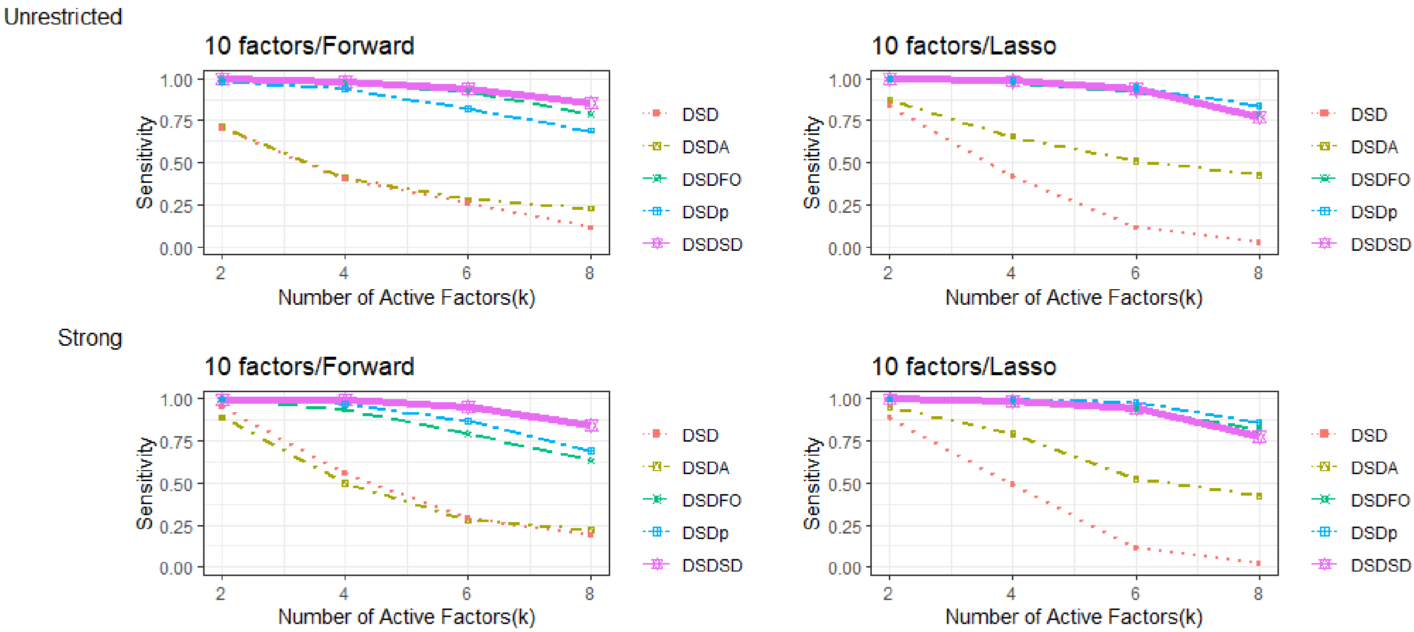

Fig. 16.: DSD+SD Interaction Term Sensitivity

4.5.2 Scenario 2: Strong Heredity Models with Active Second-Order Effects

Figure 15, Figure 16, and Figure 17's bottom two plots show the results when the models follow strong heredity. There are 10 factors with 2, 4, 6, and 8 active factors in the design with two different model selection methods. The DSD+SD has much better sensitivity than the traditional DSD. All augmented DSDs have almost 100% power to detect the main effects. The DSD+SD has clearly higher power than DSDs to detect the interaction effects, and as the number of factors increases, the differences get larger. For the quadratic terms, same as scenario 1, DSD+SD has the most powerful ability to detect corrected active quadratic terms using forward model selection even when there are many active terms in the model and shows competitive

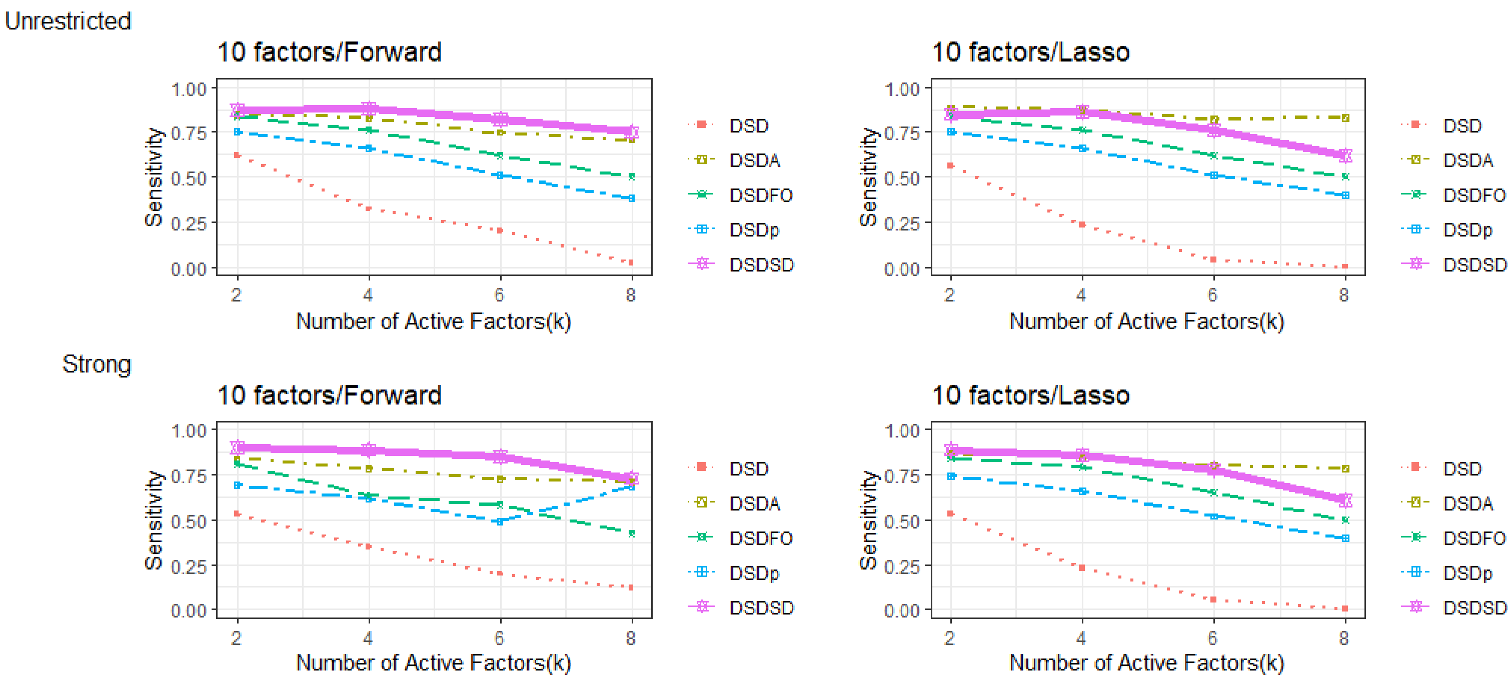

Fig. 17.: DSD+SD Quadratic Term Sensitivity

results to DSDA when using lasso model selection. They are both better than other three designs. So DSD+SD has a higher probability of finding the active effects, especially when the number of active factors increases.

Figure 18, Figure 19, and Figure 20 's bottom two graphs are the plots for comparing the specificity of the strong heredity models. The traditional DSD did well in terms of specificity. In general, the DSD+SD performed similarly to the DSD. Although DSD+SD had lower specificity compared to the DSD in most cases, they still performed well because specificity was close to 90% for these designs.

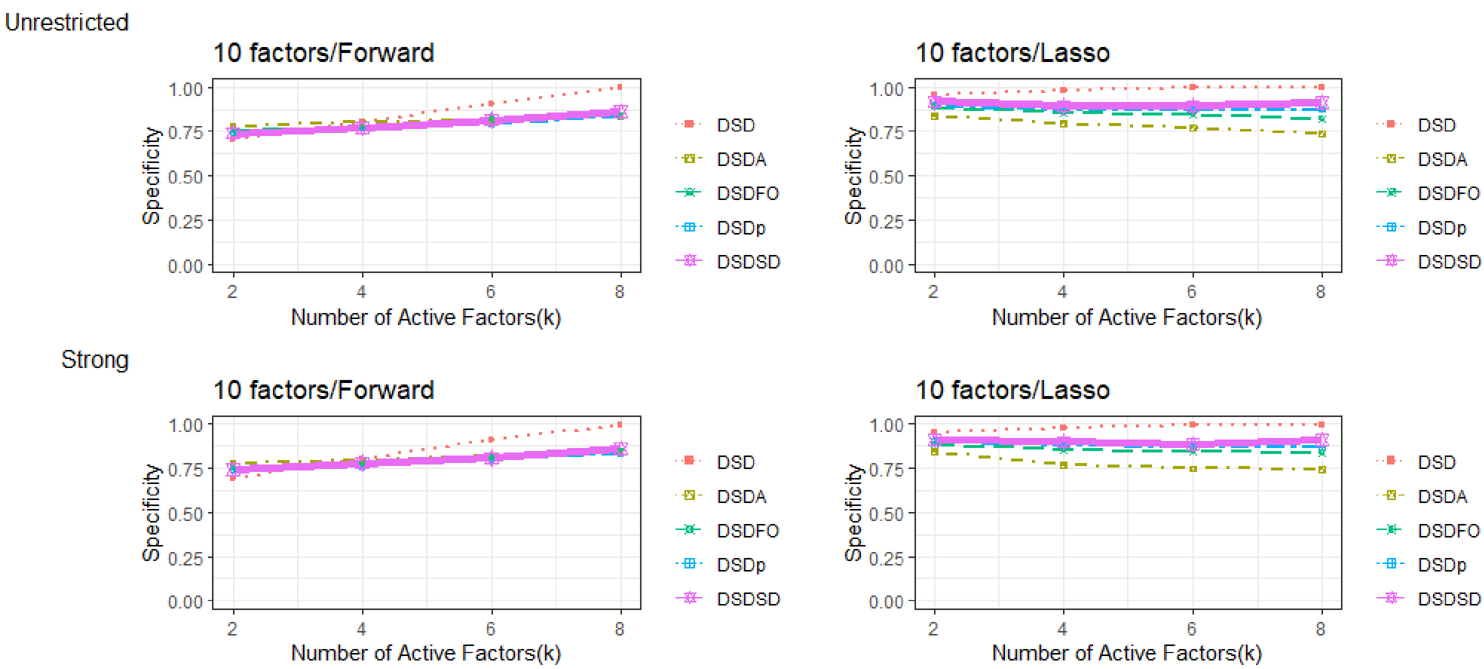

Fig. 18.: DSD+SD Linear Term Specificity

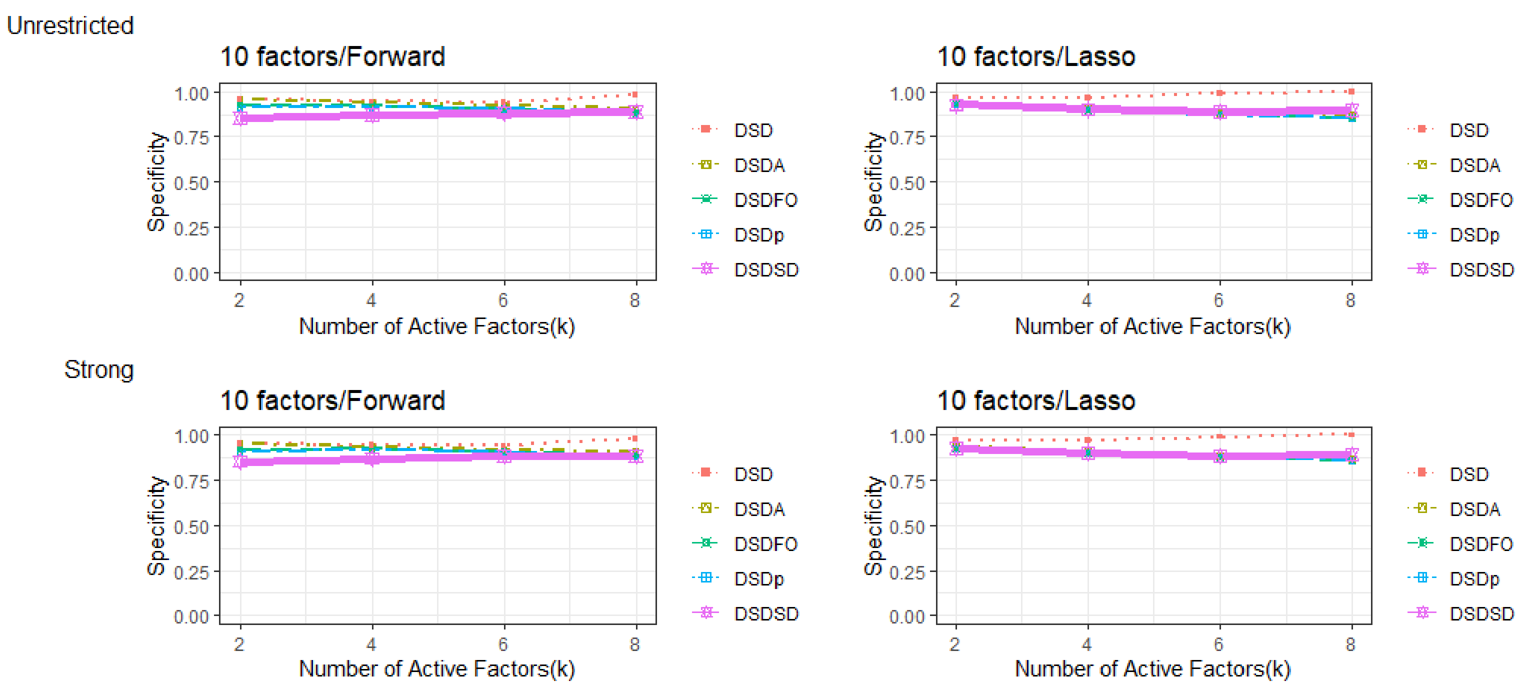

Fig. 19.: DSD+SD Interaction Term Specificity

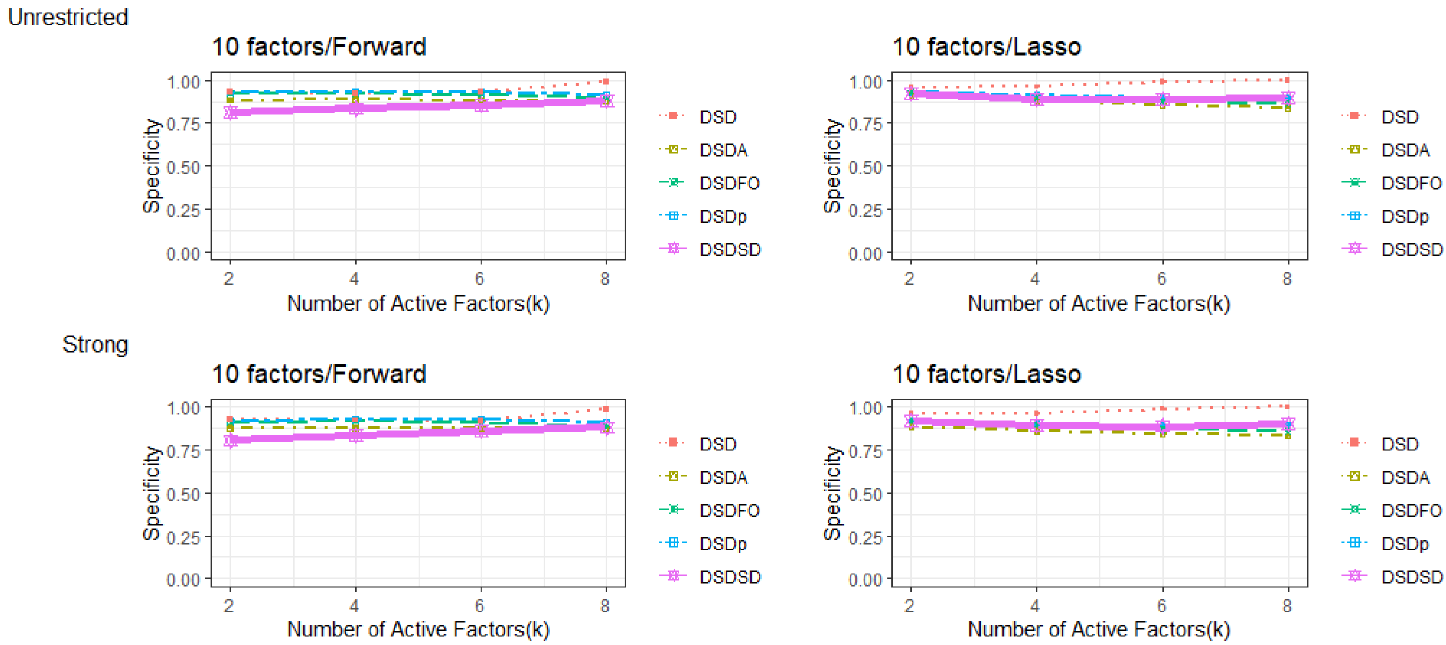

Fig. 20.: DSD+SD Quadratic Term Specificity

4.6 Case Comparison

Two cases represent two different combinations of model heredity (strong and weak) are used to compare DSDSD with DSD. We checked each model's three results; the identified corrected active terms, the incorrectly identified terms (Type I Error), and not identified terms (Type II Error).

Model I is a strong heredity model,

$$y_i = 2X_1 - 1.5X_5 + 2X_7 - 3{X_1}^2 + 2.5{X_5}^2 - 4{X_7}^2 + 4X_1X_5 + 3.5X_1X_7 - 5X_5X_7 + \epsilon_i \quad (4.2)$$

and Model II is a weak heredity model,

$$y_i = 2X_1 + 2X_5 - 1.5{X_1}^2 + 2.5{X_5}^2 - 3.5X_1X_5 + 4X_1X_7 - 5X_5X_7 + \epsilon_i \tag{4.3}$$

In Table 14, the DSD+SD in both regression methods can find all the active terms, including high order terms like quadratic terms. However, DSD+SD also has incorrectly identified some interaction terms. DSD only identified all the linear terms and one interaction term. It missed all quadratic terms and other interaction terms in the forward-step wise regression method. As for the lasso method, DSD missed all active terms. Results for the weak heredity model are in Table 15, DSD+SD still can find all the active terms. However, DSD can only identify all the linear terms and one interaction term; it missed all quadratic terms and other interaction terms in the forward step-wise regression method. For the lasso method, DSD missed all active quadratic terms.

Model I				
	DSD		DSDSD	
	Forward Step-wise	Lasso	Forward Step-wise	Lasso
Identified	X_1, X_5, X_7, X_1X_5	NA	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$
Type I Errors	$X_9, X_{10}, {X_8}^2, X_4X_{10}, X_2X_{10}$ $X_6X_8, X_3X_5, X_4X_5, X_7X_8$	X_4X_{10}	$X_4X_8, X_3X_{10}, X_7X_{10}$ X_1X_2, X_3X_4, X_{10}	X_3X_4, X_4X_5, X_4X_8 X_4X_{10}, X_6X_{10}
Type II Errors	X_1^2, X_5^2, X_7^2 X_1X_7, X_5X_7	$X_1, X_5, X_7, X_1^2, X_5^2, X_7^2$ X_1X_5, X_1X_7, X_5X_7	NA	NA

Table 14.: DSD+SD Strong Heredity Model Results

Model II				
	DSD		DSDSD	
	Forward Step-wise	Lasso	Forward Step-wise	Lasso
Identified	X_1, X_5, X_1^2	$X_1, X_5, X_1X_5, X_1X_7, X_5X_7$	X_1, X_5, X_1X_5, X_5X_7 X_1X_7, X_5^2, X_1^2	$X_1, X_5, X_1X_5, X_1X_7, X_5X_7, X_1^2,$ X_5^2
Type I Errors	$X_4X_8, X_8X_{10}, X_2X_9$ $X_7X_8, X_3X_{10}, X_{10}$	$X_1X_9, X_2X_{10}, X_4X_6, X_4X_8$	$X_{10}, X_4X_8, X_3X_{10}$ $X_7X_{10}, X_3X_9, X_1X_2$	X_1X_2, X_3X_4, X_4X_5 X_7X_{10}, X_8X_{10}
Type II Errors	X_5^2, X_1X_5, X_1X_7 X_5X_7	X_1^2, X_5^2	NA	NA

Table 15.: DSD+SD Weak Heredity Model Results

4.7 Summary and conclusions

The popularity of definitive screening designs (DSD) has risen rapidly. However, only the linear main effects and perhaps the largest second-order term can be identified by an initial DSD. When we have many main effects, DSD may cause an under-fit model. DSD also does not allow for the efficient estimation of the full quadratic model in any more than three factors. Due to the low accuracy of the DSD for pure quadratic estimates and the potential bias of second-order estimators, we created a new augmented design based on another popular subset design. Our new augmented DSD has better precision for pure quadratic estimates and increases the ability to estimate more than three factors in a full quadratic model. Through augmented runs, we increased the design power to identify the active model terms. Therefore, with the augmented DSD designs, we can efficiently estimate a response surface in one experiment.

DSD+SD shows improvement in the PEC and PIC criteria compared with other augmented designs. In the variance estimation, DSD+SD has the smallest variance on linear, interaction, and quadratic terms in all augmenting designs. It also has a very competitive sensitivity and specificity ability in the simulation study.

CHAPTER 5

AUGMENTING DEFINITIVE SCREENING DESIGNS WITH UNIFORM DESIGNS

5.1 Uniform Designs

When using optimality criteria to select a design, the optimal design is based on a pre-specified regression model, for example

$$Y = \sum_{i=1}^{m} \beta_i f_i(x_1, \ldots, x_k) + \epsilon. \tag{5.1}$$

where $x_1, \ldots, x_k$ are k input factors, $f_i s$ are known functions, $\beta_i s$ are unknown parameters and ϵ is the random error. In most cases, the true function we are trying to estimate is unknown, and we approximate this function with our pre-specified model. The true unknown function can be represented as :

$$Y = g(x_1, \ldots, x_k) + \epsilon. \tag{5.2}$$

We want to estimate the average value $E(g(x))$ over the experimental domain. $E(g(x))$ can be estimated by the mean $\bar{h} = \frac{1}{n} \sum_{x \in p} g(x)$, where p is a set of n experimental points. Thus, we look for an experimental design that can estimate $E(g(x))$ efficiently. There are several methods of designs, one is called Latin hypercube sampling proposed by McKay and Conover 1979, which provides an efficient estimate of the overall mean of the response. It has the best performance with respect to the radial-basis functions (Buhmann 2000). These functions were shown to have better performance than the polynomial model. Another design is proposed by Fang 1980, which is called the uniform design. In the uniform design, all the experimental points are uniformly scattered on the domain. An example is found in Bursztyn and Steinberg 2006. A third design is called the sphere-packing design, also known as the maxi-min design, which maximizes the minimum distances between pairs of design points Johnson, Moore, and Ylvisaker 1990. An example of this application can be found in Chen et al. 2006. Yet another design is the maximum entropy design developed by Shewry and Wynn 1987. It uses entropy as the optimality criterion. Entropy is a measure of the amount of information contained in the distribution of a data set. If the data are assumed to be normally distributed, then the design maximizes the determinant of the correlation of the design matrix. All four of the designs discussed above are space-filling experimental designs.

When the experimental domain is continuous, the points in the uniform design are selected from the center of the cells in a deterministically uniform manner. Suppose there are m factors of interest over a domain C^m. The goal is to choose points from a set of n points $P_n = (x_1, \ldots, x_n) \subset \mathrm{C}^m$ such that these points are uniformly scattered on C^m (Fang, Lin, et al. 2000). Let $F_n(x)$ be the empirical distribution function of P_n, $F_n(x) = \frac{1}{n}\sum_{i=1}^{n} I_{x_i \leq x}$,where I is the indicator function. Define $D_p(P_n) = \left[\int_{C^m} |F_n(x) - F(x)|^P dx\right]^{1/p}$, where $F(x)$ is the uniform distribution function on C^m. It can be re-expressed as follows: $D_{(P_n)} = \sup_{x \subset C^m} |F_n(x) - F(x)|$. For the case where m=1, the uniform design under D is $P_n^* = \{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\}$ with $D = \frac{1}{2n}$ (Fang, Lin, et al. 2000). When $m > 1$, it is more difficult to find a uniform design. There are $U-$type uniform designs, where $U_{n,s} = (u_{ij})$ is an n $\times$ s matrix and each column is a permutation of $\{1, 2, \ldots, n\}$. More specifically, a U-type design,$U_{n,s}$, with rank s whose induced matrix has the smallest discrepancy over $X_{n,s}$ is called a U uniform design and can be denoted by $U_n(n^s)$ (Fang, Lin, et al. 2000).

The final focus of this research is using an augmented DSD with a uniform design to get better efficiency for the quadratic terms. The uniform design has two properties: (1) some significant information can be obtained for exploring the relationships between the response and the contributing factors, and (2) it performs well even if the form of the regression model is not known. But unlike the fractional factorial design, a uniform design is not orthogonal. In reality, we do not know the input function. So, the uniform design can provide a good spread of design points over the entire design space, allowing us to explore the relationship between the output and input variables. The theory behind the uniform design is the theory of numbers and the Quasi-Monte Carlo method (Fang, Lin, et al. 2000). Suppose that we need to evaluate the integral

$$\int_D m(X)d_X \tag{5.3}$$

where X is an s-dimension vector, m(X) is a known function, and D is the domain of integration. Then, when X has a uniform distribution over D, the expected value of m(X) is

$$E\{m(X)\} = \int_D \frac{m(X)d_X}{|D|} \tag{5.4}$$

A numerical method that can be used to evaluate the integral is the Monte Carlo Method, which generates n points $P = \{X_1, \ldots, X_n\}^{1/n}$ that are independently and identically distributed over D with a uniform design. Then,

$$\bar{h} = \frac{1}{n} \sum_{X \in P} m(X) \tag{5.5}$$

is an estimate of $E\{m(X)\}$. The Central Limit Theorem (CLT) shows that the rate of convergence of the Monte Carlo method is $n^{-1/2}$. Table 16 shows an example of a $U_8(8^4)$ uniform design with a domain from [-1,1].

Uniform Design				
No. Run	$U_8(8^4)$			
	1	2	3	4
1	0.0923403342	-0.844852364	-0.367414176	-0.367414274
2	0.8213568818	0.1246386386	-0.600651522	-0.600651522
3	-0.08707149	0.8132735427	0.5641017331	-0.813273308
4	-0.613010463	0.3053750085	0.8374501039	0.0670530766
5	0.6232522007	-0.395477565	0.1541016391	-0.093445338
6	0.3956575014	-0.11184812	0.416544874	0.620564738
7	-0.810953035	-0.593616518	-0.104503052	0.8109530347
8	-0.337655646	0.6082597748	-0.822230642	0.3771222913

Table 16.: Uniform Design

5.2 Augmenting DSDs with Uniform Designs

The notation $U_n(n^s)$ is purposely chosen to mimic that commonly used for orthogonal designs $L_n(q^s)$, where n is the number of experiments, s is the number of factors, and q is the number of levels for each factor. The first column of $U_n(n^s)$ can always be taken as $(1, 2, \ldots, n)'$. There are $n! - 1$ possible permutation of $\{1, 2, \ldots, n\}$ for the second column,$n! - 2$ choices for the third column, and so on. The DSDs augmented with these types of designs will be compared to the traditional DSDs in terms of efficiency of the quadratic terms. A fully detailed 6 factor design structure appears in Table 17. To evaluate the DSD + Uniform design, first, the number of runs to consider must be selected for the uniform design. We know the uniform design can have a lot of permutation combinations based on the number of factor levels. However, increasing the number of runs will increase the experimental cost, and we would prefer to keep the run size low. Table 18 illustrates the designs generated with their

DSD+Uniform Design						
No.Run	6 factor DSDs+$U_{13}(13^6)$					
	1	2	3	4	5	6
1	0	1	1	1	1	1
2	0	-1	-1	-1	-1	-1
3	1	0	-1	1	1	-1
4	-1	0	1	-1	-1	1
5	1	-1	0	-1	1	1
6	-1	1	0	1	-1	-1
7	1	1	-1	0	-1	1
8	-1	-1	1	0	1	-1
9	1	1	1	-1	0	-1
10	-1	-1	-1	1	0	1
11	1	-1	1	1	-1	0
12	-1	1	-1	-1	1	0
13	0	0	0	0	0	0
14	0.8066	-0.7346	-0.2717	-0.3064	0.8662	-0.5991
15	0.3224	-0.2677	0.8219	-0.4000	-0.5462	-0.7717
16	-0.9003	0.8451	0.5805	0.2740	-0.5841	0.0824
17	-0.6604	0.6520	0.3228	-0.6074	0.1921	-0.8587
18	0.5964	0.3941	0.9466	-0.0639	0.4730	0.4309
19	-0.2507	-0.4557	0.6573	-0.5153	0.7830	0.8686
20	0.5411	0.7721	-0.5877	0.7712	0.7436	-0.2519
21	-0.5940	-0.2854	-0.6274	0.3185	0.5372	0.2968
22	-0.7953	0.4359	-0.8349	-0.3742	-0.8926	-0.3488
23	-0.3394	-0.7753	-0.1857	-0.6838	-0.7691	0.1940
24	0.2079	0.6236	-0.7708	-0.8904	-0.2011	0.5095
25	-0.4262	-0.6526	0.8781	0.5747	0.2540	-0.4429
26	0.8196	-0.1939	0.4283	0.4259	-0.8369	0.7371

Table 17.: Six factor DSD+Uniform Design

respective number of runs. For the augmented run size using uniform design, we will still try two strategies. One is using the same run size candidate points as DSD, and another is using half the run size of DSD to find the best combination pattern. Evaluation will use the PEC and PIC criteria. Recall the following: Table 19 provides a run size comparison for different designs.

In Figure 21 and Figure 22, DSD stands for definitive screening design, DSDFO stands for DSD augmented with fold-over, CCD stands for central composite design with the axial points at $|\alpha| = 1$, DSCD stands for DSD augmented with composite designs, DSDA stands for DSD augmented with axial runs, OACD stands for

Runs Factors k	k	k+2	k+4	2k
2	6	8	10	12
3	10	12	14	20
4	15	17	19	30
5	21	23	25	42

Table 18.: Number of Runs Required for 2^{nd} order polynomial model

The number of runs for each design							
Design Name	Number of Factors						
	6	7	8	9	10	11	12
OACD	50	82	91	155	155	155	155
DSCD	45	79	81	147	149	151	153
CCD	44	78	80	146	148	150	280
DSDA	26	30	34	38	42	46	50
DSDFO	26	30	34	38	42	46	50
DSDSD	26	30	34	38	42	46	50
DSDp	26	NA	34	NA	42	NA	50
DSDUD	26	30	34	38	42	46	50
DSD	13	15	17	19	21	23	25

Table 19.: Run Size Comparision

orthogonal-array composite design, DSDSD stands for DSD augmented with subset designs, DSDp stands for Definitive Screening Designs obtained by Dropping Columns, and our new augmented DSD with uniform design is called DSDUD. Figure 21 shows DSDUD PEC can estimate all 3-6 factors main effects with their associated two-level interactions. This is an excellent performance of DSDUD. However, Figure 22 shows in the 3, 4, 5, and 6 factor projections, the PIC values of DSDUD are not

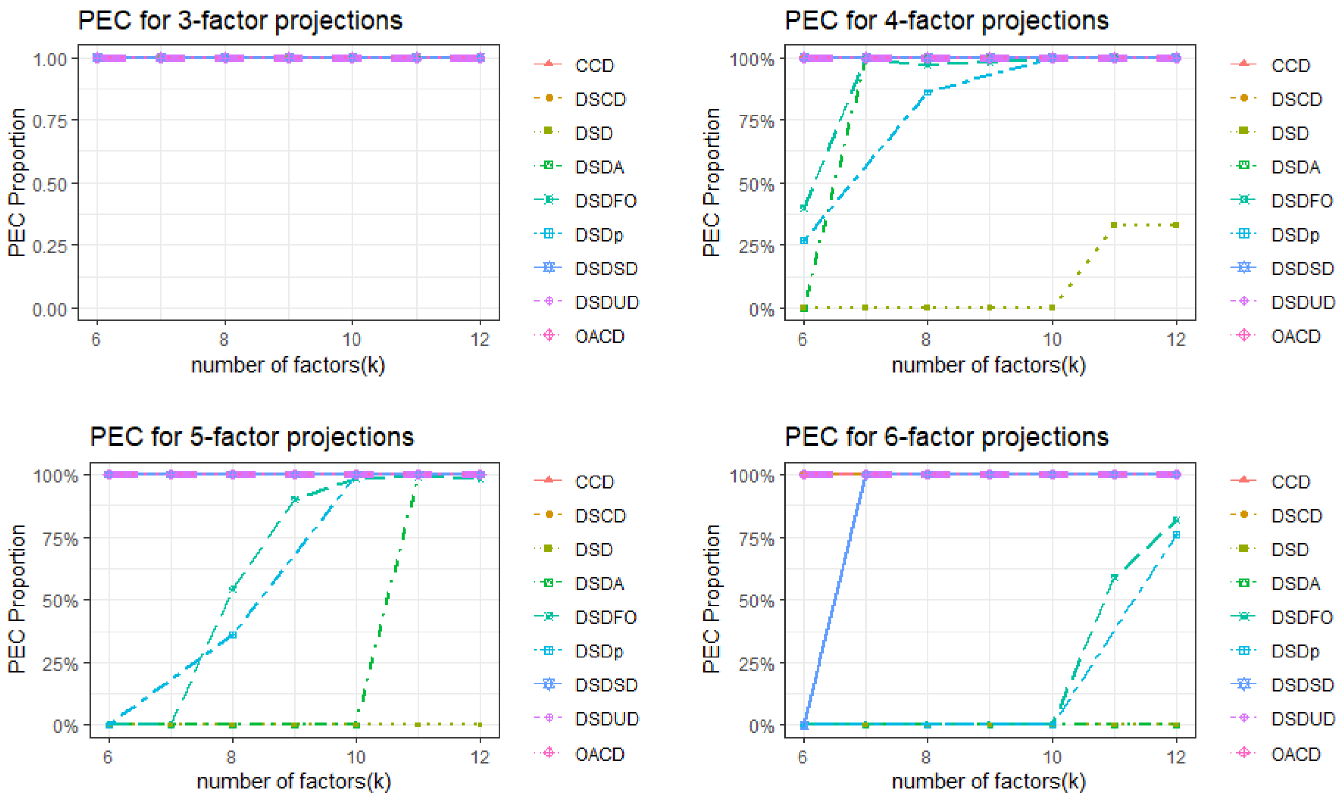

Fig. 21.: DSDUD PEC Comparison for 3-6 factor projections

as competitive as DSD+SD. For the augmentation run sizes we choose from uniform designs, we used the same strategies in section 4. One is the full-size runs match to the DSD, another is half-size runs of the DSD run sizes. In this chapter examples, we used full run size n. For the augmentation run sizes comparison, n and $n/2$ will be introduced in the Appendix section.

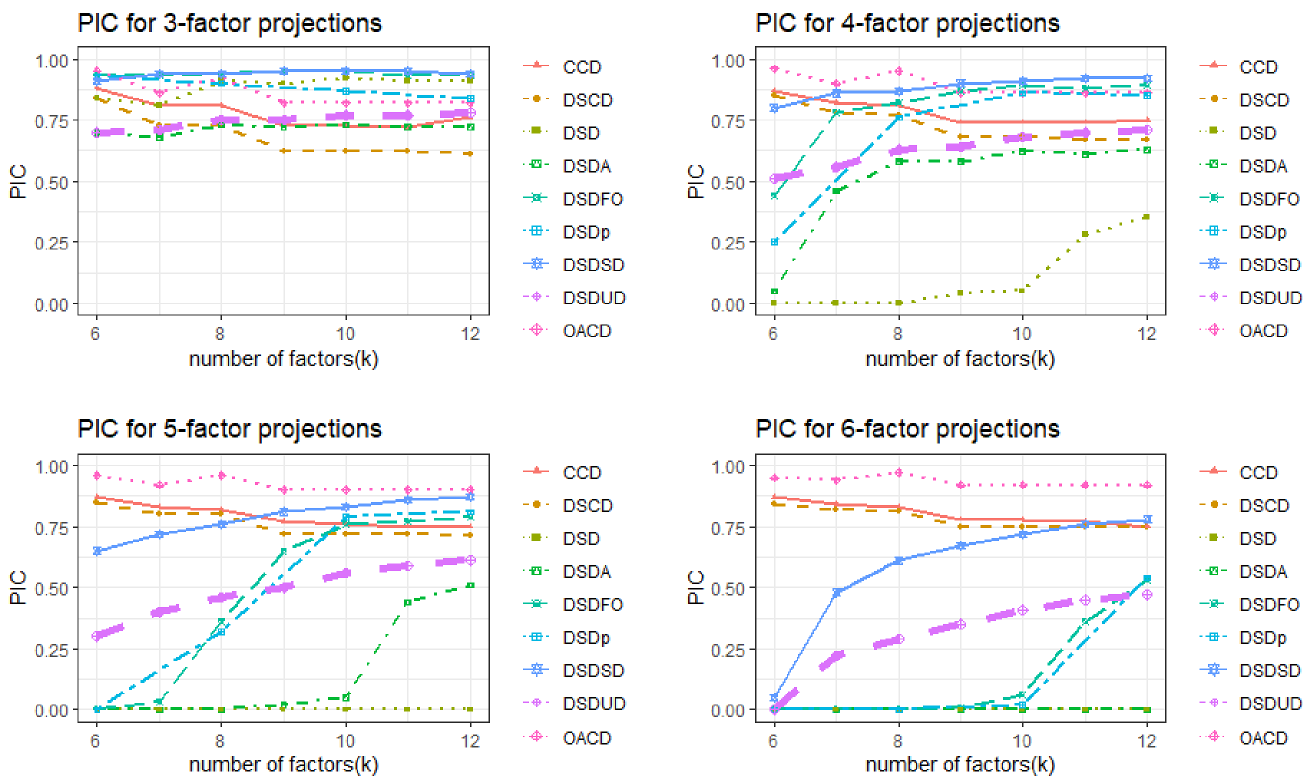

Fig. 22.: DSDUD PIC Comparison for 3-6 factor projections

5.3 Variance Comparisons

We compared OACD, DSDA, DSCD, DSDFO, DSDSD, DSDp, CCD, and DSDs with our new augmented DSD with uniform design (DSDUD). Figure 23 shows the variance of estimation comparison. We can clearly see, in quadratic terms, the DSD shows a large variance as compared with DSDUD. However, the variance of estimation is not as low as DSD+SD.

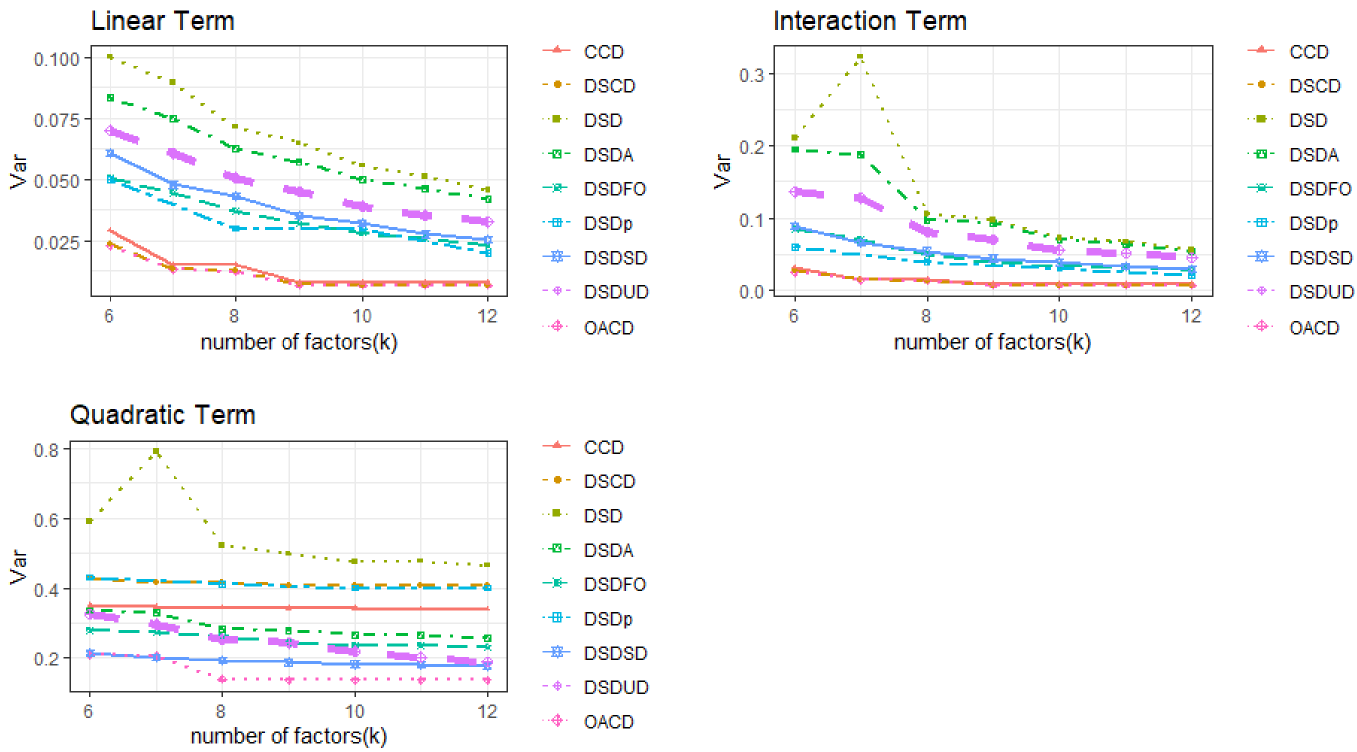

Fig. 23.: DSDUD Variance Estimation Plots

5.4 D-efficiency Comparisons

Figure 24 shows the D-efficiency comparison. On the top left, DSDUD has a comparable D-efficiency for the whole model, it is above 70%. However, with the exception of quadratic effects, D-efficiency values are not competitive with other augmentation strategies.

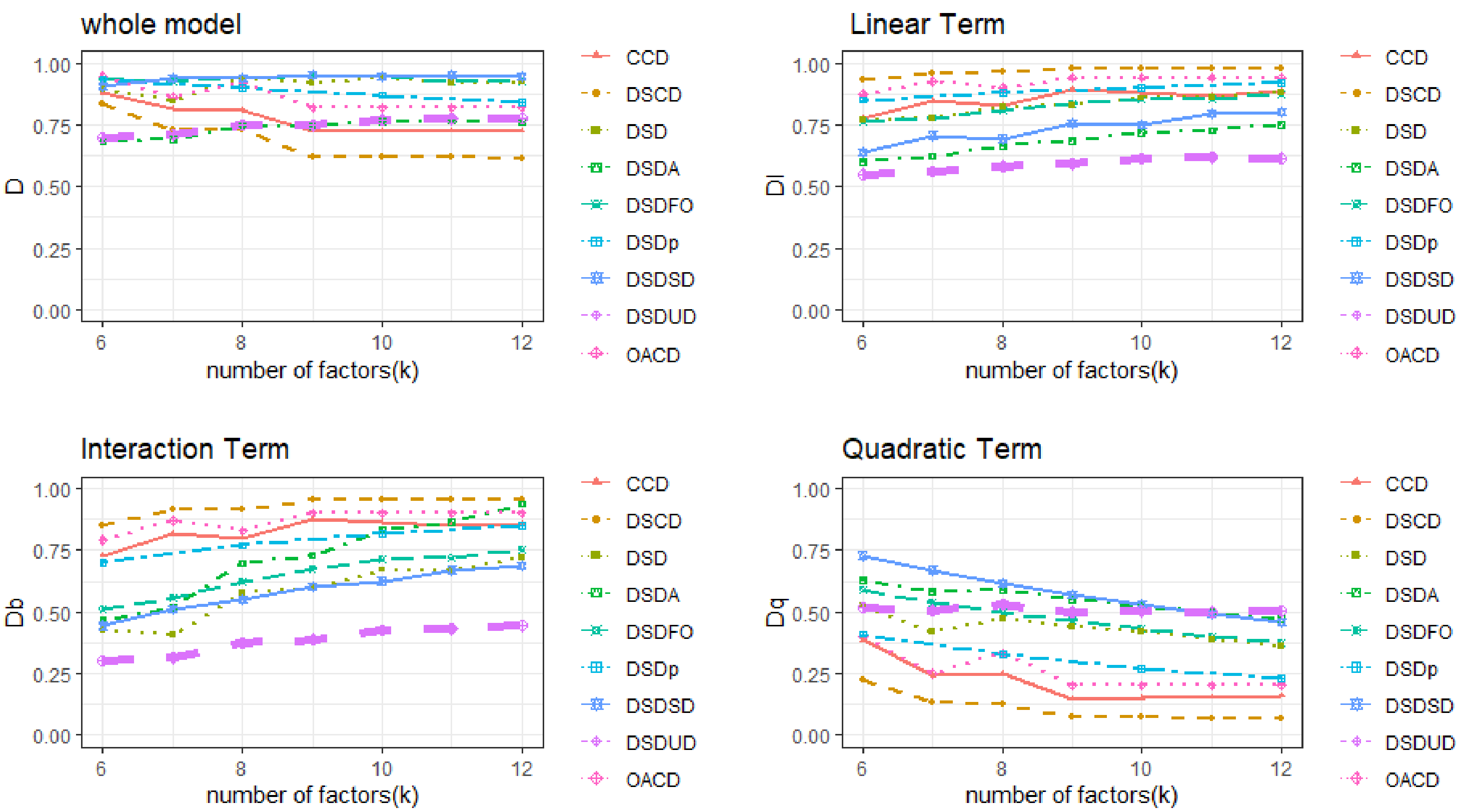

Fig. 24.: DSDUD D Efficiency Plots

5.5 Sensitivity and Specificity Analysis

We want to assess the performance of the DSDUD in terms of sensitivity and specificity rates compared with traditional DSD and some new other augmented DSDs such as DSDp, DSDA, DSDFO, and DSDSD. We constructed the same simulation study with all possible combinations of scenarios as in the previous chapters. We calculated the ratio of the number of selected active effects over the total number of active effects to perform a power analysis.

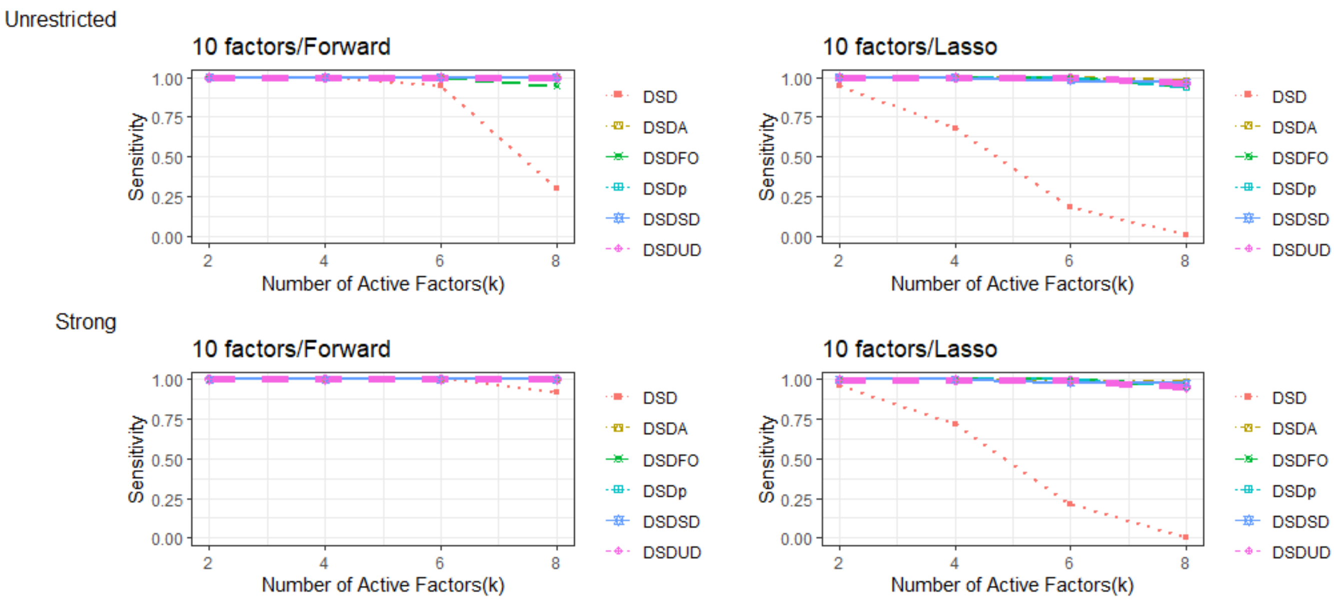

Fig. 25.: DSDUD Linear Term Sensitivity

5.5.1 Scenario 1 : Unrestricted Models with Active Second-Order Effects

Figure 25, Figure 26, and Figure 27's top two plots show the power analysis results for a total of 10 factors with 2, 4, 6, and 8 active factors in the design and for two different model selection methods. Based on these results, for the linear and interaction terms, with the exception of the traditional DSDs, all other augmented DSDs have a strong power ability to identify the active term. For the quadratic terms, DSDUD has the 3rd highest (very close to DSDFO) power ability to detect corrected active quadratic terms, it outperforms than DSDp and DSD. Finally, DSDUD has much better sensitivity than the traditional DSD. Therefore, these designs also have a better chance of finding the truly active effects, especially when the number of truly active factors is increasing. Figure 28, Figure 29, and Figure 30's top two graphs are

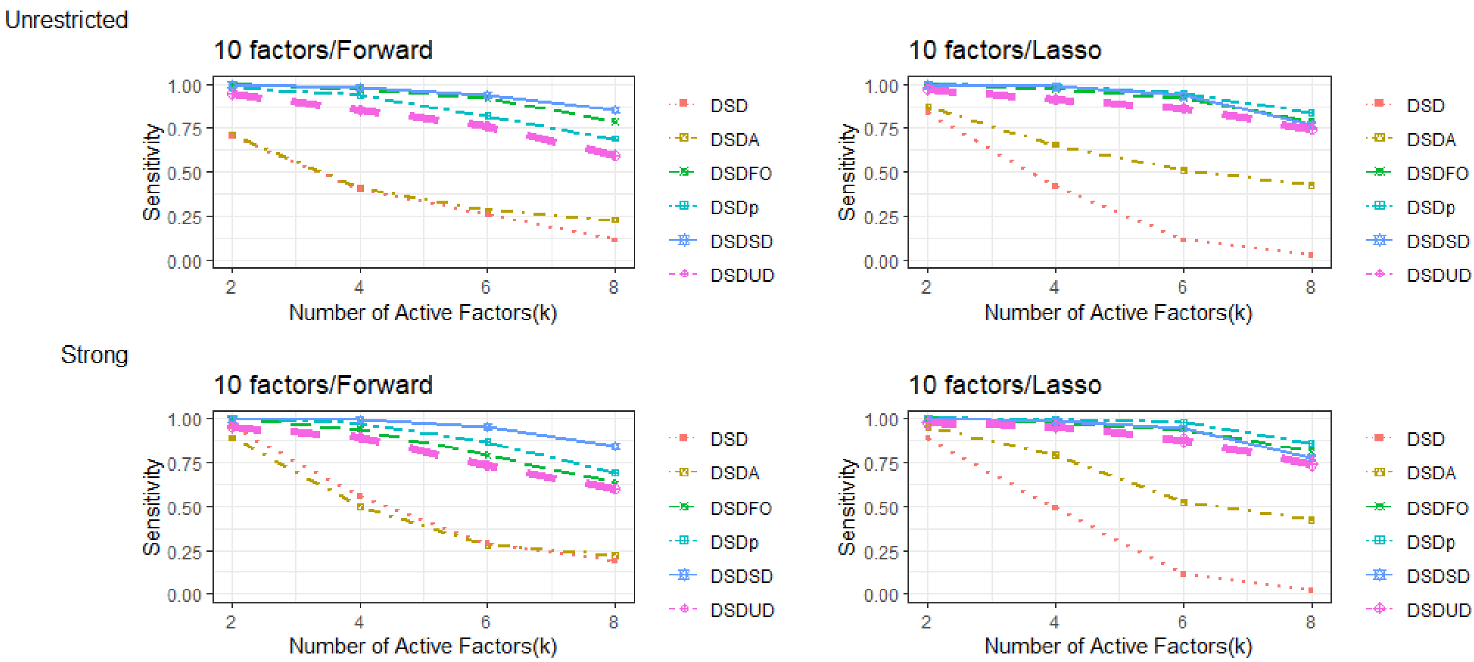

Fig. 26.: DSDUD Interaction Term Sensitivity

the plots for comparing specificity of the unrestricted models. The traditional DSD did well in terms of specificity. In general, the DSDUD performed similarly to the DSD. It performed well because specificity was close to 90% for these designs.

5.5.2 Scenario 2 : Strong Heredity Models with Active Second-Order Effects

Figure 25, Figure 26, and Figure 27's bottoms two plots show the results when the models are following strong heredity. There are 10 factors with 2, 4, 6, and 8 active factors in the design with two different model selection methods. The DSDUD has much better sensitivity than the traditional DSD. They perform competitively with other augmentation strategies to detect the main effects. The DSDUD has more

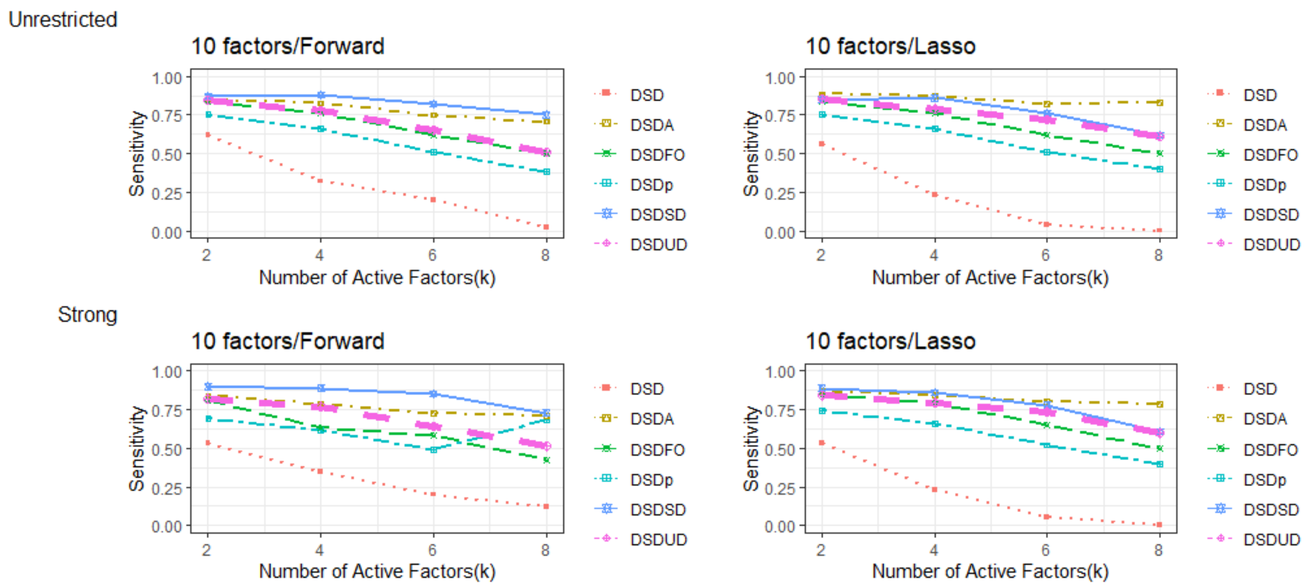

Fig. 27.: DSDUD Quadratic Term Sensitivity

power than DSD and DSDA to detect the interaction effects, and as the number of factors increases, the percentage differences gets larger. DSDUD had a competitive performance on quadratic effects, it is slight better than DSDp and DSDFO, and much better than DSD. So DSDUD has a higher probability of finding the active effects, especially when the number of active factors is increasing.

Figure 28, Figure 29, and Figure 30 's bottom two graphs are the plots for comparing specificity of the strong heredity models. The traditional DSD did well in terms of specificity. In general, the DSDUD performed similarly to the DSD. Although DSDUD had lower specificity when compared to the DSD in most cases, they still performed well because specificity was close to 90% for these designs.

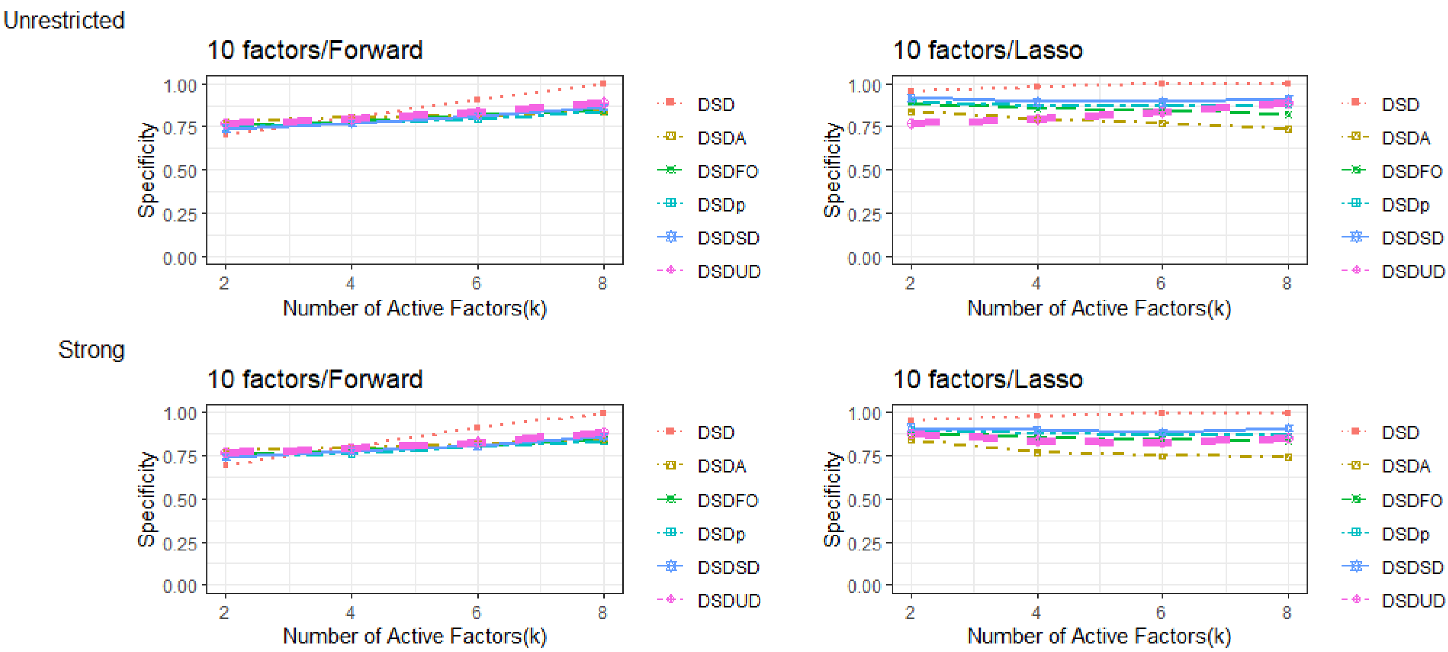

Fig. 28.: DSDUD Linear Term Specificity

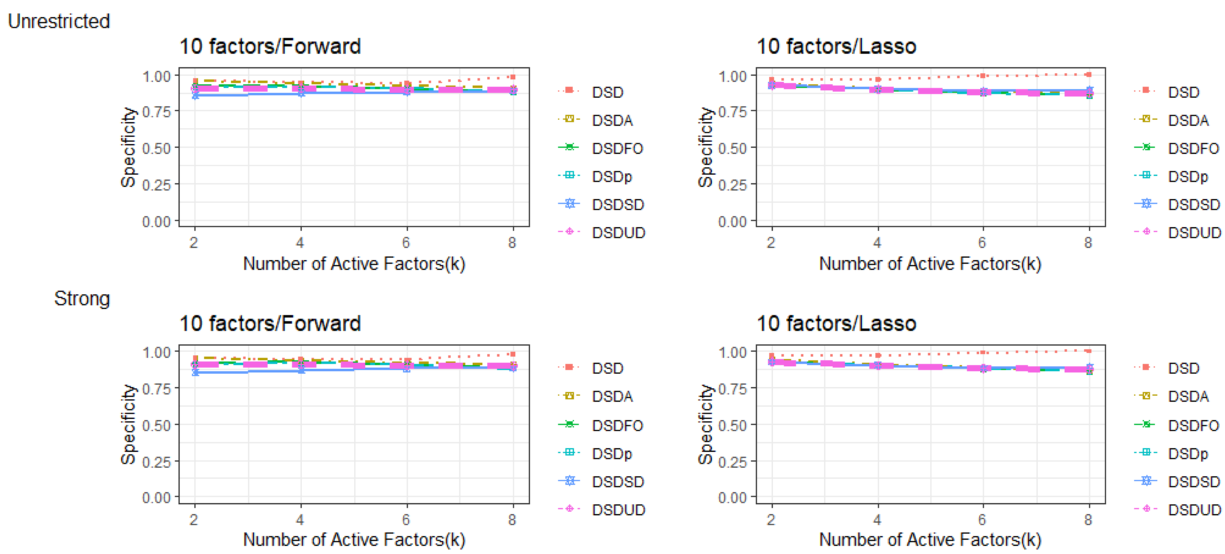

Fig. 29.: DSDUD Interaction Term Specificity

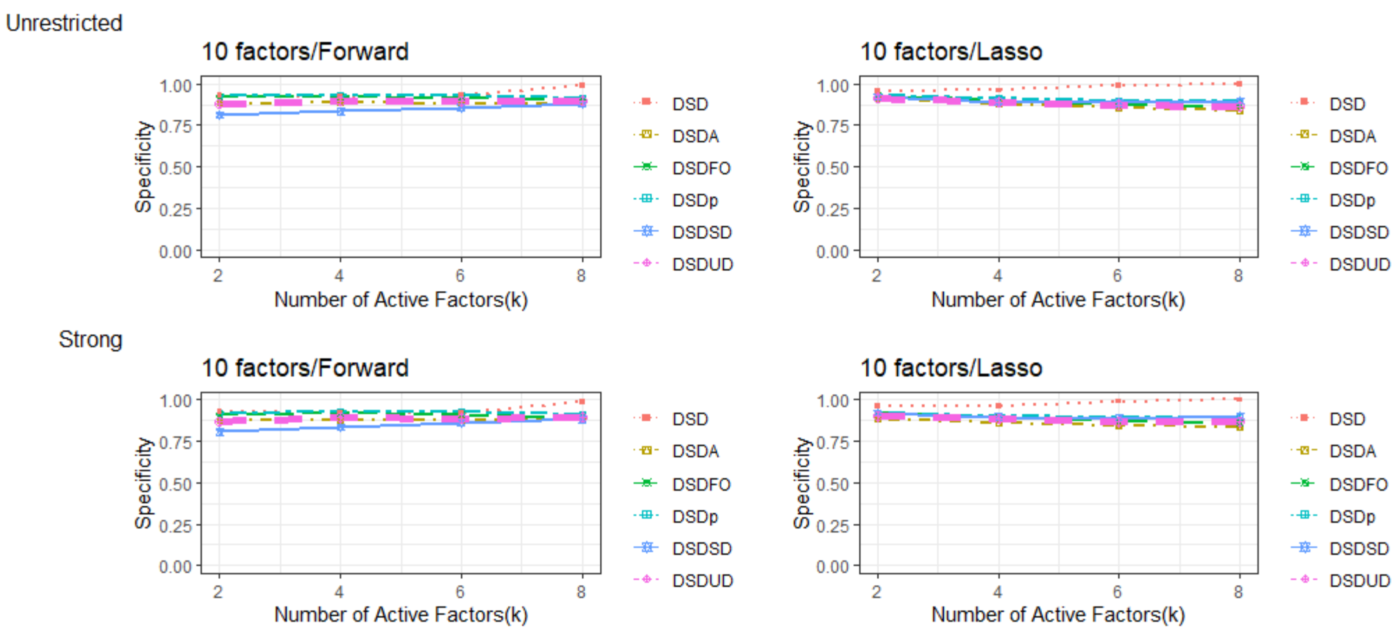

Fig. 30.: DSDUD Quadratic Term Specificity

5.6 Case Comparison

Two cases were used to compare DSDUD with DSD, representing two different combinations of model heredity (strong and weak). We checked three results for each model: the identified correctly active terms, incorrectly identified terms (Type I Error), and not identified terms (Type II Error).

Model I is a strong heredity model:

$$y_i = 2X_1 - 1.5X_5 + 2X_7 - 3{X_1}^2 + 2.5{X_5}^2 - 4{X_7}^2 + 4X_1X_5 + 3.5X_1X_7 - 5X_5X_7 + \epsilon_i \tag{5.6}$$

In Table 20, when the USDUD is using the forward step-wise method, it can exactly find the active terms and high order terms. When using the lasso method, DSDUD did not identify X_5^2. Comparing to DSD, DSDUD finds more active terms than DSD. DSDUD and DSDs both have some incorrectly identified interaction terms. DSD only identified all the linear terms and one interaction term. It missed all quadratic terms and other interaction terms in the forward step-wise regression method. For the lasso method, DSD missed all active terms.

Model II is a weak heredity model:

$$y_i = 2X_1 + 2X_5 - 1.5{X_1}^2 + 2.5{X_5}^2 - 3.5X_1X_5 + 4X_1X_7 - 5X_5X_7 + \epsilon_i \tag{5.7}$$

With results presented in Table 21. DSDUD still can exactly find all the active terms, while DSD also can only identify all the linear terms and one interaction term. It missed all quadratic terms and other interaction terms in the forward step-wise regression method. Using the lasso method, DSD missed all active quadratic terms.

Model I				
	DSD		DSDUD	
	Forward Step-wise	Lasso	Forward Step-wise	Lasso
Identified	X_1, X_5, X_7, X_1X_5	NA	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	$X_1, X_5, X_7, X_1X_5, X_1X_7$ X_5X_7, X_1^2, X_7^2
Type I Errors	$X_9, X_{10}, {X_8}^2, X_4X_{10}, X_2X_{10}$ $X_6X_8, X_3X_5, X_4X_5, X_7X_8$	X_4X_{10}	$X_9, X_{10}, X_1X_2, X_1X_8, X_1X_9$ $X_2X_6, X_3X_7, X_3X_8, X_7X_9$	$X_2X_3, X_2X_6, X_3X_7X_6X_7$ $X_6X_{10}, X_7X_8, X_7X_9, X_{10}^2$
Type II Errors	X_1^2, X_5^2, X_7^2 X_1X_7, X_5X_7	$X_1, X_5, X_7, X_1^2, X_5^2, X_7^2$ X_1X_5, X_1X_7, X_5X_7	NA	X_5^2

Table 20.: DSDUD Strong Heredity Model Results

Model II				
	DSD		DSDUD	
	Forward Step-wise	Lasso	Forward Step-wise	Lasso
Identified	X_1, X_5, X_1^2	$X_1, X_5, X_1X_5, X_1X_7, X_5X_7$	X_1, X_5, X_1X_5, X_5X_7 X_1X_7, X_1^2, X_5^2	$X_1, X_5, X_1X_5, X_1X_7, X_5X_7, X_1^2$ X_5^2
Type I Errors	$X_4X_8, X_8X_{10}, X_2X_9$ $X_7X_8, X_3X_{10}, X_{10}$	$X_1X_9, X_2X_{10}, X_4X_6, X_4X_8$	X_9, X_4X_{10} X_3^2	$X_{10}, X_3X_4, X_6X_{10}$ X_7X_8, X_3^2
Type II Errors	X_5^2, X_1X_5, X_1X_7 X_5X_7	X_1^2, X_5^2	NA	NA

Table 21.: DSDUD Weak Heredity Model Results

5.7 Summary and conclusions

Even though we improved the precision to identify quadratic terms, the procedures are still misleading in identifying the interaction terms. But for our design goal, we need to find all the right active terms in our design model, so we will not miss important information for the analysis step. Our new augmented DSD can achieve this goal. DSD can be used to identify the main effects and some second-order terms. When we have many main effects, DSD may cause an under-fit model. DSD also cannot allow for the efficient estimation of the full quadratic model in any more than three factors. Our augmented DSD has better precision for pure quadratic estimates, and increases the ability to estimate more than three factors in a full quadratic model. Therefore, with the augmented DSD designs, we can efficiently estimate a response surface in one experiment. While DSDUD does well with respect to the estimation of 2nd-order models, they did not outperform other augmentation strategies with respect to information and variance measure.

CHAPTER 6

SUMMARY

6.1 Summary of Research

For a second order polynomial model, a design must have enough degrees of freedom to estimate all effects. For example, if we have k factors, then we will need $\frac{(k+1)(k+2)}{2}$ design runs. Jones and Nachtsheim 2011 proposed the three-level DSD for screening the continuous factors in the presence of active second order effects. Dougherty et al. 2015, however, showed the DSD lacked the power to separate active second order effects when both two factor interactions and pure quadratic effects are active. For $k \geq 6$, the DSD can only project down to a full quadratic model in any three factors. We introduced three ways to augment the DSD, which increase the detection performance of active second-order effects. Our approach took the run efficient DSD as a baseline, and our augmented designs can improve effect estimablity. So far, DSDFO, DSDSD, and DSDUD all show much better projection capacity than DSD. They also show that augmenting DSDs is better than the standard DSDs with regard to identifying active effects, especially pure-quadratic effects, and have better power to identify active model terms. Therefore, with the augmented DSD designs, we can efficiently estimate a response surface in one experiment. If the primary interest focuses on quadratic terms, DSD+SD is preferred over other augmentation DSD.

6.2 Recommendations for Future Research

This research focused on better estimation efficiency of existing second-order models and quadratic effects. It is important to review alternative methodologies of analysis to see if performance can be attributed to the design structure or analytical methodologies for the identification of active results. DSDFO and DSDSD both can fit more second order models in more than three factors; meanwhile, they have better estimation efficiency in quadratic effects and better power to identify active model terms with a good cost-performance ratio. While DSDUD also increased the ability to fit more second order models in more than three factors and did a better estimation efficiency in quadratic effects, it poorly estimated the linear and interaction terms. That will decrease the whole model efficiency. It would be interesting to try some different run size from uniform design to check the effect. For the DSDUD, we can try some different run sizes from uniform design. For the DSDSD, we can combine with runs from other orbits(S_r).

Appendix A

ABBREVIATIONS

DSDFO	Augmented Definitive Screening Design with fold over and column permutation
BBD	Box-Behnken Design
CCD	Central Composite Design
SCD	Small Composite Designs
VCU	Virginia Commonwealth University
DSDs	Definitive Screening Designs
DOE	Design of Experiments
DSDA	DSD with axial runs
DSCD	DSD with a two-level orthogonal array composite design
DSDp	Definitive Screening Designs Obtained by Dropping Columns
RSD	Response Surface Design
PIC	Projection Information Capacity
PEC	Projection estimation capacity
OACDs	Orthogonal-array composite designs
DSDSD	Definitive Screening Designs with Subset designs
DSDUD	Definitive Screening Designs with Uniform Design

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Appendix B

APPENDIX

B.0.1 DSD+SD n and n/2 Augmentation Discussion

Figure 31 showed a PIC value comparison between full-size augmented run and half-size augmented run. Full size means the same number of run sizes as the DSDs structured used. Half-size is half of it. From Figure 31, when the designer tries to project on less than or equal to four factors, we can consider using a half-size run for augmenting. It did not show an enormous difference when using full size. Each experiment run in the real world problem will be expensive; a half-size augmented run can have better budget control and more economical. Table 22 and Table 23 show a consistent result like the PIC plot. For each k factors in the design, augmented half-size runs can estimate almost all the $k-2$ main effects with their associated two-level interactions. When the design factor is getting larger, it can estimate six main effects with their associated two-level interactions.

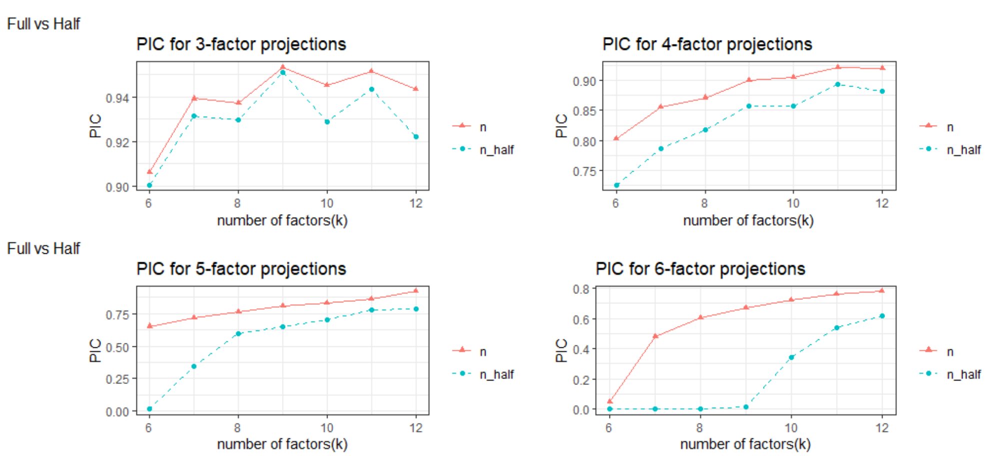

Fig. 31.: DSD+SD PIC run size Comparison

B.0.2 DSD+SD Supplement Tables

PEC(Projection Estimation Capacity)						
Factor	Projection Estimation Capacity					
	P_3	P_4	P_5	P_6	P_7	P_8
k=6	20/20	15/15	6/6	0/1	NA	NA
k=7	35/35	35/35	21/21	7/7	0/1	NA
k=8	56/56	70/70	56/56	28/28	0/8	0/1
k=9	84/84	126/126	126/126	84/84	36/36	0/9
k=10	120/120	210/210	252/252	210/210	120/120	0/45
k=11	165/165	330/330	462/462	462/462	330/330	0/165
k=12	220/220	495/495	792/792	924/924	792/792	495/495

Table 22.: DSD+SD Full Size Run Augmented PEC

PEC(Projection Estimation Capacity)						
Factor	Projection Estimation Capacity					
	P_3	P_4	P_5	P_6	P_7	P_8
k=6	20/20	15/15	0/6	0/1	NA	NA
k=7	35/35	35/35	21/21	0/7	0/1	NA
k=8	56/56	70/70	56/56	0/28	0/8	0/1
k=9	84/84	125/126	121/126	0/84	36/36	0/9
k=10	120/120	209/210	246/252	149/210	0/120	0/45
k=11	165/165	330/330	462/462	458/462	0/330	0/165
k=12	220/220	495/495	792/792	923/924	0/792	0/495

Table 23.: DSD+SD Half Size Run Augmented PEC

B.0.3 DSDUD n and n/2 Augmentation Discussion

Figure 32 showed a PIC value comparison between full-size augmented run and half-size augmented run. Full size means the same number of run sizes as the DSDs structured used. Half-size is half of it. From Figure 32, when the designer tries to project on less than or equal to five factors, we can consider using a half-size run for augmenting. It did not show an enormous difference when using full size, even it is better when projecting on three factors. Table 24 and Table 25 show a consistent result like the PIC plot. For each k factors in the design, augmented half-size runs can estimate almost all the 6 main effects with their associated two-level interactions when having 12 factors in the model.

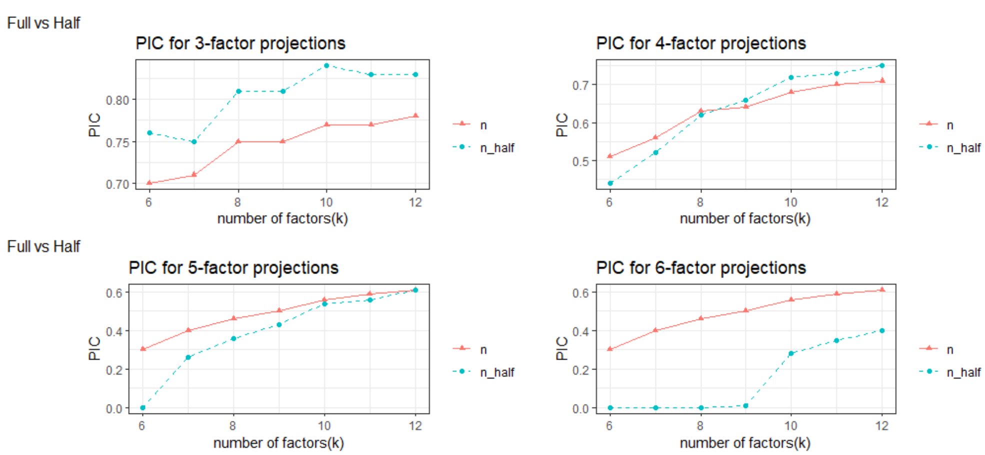

Fig. 32.: DSDUD PIC run size Comparison

B.0.4 DSDUD Supplement Tables

PEC(Projection Estimation Capacity)						
Factor	Projection Estimation Capacity					
	P_3	P_4	P_5	P_6	P_7	P_8
k=6	20/20	15/15	6/6	0/1	NA	NA
k=7	35/35	35/35	21/21	7/7	0/7	NA
k=8	56/56	70/70	56/56	28/28	0/8	0/1
k=9	84/84	126/126	126/126	84/84	36/36	0/9
k=10	120/120	210/210	252/252	210/210	120/120	0/45
k=11	165/165	330/330	462/462	462/462	330/330	0/165
k=12	220/220	495/495	792/792	924/924	792/792	495/495

Table 24.: DSDUD Full Size Run Augmented PEC

PEC(Projection Estimation Capacity)						
Factor	Projection Estimation Capacity					
	P_3	P_4	P_5	P_6	P_7	P_8
k=6	20/20	15/15	0/6	0/1	NA	NA
k=7	35/35	35/35	21/21	0/7	0/1	NA
k=8	56/56	70/70	56/56	0/28	0/8	0/1
k=9	84/84	126/126	126/126	0/84	0/36	0/9
k=10	120/120	210/210	252/252	210/210	0/120	0/45
k=11	165/165	330/330	462/462	462/462	0/330	0/165
k=12	220/220	495/495	792/792	924/924	0/792	0/495

Table 25.: DSDUD Half Size Run Augmented PEC

B.0.5 All Augmented Definitive Screening Designs Sensitivity and Specificity Analysis

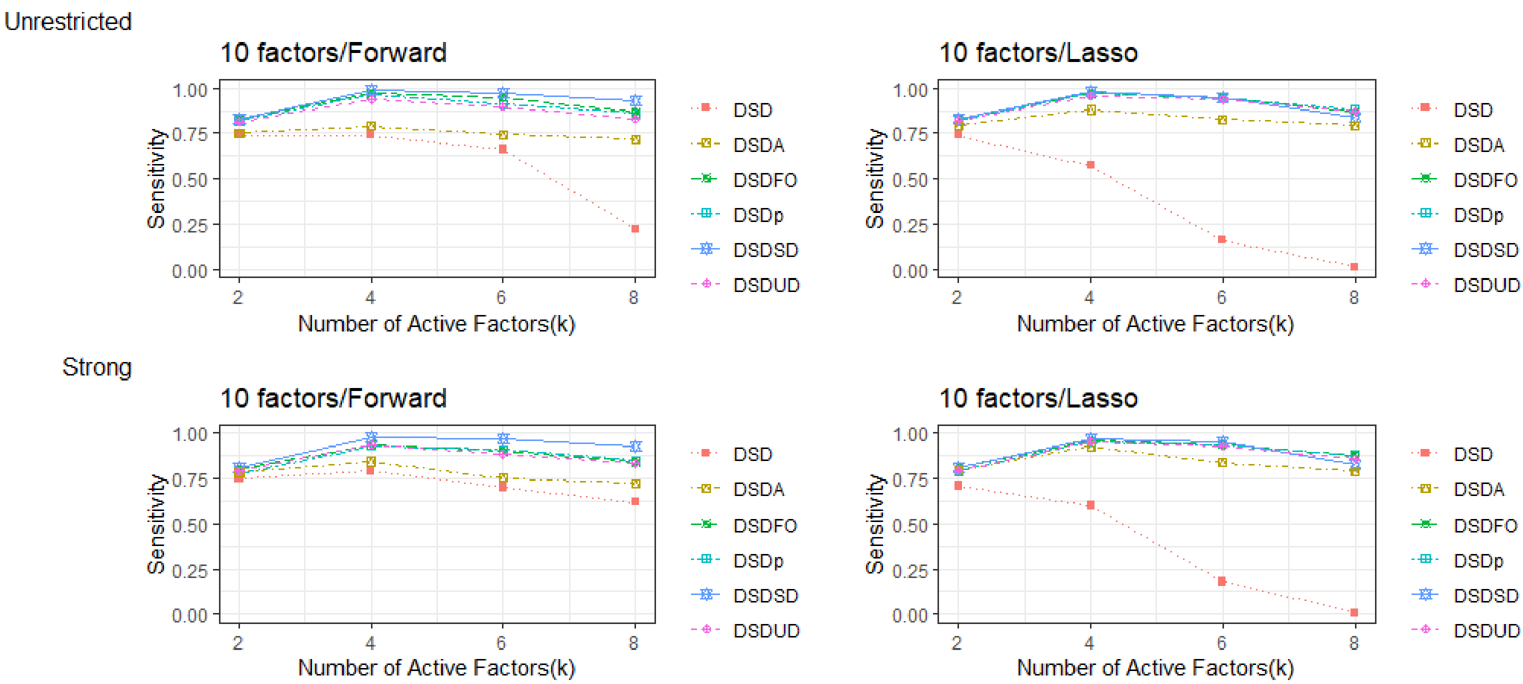

Fig. 33.: All augmented DSDs Full Model Sensitivity

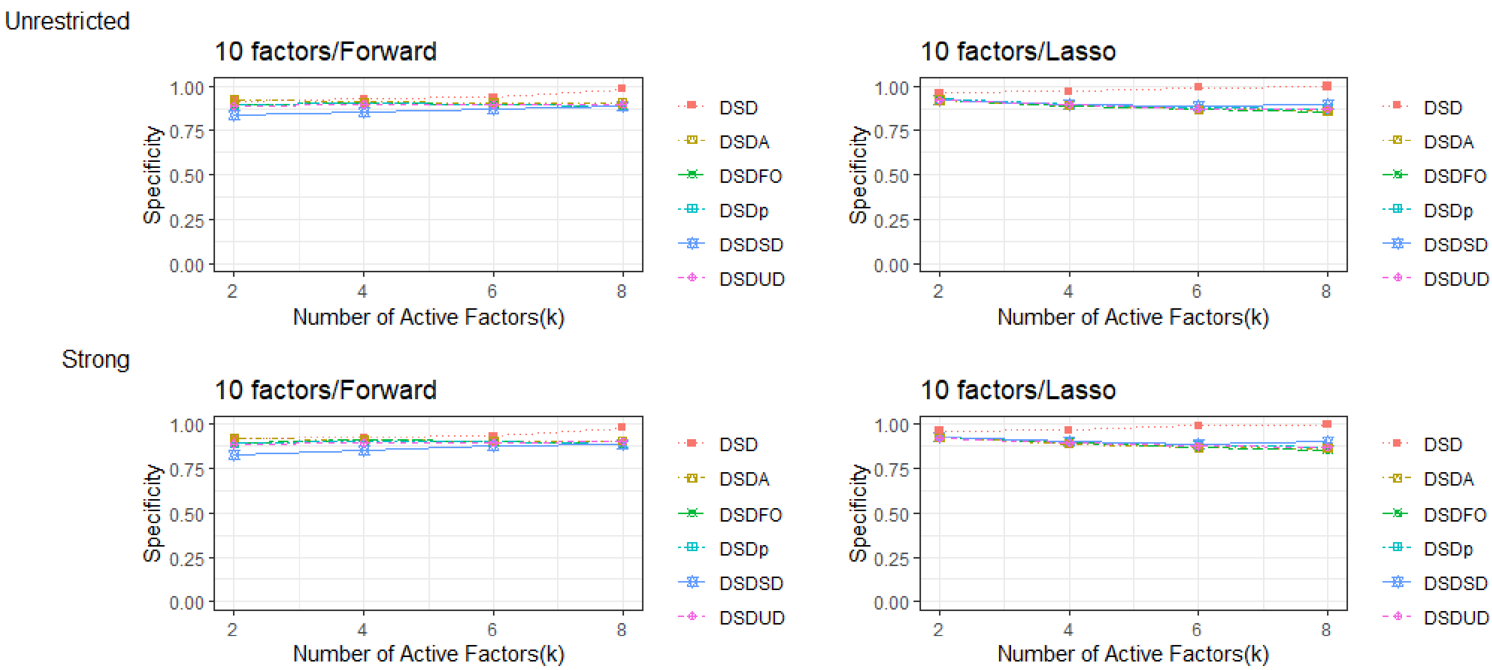

Fig. 34.: All augmented DSDs Full Model Specificity

B.0.6 All Augmented Definitive Screening Designs Comparison Supplement Table

DSD+SD can have consistent results for Type II error than other augmented DSDs.

Model I				
Design	Model Selection	Identified	Type I Error	Type II Error
DSDUD	Forward	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	$X_9, X_{10}, X_1X_2, X_1X_8, X_1X_9$ $X_2X_6, X_3X_7, X_3X_8, X_7X_9$	NA
	Lasso	$X_1, X_5, X_7, X_1X_5, X_1X_7$ X_5X_7, X_1^2, X_7^2	$X_2X_3, X_2X_6, X_3X_7, X_6X_7$ $X_6X_{10}, X_7X_8, X_7X_9, X_{10}^2$	X_5^2
DSDA	Forward	X_1, X_5, X_7, X_1^2 X_5^2, X_7^2	$X_4X_{10}, X_3X_{10}, X_4X_6, X_4X_5$ $X_5X_{10}, X_7X_9, X_1X_{10}, X_9, X_{10}$	X_1X_5, X_1X_7 X_5X_7
	Lasso	X_1, X_5, X_1^2, X_5^2 X_1X_5, X_1X_7, X_5X_7	$X_9, X_{10}, X_2X_{10}, X_4X_6$ X_4X_8, X_5X_7, X_7X_9	NA
DSDp	Forward	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	$X_3, X_9, X_6X_9,$ X_8X_9, X_9^2	NA
	Lasso	X_1, X_5, X_7, X_1X_5 $X_1X_7, X_5X_7, X_1^2, X_7^2$	X_2X_6, X_2X_7, X_3X_7 X_4X_{10}, X_5X_8	X_5^2
DSDFO	Forward	X_1, X_5, X_7, X_1X_5 X_1X_7, X_5X_7, X_7^2	$X_2X_5, X_2X_{10}, X_4X_7$ $X_5X_6, X_7X_{10}, X_{10}^2$	X_1^2, X_5^2
	Lasso	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	$X_2X_4, X_2X_8, X_2X_9, X_2X_{10}$ $X_4X_{10}, X_6X_8, X_3^2, X_9^2$	NA
DSDSD	Forward	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	$X_4X_8, X_3X_{10}, X_7X_{10}$ X_1X_2, X_3X_4, X_{10}	NA
	Lasso	$X_1, X_5, X_7, X_1X_5, X_1X_7$ $X_5X_7, X_1^2, X_5^2, X_7^2$	X_3X_4, X_4X_5, X_4X_8 X_4X_{10}, X_6X_{10}	NA

Table 26.: All augmented DSDs Strong Heredity Model Results

Model II				
Design	Model Selection	Identified	Type I Error	Type II Error
DSDUD	Forward	X_1, X_5, X_1X_5, X_5X_7 X_1X_7, X_1^2, X_5^2	X_9, X_4X_{10} X_3^2	NA
	Lasso	X_1, X_5, X_1X_5, X_1X_7 X_5X_7, X_1^2, X_5^2	$X_{10}, X_3X_4, X_6X_{10}$ X_7X_8, X_3^2	NA
DSDA	Forward	X_1, X_5, X_1^2 X_5^2, X_5X_7	$X_4X_8, X_8X_{10}, X_2X_9, X_7X_8$ $X_3X_{10}, X_3X_7, X_9, X_{10}$	X_1X_7, X_1X_5
	Lasso	X_1, X_5, X_1^2, X_5^2 X_5X_7, X_1X_5, X_1X_7	$X_9, X_10, X_2X_10, X_4X_6$ X_4X_8, X_5X_7, X_7X_9	NA
DSDp	Forward	X_1, X_5, X_1^2, X_5^2 X_5X_7, X_1X_7, X_1X_5	X_9^2, X_9, X_3 X_8X_9, X_6X_9	NA
	Lasso	X_1, X_5, X_1X_5 X_1X_7, X_5X_7, X_5^2	X_8X_9	X_1^2
DSDFO	Forward	X_1, X_5, X_1X_5, X_5X_7 X_1X_7, X_1^2, X_5^2	X_7, X_9, X_2X_9 X_5X_8	NA
	Lasso	X_1, X_5, X_1X_5, X_1X_7 X_5X_7, X_5^2	$X_1X_6, X_2X_{10}, X_3X_7$ X_7X_{10}, X_{10}^2	X_1^2
DSDSD	Forward	X_1, X_5, X_1X_5, X_5X_7 X_1X_7, X_5^2, X_1^2	$X_{10}, X_4X_8, X_3X_{10}$ $X_7X_{10}, X_3X_9, X_1X_2$	NA
	Lasso	X_1, X_5, X_1X_5, X_1X_7 X_5X_7, X_1^2, X_5^2	X_1X_2, X_3X_4, X_4X_5 X_7X_{10}, X_8X_{10}	NA

Table 27.: All augmented DSDs Weak Heredity Model Results

VITA

Tianchi Zhang is an international student originally from China. He came to the United States to seeking his Bachelor's degree in Art and Science in 2010. He got his Bachelor's degree in construction management and minor in Statistics in 2013. Then he earned a full scholarship from Miami University at Ohio, studying statistics for two years as a master's degree.

Tianchi Zhang began his doctoral studies at VCU in 2015. He conducted his dissertation research in experimental design under the guidance of Dr. David J Edwards. Upon graduation, he will be a statistician in the pharmaceutical field.