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D-OPTIMAL MINIMAX CRITERION FOR TWO-LEVEL FRACTIONAL FACTORIAL SPLIT PLOT DESIGNS

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ABSTRACT. In this paper, the D-optimal minimax criterion of two-level fractional factorial split-plot designs were constructed and a general form of the loss function for the criterion was provided. This was used in searching for optimal designs. The optimum designs were obtained via the algorithm developed in python programming language among many designs constructed. As such, the resulting designs are called D-optimal minimax two-level fractional factorial split plot designs. The efficiency of D-optimal minimax designs was felt when compared with both A- and D-optimal designs.

1. INTRODUCTION

Factorial designs are useful to study the effects of two or more factors with their interactions effects in an experiment. In every complete trial or replicate of an experiment, all possible combinations of the levels of the factors are investigated. As the numbers of factors increase, the numbers of runs required for a full replicate of the design rapidly outgrows the resources of experimenters. As such, fractional factorial designs are then employed to screen the factors and identify those with significant effects. At times, it may be impossible to perform the trial in a complete random

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form, due to costs, nature of the process or experimental venue, this results in fractional factorial (FF) designs with randomization restrictions and this give rise to fractional factorial split-plot (FFSP) designs.

Fractional factorial split-plot designs are used in industrial experiments where some factors may require larger experimental units than others or their levels are more difficult to change. This design is also applicable to industrial experiments with multiple processing stages where the levels of the factors are assigned at different stages. For more examples see [9], [8] and [10].

In the design of experiments, optimal designs is a group of experimental designs that are the best with respect to a statistical criterion. An Optimal design uses the best factor levels combinations, that are selected from reducing the experimental runs in the original design. Optimal design enables parameters to be estimated without bias and with minimum variance. An alternative criterion called the maximal rank-minimum aberration criterion for selecting optimal fractional factorial split plot designs was suggested by [11]. The study also shown how this alternative criterion performed in terms of selecting the optimal designs and making comparison to the minimum aberration criterion.

Researchers such as [1, 2, 4] and [11] used the minimum aberration criterion to rank fractional factorial split plot designs, and also [6] introduced the minimum secondary aberration to distinguish between non-isomorphic minimum aberration fractional factorial split plot design designs.

Meanwhile, [5] ranked the designs based on the maximum number of clear two factor interactions (2FI's). These criteria are based on the effect of hierarchal principle; (i) lower order effects are more likely to be significant than higher order ones, (ii) factorial effects of the same-order are equally likely to be important. Also, [3] ranked fractional factorial split plot designs using the D-optimality criterion.

The minimum aberration criterion produces optimal design that minimizes the alias of the important effects. Although the minimum aberration criterion and the D-optimal criterion are mostly used for constructing optimal fractional factorial split-plot designs, the optimal designs selected by the two criteria may have large mean square error (MSE). The minimum aberration criterion focuses on minimizing the bias of the estimation but less concerns about minimizing the variances and covariances. In [12], construction of foldovers of two-level fractional factorial split-plot designs were considered and a catalog of optimal foldover plans for initial minimum aberration fractional factorial split-plot designs consisting of 16 and 32 runs were equally provided. Some theoretical results to construct FFSP designs with weak minimum aberration, which further shown that quite a few of them are also minimum aberration designs was discussed by [13]. Therefore, the optimal fractional factorial split-plot design constructed by this criterion may have higher mean square error due to higher variances or covariances of the estimation. On the contrary, the D-optimal criterion aims to minimize the variances and covariances but does not consider the bias of the estimation.

In this paper, the focus is on regular two-level fractional factorial split plot designs, where the factors are classified into two, that is hard to change and easy to change also refer to as whole plot factors and sub-plot factors respectively. Importantly, the D-optimal minimax criterion proposed by [7] for two-level fractional factorial design is extended to construct two-level fractional factorial split plot design for estimating the parameters of the design and compare the D-optimal minimax design with the existing designs. The D-optimal minimax criterion considered the variance, covariance and the bias of the estimator if the model is misspecified, that is there are some significant effects that are not included in the model. This is a model-based criterion which minimizes the largest determinant of the mean squared error of the generalized least square estimator. When there is limited resources to run the full replicate of the factorial design and also the experiment cannot be performed in a completely random order, the D-optimal minimax criterion is used to select the best treatment combinations for optimal fractional factorial split plot designs.

2. Linear Model and D-Optimal Minimax Criterion

Let S be a 2^k factorial design involving k factors $F_1, \cdots, F_k$ each at two level coded as -1 and $+1$ where $N = 2^k$ runs is the total number of runs in a full factorial design. Let $\mathbf{H}$ denote the $N \times N$ design matrix for the full factorial design whose first column is all ones for the grand mean term and

the other $N-1$ columns represent all the main effects and the interaction effects. Suppose that among the k factors there are k_1 whose level are hard to change (i.e whole plot) and $k_2 = (k-k_1)$ factors are easy to change (i.e subplot). A fractional factorial split plot design D with n runs may be selected from N when it is not feasible to run the full factorial experiment in a complete random order.
Let R be a requirement set containing t effects which usually includes main effects and some interaction effects, then the linear model for R is

$$\mathbf{Y} = \mathbf{X}_1\beta_1 + \mathbf{Z}\gamma + \epsilon \tag{2.1}$$

where $\mathbf{Y}$ is the $n \times 1$ vector of response, $\mathbf{X}_1$ represents the $n \times t$ design matrix, β is the $t \times 1$ vector of mean and factor effects, $\mathbf{Z}$ is an $n \times b$ matrix which indicates the whole plot each run belongs to, γ is the $b \times 1$ vector of random whole plots error and ϵ is the $n \times 1$ vector of random subplot errors. It is assumed that γ and ϵ are independent and have mean zero and variance- covariance matrix $\sigma^2_\gamma \mathbf{I}_n$ and $\sigma^2_\epsilon \mathbf{I}_n$ respectively.
Under these assumptions, the covariance matrix of the reponses, $\mathbf{Y}$ is

$$\mathbf{\Sigma} = \sigma^2_\epsilon(\mathbf{I}_n + d\mathbf{Z}\mathbf{Z}^\mathbf{T}) \tag{2.2}$$

where $d = \sigma^2_\gamma/\sigma^2_\epsilon$. If the entries of Y are grouped by whole plots, then equation (2.2) can be written as the $n \times n$ block diagonal matrix

$$\mathbf{\Sigma} = diag[\mathbf{\Sigma}_1 ... \mathbf{\Sigma}_b]\,,$$

where $\mathbf{\Sigma}_i = \sigma^2_\epsilon(\mathbf{I}_{n_i} + d\mathbf{1}_{n_i}\mathbf{1'}_{n_i})$ for $i = 1, 2, \ldots, b$, and n_i is the number of subplot. The generalised least square estimator of β is:

$$\hat{\beta}_1 = (\mathbf{X}_1^T\mathbf{\Sigma}^{-1}\mathbf{X}_1)^{-1}\mathbf{X}_1^T\mathbf{\Sigma}^{-1}\mathbf{Y}\,, \tag{2.3}$$

and the variance-covariance matrix of $\hat{\beta}_1$ is:

$$Cov(\hat{\beta}_1) = (\mathbf{X}_1^T\mathbf{\Sigma}^{-1}\mathbf{X}_1)^{-1}\,.$$

If there exist significant effects that are not included in R, the model can be written as

$$\mathbf{Y} = \mathbf{X}_1\beta_1 + \mathbf{X}_2\beta_2 + \mathbf{Z}\gamma + \epsilon\,, \tag{2.4}$$

where $\mathbf{X}_2$ is the model matrix for the effects not in R, and β_2 is the unknown parameter vector of effects not in R.

When $n = N$, we define

$$\mathbf{V}_1 = \mathbf{H}_1^T \mathbf{H}_1$$
$$\mathbf{V}_2 = \mathbf{H}_2^T \mathbf{H}_2$$

where $\mathbf{H}_1$ is the $N \times p$ submatrice of $\mathbf{H}$ which represents those effects that are in the requirement set R and $\mathbf{H}_2$ is the $N \times (N-p)$ submatrix of $\mathbf{H}$ which represents those effect that are not in R. since the column of $\mathbf{H}$ are orthogonal. We have:

$$\mathbf{H}^T \mathbf{H} = diag[\mathbf{V}_1 \mathbf{V}_2] \,.$$

The unknown parameter vector β_2 is assumed to satisfy the condition

$$\frac{1}{N} \beta_2^T V_2 \beta_2 \leq \alpha^2 \,.$$

For two level fractional factorial designs,

$$\mathbf{V}_1 = \mathbf{H}_1^T \mathbf{H}_1 = N\mathbf{I}$$
$$\mathbf{V}_2 = \mathbf{H}_2^T \mathbf{H}_2 = N\mathbf{I},$$

then we have the length of the unknown parameter vector β_2 to be $\|\beta_2\| \leq \alpha$. If $\alpha = 0$, the model is correct. When the model is misspecified, $\alpha > 0$, then the generalized least squares estimate of $\hat{\beta}_1$ is biased.

$$bias(\hat{\beta}_1) = E(\hat{\beta}_1) - \beta_1 = (\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)^{-1} \mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_2 \beta_2 \,.$$

Then, the mean square error of $\hat{\beta}_1$ is:

$$\begin{aligned} MSE(\hat{\beta}_1, \mathbf{X}_1, \beta_2) &= cov(\hat{\beta}_1) + bias(\hat{\beta}_1) bias(\hat{\beta}_1)^T \\ = (\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)^{-1} &+ (\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)^{-1} \mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_2 \beta_2 \beta_2^T \mathbf{X}_2^T \mathbf{\Sigma}^{-1} \mathbf{X}_1 (\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)^{-1} \,. \end{aligned}$$

To search for an optimal fractional factorial split plot, we proposed a D-optimal minimax criterion based on the MSE of the generalized least squares estimate, we define the loss function D with respect to the requirement set R as:

$$L_R(D) = \underset{\beta_2 \leq \alpha^2}{max} \det MSE(\hat{\beta}_1, \mathbf{X}_1, \beta_2) \,. \tag{2.5}$$

The loss function in equation (2.5) equals

$$L_R(D) = \frac{1 + (N - \lambda_{min}(\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1))}{\det (\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)} \,, \tag{2.6}$$

where $\lambda_{min}(\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)$ is the smallest eigenvalue of $(\mathbf{X}_1^T \mathbf{\Sigma}^{-1} \mathbf{X}_1)$.

3. Algorithm and Optimal Designs

3.1. **Algorithm.** Below are the procedures required in the constructions to obtain optimal designs with run size as n selected from N :

(i) Select the numbers of factors;
(ii) Select the number of generators;
(iii) Select the number of wholeplot factors;
(iv) Select the number of subplot factors;
(v) Select the numbers of designs you want to generate;
(vi) Generate random designs with desired run size and design matrix;
(vii) Generate the covariance matrix $\boldsymbol{\Sigma}$;
(viii) Compute the loss function, check for the minimum value of all the designs generated; and
(ix) the design with the minimum loss funcion is chosen as the best or optimal design.

The algorithm above was developed into a programme, which further generates the designs and finally search for the optimum designs .

3.2. **Optimal Designs.** The algorithm in Section 3 is applied to construct optimal fractional factorial split plot designs for various requirement sets. The value for the A-optimal $A(D)$ and D-optimal $D(D_n)$ criteria are compared with the loss function value $L_R(D)$. Codes were written in Python program to compute the optimal designs. The resulting designs are represented using numbers $1, 2 \cdots, N$ where $N = 2^k$, k_1 is the number of whole plot factors,$k_2$is the number of subplot factors, p_1 is the number generators for the whole plot and p_2 is the number of generators for the subplot. We represent the whole plot factors with capital letters $A - H$ and the subplot factors with small letters $p - u$. To search for the D-optimal minimax fractional factorial split plot design. We set $\alpha = 1$ and $d = 1$.

Example 1. *Construction of fractional factorial split plot design with five factors and* $R =$ *(the set of all the main effects). For a fractional factorial split plot design with five factors, the requirement set* R *is the set of all the main effects. The number of effects in the requirement set* R *is* $t = 5$*, and* $N = 2^5 = 32$*. The optimal designs constructed are presented in Table 1. The D-optimal minimax designs are also A-optimal and D-optimal.*

TABLE 1. Optimal Design for $R =$ (all main effects)

Design	Run size n	k_1	k_2	p_1	p_2	Trt. Comb.	A(D)	$D(D_n)^{1+t}$	$L_R(D)^{1+t}$
1	16	3	2	0	1	5,6,7,10 11,12,16,18 19,20,21,24 25,29,30,31	92.0	10.2971	0.1478
2	16	2	3	0	1	3,5,6,8,9 12,18,19,20 21,23,25,26 30,31,32	176.6	11.3285	0.1555

Example 2. *Construction of fractional factorial split plot design with five factors and $R =$ (the set of all the main effects and some interaction effects.) For a fractional factorial split plot design with five factors, the requirement set R is the set of all the main effects and some interaction effects. Table 2 shows the results for*

(i) *run size $n = 16$ with $R = (A, B, C, p, q, AC, Ap)$; and*
(ii) *run size $n = 16$ with $R = (A, B, p, q, r, AB, Ap)$*

The D-optimal minimax designs constructed are also D-optimal designs but not A-optimal.

TABLE 2. Optimal Design for $R =$ (all main effects and some interaction effects)

Design	Run size n	k_1	k_2	p_1	p_2	Trt. Comb.	A(D)	$D(D_n)^{1+t}$	$L_R(D)^{1+t}$	R
3	16	3	2	0	1	3,4,5,6,8 11,12,16,17 18,22,23,24 26,29,31	96.0	10.3086	0.1494	(A,B,C,p, q,AC,Ap)
4	16	2	3	0	1	1,4,6,7,9 10,13,15,16 19,20,21,22 23,27,28	106.3990	11.4569	0.1335	(A.B,p, q,r,AB,Ap)

Example 3. *Construction of fractional factorial split plot design with six factors and R = (A, B, C, p, q, r). For a fractional factorial split plot design with sixteen and thirty-two runs, we have six factors; A, B, C, p, q, r, where A, B, C are the whole plot factors and p,q,r are the subplot factors. The requirement set R is (A, B, C, p, q, r). The optimal designs constructed are presented in Table 3. The resulting D-optimal minimax designs are also D-optimal designs but not A-optimal.*

TABLE 3. Optimal Design for $R = (A, B, C, p, q, r)$

Design	Run size n	k_1	k_2	p_1	p_2	Trt. Comb.	A(D)	$D(D_n)^{1+t}$	$L_R(D)^{1+t}$
5	16	3	3	0	2	6,7,10,16,17 22,25,27,33 39,43,45,49 52,63,64	80.0	10.2456	0.1752
6	32	3	3	0	1	1,3,8,9,11,12,13 14,16,19,21,23,25 26,28,30,34,38,39 41,42,43,44,50,52 53,56,57,58,61,63	177.6	22.3385	0.0801

Example 4. *Construction of fractional factorial split plot design with six factors and R =(all the main effects). For a fractional factorial split plot design with sixteen and thirty-two run sizes and six factors, using different numbers of whole plot and subplot factors. The requirement set R includes all the main effects. This results are shown in Table 4.*

(i) *the first design with $n = 16$, $k_1 = 2$, $k_2 = 4$, $p_1 = 0$, and $p_2 = 2$. The design is a D-optimal minimax designs and also D-optimal designs but not A-optimal;*
(ii) *while the remaining designs are D-optimal minimax designs, A-optimal and D-optimal.*

The D-optimal minimax designs are also A-optimal and D-optimal.

TABLE 4. Optimal Design for $R =$(all main effects)

Design	Run size n	k_1	k_2	p_1	p_2	Trt. Comb.	A(D)	$D(D_n)^{1+t}$	$L_R(D)^{1+t}$
7	16	2	4	0	2	6,9,12,15,18 23,28,29,33 36,37,46,50 53,59,64	92.0	11.2424	0.1603
8	32	2	4	0	1	1,2,3,4,6,7,11,12 13,14,15,17,18,19 20,22,23,24,25,32 33,36,38,39,42,44 45,52,53,56,58,59	186.6667	22.1875	0.0812
9	16	4	2	1	1	3,4,10,13,15 17,22,26,28 30,31,38,41 43,61,64	81.333	9.9076	0.1816
10	32	4	2	0	1	3,4,5,8,9,13,15,16 19,21,22,26,30,32 34,38,40,41,42,43 44,45,50,52,56,57 58,59,60,62,63,64	168.0	21.5846	0.08214

Example 5. *Construction of fractional factorial split plot design with six factors and R = (the set of all the main effects and some interaction effects). For a fractional factorial split plot design with six factors, the requirement set R is the set of all the main effects and some interaction effects. The resulting designs are presented in Table 5, the designs are D-optimal minimax designs and also D-optimal designs but not A-optimal.*

TABLE 5. Optimal Design for $R =$(all main effects and some interaction effects)

Design	Run size n	k_1	k_2	p_1	p_2	Trt. Comb.	A(D)	$D(D_n)^{1+t}$	$L_R(D)^{1+t}$	R
11	16	3	3	0	2	4,5,11,12,18 24,29,33,37 45,48,51,52 54,58,63	104.0	9.8255	0.1608	(A,B,C,p,) q,r,AC,BC
12	16	2	4	0	2	7,8,10,11,12 14,32,35,38 41,47,49,52, 60,61,62	132.0	10.3005	0.1469	(A,B,p, q,r,s,AB, Ap,Aq)

4. CONCLUSION

D-optimal minimax criterion for regular two-level fractional factorial split plot designs with model misspecification has been studied. Fractional factorial split plot designs were constructed using different design generators. The application of D-optimal mimnmax criterion to the two-level fractional factorial split plot design was extended and implemented to the introduction of a general form of the loss function for this criterion.

The loss function was used in searching for optimal two-level fractional factorial split plot design. Indeed the development of an algorithm using Python programming language to increase the search for optimal designs was introduced; adequate and efficient. The resulting designs are called D-optimal minimax two-level fractional fractorial split plot design. This can be used to estimate the parameters of a linear model including the main and some specified interactions effects.

Importantly, the D-optimal mimnmax criterion introduced in this study is a suitable tool that minimizes the variance, covariance and the bias of the estimations of the optimal fractional factorial split plot designs constructed.

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