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Screening Designs that Minimize Model Dependence

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Screening Designs that Minimize Model Dependence

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A project submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Master of Science

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ABSTRACT

Screening Designs that Minimize Model Dependence

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When approaching a new research problem, we often use screening designs to determine which factors are worth exploring in more detail. Before exploring a problem, we don't know which factors are important. When examining a large number of factors, it is likely that only a handful are significant and that even fewer two-factor interactions will be significant. If there are important interactions, it is likely that they are connected with the handful of significant main effects. Since we don't know beforehand which factors are significant, we want to choose a design that gives us the highest probability *a priori* of being able to estimate all significant main effects with their associated two-factor interactions. This project examines the methodology of finding designs that do not rely on an assumed model. We propose a method of modifying the D-Optimality criteria that averages over models with a common set of main effects and varying subsets of two-factor interactions. We also calculate the proportion of the subsets that produce estimable designs. We use these results to find the best models for given run size and number of main effects.

Keywords: Experimental Design, Plackett-Burman Designs, Model Dependency, Optimal Designs, Model-Robust Designs

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INTRODUCTION

1.1 SCREENING DESIGNS

When approaching a new research problem, there may be many factors that may be plausible contributors to our dependent variable. Since we don't know which factors are important, we often use screening designs to determine which factors are worth exploring in more detail. The goal of the screening experiment is to study as many variables as we think are plausible contributors to the dependant variable under the assumption that all except the most important will wash out.

Having a large number of factors can be problematic because in order to study a large number of factors, along with their interactions, we also have to have a large number of runs in our experiment to get estimates for each one. This can become cost prohibitive if each experimental run is very time consuming, very expensive, or both. Ideally, we'd like to get information about the important factors without having to run an experiment that allows estimation of every possible interaction. This is a reasonable desire because if we don't believe that all the factors are important, we also will not believe that all the interactions are important.

1.2 FRACTIONAL FACTORIAL DESIGNS

One solution to the above problem is to sacrifice the ability to estimate higher level interaction terms for the benefit of having fewer experimental runs. The most basic design to reduce the number of experimental runs is the fractional factorial design. The fractional factorial design is produced by intentionally confounding certain factors with interaction terms.

Consider an example where we have four factors (A, B, C, and D), each with two levels (-1 and 1). For a full factorial design, we would generate every possible combination of each factor. This would require $2^4 = 16$ runs. If we wanted to reduce the number of runs, we could use a one half-fraction design. A one-half fraction design can be obtained by generating a full factorial of A, B and C, and setting the level of factor D to be equal to ABC. This fully confounds D with ABC, making them indistinguishable. The factor level combinations for this design are shown in Table 1.1. Note that many other one half-fraction designs are possible.

Table 1.1: Fractional Factorial - D=ABC

Run	A	B	C	D
1	-1	-1	-1	-1
2	-1	-1	1	1
3	-1	1	-1	1
4	-1	1	1	-1
5	1	-1	-1	1
6	1	-1	1	-1
7	1	1	-1	-1
8	1	1	1	1

1.3 PLACKETT-BURMAN DESIGNS

Fractional Factorial Designs are very useful designs for screening experiments because of their simplicity in both generation and interpretation. Their shortcoming is that they are limited to designs with run numbers that are powers of the number of factors levels, and any confounded effects are completely confounded and cannot be all included in the fitted model. The number of factor levels is usually two and for all designs considered for this project we will use two factors levels. Plackett and Burman (1946) propose designs to resolve this problem by creating reduced run two-factor level designs that have run numbers that are multiples of four, but not powers of two to fill in the gaps between possible factorial designs.

Plackett-Burman designs have two-factors interactions that are only partially confounded with main effects and other two-factor interactions.

Generating these models begins with an initial row of length $n - 1$ where n is the number of rows in the design. This initial row is then shifted by taking the last element and moving it to the front. This is repeated until run $n - 1$. Run n is at the low level for every factor. This method produces a design matrix that is $n \times (n - 1)$ (Table 1.2 provides an example with 12-runs and 11 columns). These designs can be used to analyze fewer factors than $n - 1$ by assigning the factors to only a subset of the total number of columns. This selection has implication in the alias structure of the design and thoughtful selection of these columns is the subject of this project.

Table 1.2: Basic 12-run Plackett-Burman Design

Run	1	2	3	4	5	6	7	8	9	10	11
1	+	-	+	-	-	-	+	+	+	-	+
2	+	+	-	+	-	-	-	+	+	+	-
3	-	+	+	-	+	-	-	-	+	+	+
4	+	-	+	+	-	+	-	-	-	+	+
5	+	+	-	+	+	-	+	-	-	-	+
6	+	+	+	-	+	+	-	+	-	-	-
7	-	+	+	+	-	+	+	-	+	-	-
8	-	-	+	+	+	-	+	+	-	+	-
9	-	-	-	+	+	+	-	+	+	-	+
10	+	-	-	-	+	+	+	-	+	+	-
11	-	+	-	-	-	+	+	+	-	+	+
12	-	-	-	-	-	-	-	-	-	-	-

1.4 HALL'S DESIGNS

Hall (1961) developed a series of five 16-run designs called Type I, II, III, IV, and V. They are given in increasing order of confounding structure complexity for their two-factor interactions. For this project we will be using Type V exclusively because the increased complexity of the confounding structure of the two-factor interactions allows us to avoid complete confounding of factors in more cases than the other Hall's designs.

1.5 MODEL DEPENDENCY

Without performing a full factorial experiment, we have no way of obtaining estimates for each factor and all possible interactions. However, when performing a screening experiment, we don't expect that all effects will be significant, and, by extension, we don't expect all that their associated interactions will be significant. Both Fractional Factorial and Plackett-Burman designs give us methods of obtaining estimates of the main effects and some interactions by assuming that other interactions are likely not significant.

A potential problem arises with fractional factorial designs when factors that are of interest are confounded in the design. For illustration, consider the four factor experiment from above. Assume that we defined $D=AB$ instead of $D=ABC$, then our design matrix would be given in Table 1.3.

Table 1.3: Fractional Factorial - $D=AB$

Run	A	B	C	D
1	-1	-1	-1	1
2	-1	-1	1	1
3	-1	1	-1	-1
4	-1	1	1	-1
5	1	-1	-1	-1
6	1	-1	1	-1
7	1	1	-1	1
8	1	1	1	1

Suppose we perform the experiment and upon analysis of the data we find that A, B, and D are all significant. Because $D=AB$, there is no way to determine whether this last significance is due to factor D, the AB interaction, or whether both of them are significant, unless we perform additional experiments.

In this scenario, had we defined $D=ABC$, $D=BC$, or $D=AC$, we would have been able to distinguish D and AB. The selection of $D=ABC$ ensures no main effects are confounded with any two-factor interactions. In more complicated designs it may not always

be as straightforward or intuitive. In practice, if an experiment is performed and important interactions are not estimable, follow-up experiments would need to be performed in order to allow estimation of all important effects. In order to avoid this situation, we would like a model that *a priori* has a minimal chance of having significant factors and interactions confounded.

Plackett-Burman designs, by their construction, have main effects that are orthogonal to each other, but have complicated confounding of interaction terms. Each interaction term may be partially confounded with a large number of other main effects and interactions. Contrast this with the fractional factorial design that has simple confounding structure of interactions completely confounded with other model terms. Plackett-Burman designs do not, however, remove the problem of confounding entirely, but often important interaction effects are only partially confounded rather than completely confounded. This project will be focusing on Plackett-Burman Designs and Hall's 16-run design type V and how we can thoughtfully assign factors to columns in the design to get the best chance of having important main effects and two-factor interactions estimable without the need for follow-up experiments.

LITERATURE REVIEW

There is considerable body of literature that has considered the subject of optimal designs. Some authors try to quantify the projection properties of the design or to group similar models together. In this chapter we will discuss some of the work that has been done on evaluating design dependence and how they contribute to this project.

2.1 DESIGN CREATION

D-Optimal Designs

There have been many approaches trying to quantify a “good” design. Generally, we want a design that can estimate the most factors in the fewest runs possible. However, not all designs are equally efficient in doing so. The most common metric for design efficiency is D-Optimality (DuMouchel and Jones 2010). A D-Optimal design attempts to minimize $\det([X'X]^{-1})$ where X is the design matrix. This minimizes the volume of the confidence ellipsoid for the parameters (DuMouchel and Jones 2010). The assumption is that if the design provides minimal variance in estimating the parameters of the model, then it should be the best design for estimating the specified model.

The most common criticism of D-Optimality is that a D-Optimization algorithm will be based on some prespecified model (DuMouchel and Jones 2010). This creates a design that is dependent on an assumed model, and the alias structure is optimized towards a model that may or may not be correct.

For this project, we assume that the effect sparsity principle holds, or in other words, that only a subset of the main effects are actually significant. D-Optimality depends on the specification of the design matrix X . We don't know beforehand which factors are significant,

so applying D-Optimality for the complete design matrix is insufficient for our needs. It is optimized for a predetermined model, but instead we want to assume that the actual model is unknown and will only be a subset of the full model. In order to use this criteria, we will have to develop a method to average its results over several potential subset models.

DuMouchel and Jones (2010) propose an extension of D-optimality using a Bayesian approach. They propose including a set of primary parameters to include in the model X_{pri} and a set of potential parameters X_{pot} . In general, it is assumed that primary terms will be main effects, and potential terms will be interaction terms. Priors are specified as $N(0, \sigma^2)$ for primary terms, and $N(0, \tau^2)$ for potential terms. The prior variance is chosen to be less informative for the primary effects and more informative for the potential effects. Potential effects tend to be less active and therefore the more informative prior tends to shrink their estimates toward zero.

S² Criteria

Because of the D-optimal design's dependence on an assumed model, (Jones and Montgomery 2010) propose the use of the S^2 criteria for selecting models. To calculate S^2 first construct a design matrix, X, where X contains a column of 1's, columns of coefficients for the main effects, and columns of coefficients for all two-factor interaction. Then

$$E(S^2) = \frac{1}{2} \sum_{i < j} (x'_i x_j)^2 / (k(k-1)),$$

where k is the number of columns in X, x_i is the i -th row of X, and x_j is j -th column of X. Minimizing $E(S^2)$ is equivalent to minimizing the sum of squares of the off-diagonal elements of the correlation matrix of X (Jones and Montgomery 2010). In other words, the S^2 criteria penalizes designs with large correlations between main effects and interactions, while it favors models with diffuse correlations among the various effects. This result is similar to the D-Optimal design in that it is dependent on the model structure, but in this case the assumed model is the one with all main effects and all two-factor interactions.

Model Classification

When using Plackett-Burman designs, there are many possible combinations of columns in the design matrix that can be assigned to various factors. However, there are limited number of non-isomorphic designs for a given number of factors being modeled (Wang and Wu 1995). When two design matrices are non-isomorphic, it means that the one design matrix cannot be formed by row and column operations on the other. The choice of columns is not arbitrary and has an impact on the estimability of two-way interactions.

For a 12-run Plackett-Burman design, for $k \leq 4$, there are enough runs to estimate all four main effects, and all $\binom{4}{2} = 6$ two-factor interactions. In the case of $n=5$ or 6 , however, there are two non-isomorphic designs (Wang and Wu 1995). For $k=5$, the first is called design 5.1, and is characterized by having a duplicate run. Design 5.2 has a mirror image run. Similarly, designs for $k=6$ (6.1 and 6.2) have the same properties. These designs alter the number of estimable two-factor interactions because a mirror image run doesn't help in separating confounded factors and interactions.

Projection Estimation Capacity

Loeppky, Sitter, and Tang (2007) introduce another approach to evaluating a design matrix. Given an $n \times m$ design matrix D , define a sequence of length m that has elements $p_k(D)$ that equal the number of subsets that have k main effects and all their associated two-factor interactions all estimable. This sequence can not generally be optimized for all k , so a design that is best for a specific number of k main effects is the optimal choice under this criterion. This method also makes the assumption that given a set of main effects, all two-factor interactions involving these main effects are likely to be important. Empirically this has not been the case as we will discuss later, and it is an assumption that we would like to relax.

2.2 DESIGN ANALYSIS

In all reduced run models with fewer runs than a full factorial of all factors, there are more factors and interactions than there are degrees of freedom. If all main effects and interactions were significant, we would not be able to obtain estimates of all these factors and interactions without performing additional runs of our experiment. We have two principles that we can appeal to however. The first is *effect sparsity*, which says that not all effects are likely to be significant (Lawson 2002). The second is the *effect heredity principle* which says that significant interactions are more likely to involve significant main effects than main effects that are not significant (Lawson 2002). In a design with a complex alias structure, we can estimate some otherwise inestimable interaction terms if we only estimate a subset of the main effects (Lawson 2002).

The modeling strategy given by both Hamada and Wu (1992) and Lin (1998-1999) is to use a forward stepwise selection in two stages. The first stage is a forward selection for the main effects and next stage is for the interaction terms. This allows as many main effects as are significant to be inserted into the model before considering interactions. As soon as additional factors do not seem statistically relevant, the process is halted.

Chipman et al. (1997) add a Bayesian approach to the variable selection method. This is accomplished by placing a normal mixture prior on each variable, a mixture of a “significant” normal and an “insignificant” normal. To apply this method the experimenter must be able to specify priors for what significant means relative to what insignificant means.

2.3 EMPIRICAL PREVALENCE OF TWO-FACTOR INTERACTIONS

The design selection methods defined previously all hinge generally on the idea that many of the two-factor interactions involving the significant main effects will also be important. Empirically this has not been the case. Bergquist, Vanhatalo, and Nordenvaad (2011) recently showed, in a literature review of a broad range of studies, that the number of two-factor interactions that they found significant was only 7 out of 174, or about 4%. Based on these

results, we do not assume that all two-factor interactions associated with significant main effects will be significant, but we would like to have a high probability that small subsets of two-factor interactions are estimable without additional runs. Table 2.1 shows the results of the literature search done by Bergquist, Vanhatalo, and Nordenvaad (2011). It shows the aggregates of the studies they examined and then the results separated into full factorial and fractional factorials.

Table 2.1: Rate of Active Contrasts in Experiments

All experiments	Tested in total	Number of active effects	Active/tested
Contrasts of effect	637	121	0.19
Main factor	160	85	0.53
Two-factor interaction	320	31	0.10
Three-factor interaction	100	2	0.02
Only full factorials	Tested in total	Number of active effects	Active/tested
Main factor	94	56	0.60
Two-factor interaction	146	24	0.16
Three-factor interaction	96	2	0.02
Only fractional factorials	Tested in total	Number of active effects	Active/tested
Main factor	66	29	0.44
Two-factor interaction	174	7	0.04
Three-factor interaction	0	0	–

Since this project is focused on reduced run experiments, we look at the fractional factorial section of Table 2.1 to see the prevalence of two-factor interactions. This empirical result is the basis for our developing a method that doesn't attempt to optimize toward a model that contains all the two-factor interactions or an arbitrary subset of them.

The purpose of this study is to find reduced-run designs that maximizes the probability that we can estimate a small subset of two-factor interactions that correspond to the main effects that are significant in an experiment. Since we don't believe that all two-factor interactions will be significant, our reduced-run experiments try to find important effects and interactions without exploring every possible effect and interaction. The result of the methods presented here will be to show that we can find useful, reduced run designs for evaluating the important main effects and two-factor interactions that have maximum *a priori* chance of not needing additional runs.

3.1 VARIATION OF D-OPTIMALITY

D-Optimality, that is the minimization of $\det([X'X]^{-1})$, has the limitation of being tied to the specific assumed model represented by the design matrix X . This is equivalent to maximizing $\det([X'X])$ which is computationally simpler and will be used for this project. Our goal is to avoid the limitation of having an assumed model.

To do this we need to create a metric that accounts for the fact that only a handful of two-factor interactions are likely significant, as stated by Bergquist et al. (2011). For a given number of main effects, which will vary according to the experiment, we want to consider a reasonable number of possible two-factor interactions that we will call t . Reasonable in this sense is based on the literature search done by Bergquist et al. (2011) indicating empirically that it is unlikely that a large proportion of possible two-factor interactions will be significant.

For a given set of s main effects, we will consider every possible combination of the main effects combined with t of the associated two-factor interactions. For each combination we calculate $D_{ij} = \log(\max(\det([X'_{ij}X_{ij}]), 1))$ where X_{ij} is the design matrix of the main

effects i with two-factor interactions j . We then sum over j to get $D_i = \sum_j D_{ij}$. This is a monotone transform of a geometric average, except in the case where we have a singular $X'_{ij}X_{ij}$ matrix where we multiply by 1 instead of 0.

For example, for a Plackett-Burman design of 12 runs, there are 11 columns in the design matrix. If we begin by taking 5 main effects and want to consider the scenario where we have potentially 3 significant two-factor interactions without knowledge of what they are beforehand, then there are $\binom{5}{3} = 120$ combinations of sets of 3 two-factor interactions. For each of the 120 combination of 3 two-factor interactions, we construct the design matrix X_{ij} , and calculate $D_{ij} = \log(\max(\det([X'_{ij}X_{ij}], 1), 1))$ and then sum over $j = 1, \dots, 120$ to get $D_i = \sum_{j=1}^{120} D_{ij}$.

In general, we can perform this analysis for s main effects and t two-factor interactions as long as the number of main effects plus the number of two factor interactions is less than the number of runs in the experiment, that is $n > s + t$. For this case we will have $\binom{s}{2}$ total two-factor interactions and we will look at each combination of t of them for a total of $\binom{\binom{s}{2}}{t}$ total subset models. For each subset of two-factor interactions combined with the main effects, we will calculate D_{ij} and add them together.

The sum D_i represents the value for a particular subset of main effects. If we evaluate D_i for every $\binom{n-1}{s}$ possible subset of s main effects, we can determine which design *a priori* has the highest likelihood of having estimable two-factor interactions without having to perform additional runs.

3.2 PERCENTAGE OF ESTIMABLE SUBSETS

Another approach is to determine the number of subsets of main effects and 3 two-factor interactions that are estimable. In the Variation of D-Optimality method (Section 3.1), we calculated a log sum of determinants, but it would also be useful to know the percentage of subset designs that had non-zero determinants. This represents the probability that we do not have to perform additional runs under the assumed number of main effects and two-factor

interactions. This is performed simply by counting the number of non-zero determinants when calculating D_i and dividing by the total number of subsets, $\binom{s}{t}$.

3.3 PROJECT ALGORITHM

For this project we will produce a series of design matrices that, for a given number of main effects and two-factor interactions, have the maximum probability of being able to estimate the corresponding subset model without further runs. We will do this for the common run sizes of 12, 16, and 20. The complexity of this problem increases dramatically as the number of runs in the design matrix increases. To find the best design we consider each of $\binom{n-1}{s}$ possible combinations of s main effects. Each set of s main effects has $\binom{s}{2}$ potential two factor interactions for which, for this project, we consider only 3 at a time for a total of $\binom{\binom{s}{2}}{3}$ subset designs. We will preserve only the best design and compile a list of the best designs for each number of runs. The algorithm steps are enumerated in Table 3.1.

Table 3.1: Project Algorithm

1. Find every $\binom{n-1}{s}$ combinations of s main effects from the design matrix, $i = 1, \dots, I$ where $I = \binom{n-1}{s}$.
2. For each combination of main effects, consider all possible combinations of t two-factor interactions, $j = 1, \dots, J$ where $J = \binom{\binom{s}{2}}{t}$, where $t=3$.
3. Calculate the modified D-Optimality criterion $D_{ij} = \log(\max(\det([X'_{ij}X_{ij}]), 1))$ and note whether the determinant is zero or non-zero.
4. Sum over j to find D_i and compute the proportion of non-zero determinants.
5. For the maximum D_i , store the associated columns from the design matrix that correspond to those main effects.

Given the stored best designs, we can then choose the optimal columns from the design matrix for a given run size. There are a number of possible combinations of main effects and two-factor interactions that are possible for a given run size. In Table 3.2 we have a list of designs we would like to explore that we believe are reasonable based on Bergquist

et al. (2011). Their work has shown that about 4% of interactions empirically turn out to be significant. We chose the number 3 as the number of interactions to investigate as it is a reasonable number across the range of run sizes and main effect numbers that we will be investigating. The combinations of run size, main effects, and two-factor interactions to explore are found in Table 3.2. These are reasonable number of main effects to explore for each run size and the number of two-factor interactions are reasonable according to the approximately 4% of significant two-factor interactions from Bergquist, Vanhatalo, and Nordenvaad (2011).

Table 3.2: Designs to Explore

Number of Runs	Number of Main Effects, s	Two-Factor Interactions, t
12	5	3
	6	3
	7	3
	8	3
16	6	3
	7	3
	8	3
	9	3
	10	3
	11	3
20	9	3
	10	3
	11	3
	12	3
	13	3
	14	3
	15	3

RESULTS

One of the most notable results that we found was the fact that though there were numerous subset designs there was only a relatively small set of unique D_i values. Therefore, there is not a single "best" design, but there are a set of designs that are equivalent in their D_i values. When running the algorithm, we kept track of the result that was the best so far, so our reported result is the first in the set of "best" possible choices of columns.

Using these results found in Tables 4.1 – 4.3, an experimenter can select the desired number of experimental runs and main effects to explore, and then select the corresponding columns as specified in Tables 4.1 – 4.3. These designs cover the likely numbers of two-factor interactions and thereby minimize the chance of needing to perform additional runs. These results relax one of the most binding restrictions in the area of optimal design, which is that every two-factor interaction involving a significant main effect is important and should be estimable. On the other hand, we only seek to maximize the chance that any given subset of 3 two-factor interactions are estimable.

4.1 OPTIMAL DESIGNS

In Tables 4.1 – 4.3 we have the results of our study along with the design matrix used to generate them. For each design matrix, we have results for each of the combinations of run size with number of main effects. On each row we have the optimal column selection from the design matrix for that number of main effects, the D_i score for the optimal combination, and the proportion of subsets that are estimable for that combination. The D_i scores on each row are only comparable to other designs of the same run size and the same number of main effects.

4.2 USE OF TABLES 4.1 - 4.3

In order for an experimenter to use the result in the from Tables 4.1 – 4.3, they should do the following

1. Determine the number of main effects to explore.
2. Decide the number of experimental runs to perform (cost vs estimability).
3. In the appropriate table (4.1 – 4.3), select the columns from the design matrix that correspond to the recommended columns. For example, columns {1 2 3 4 5 6 8 10 13 14 16 17} for a 20-run Plackett-Burman design with 12 main effects.
4. Conduct the experiment using those columns to choose factors levels for each run.
5. Use forward selection to determine significant effects in the model.

Table 4.1: 12-Run Plackett-Burman Design

Run	1	2	3	4	5	6	7	8	9	10	11
1	+	-	+	-	-	-	+	+	+	-	+
2	+	+	-	+	-	-	-	+	+	+	-
3	-	+	+	-	+	-	-	-	+	+	+
4	+	-	+	+	-	+	-	-	-	+	+
5	+	+	-	+	+	-	+	-	-	-	+
6	+	+	+	-	+	+	-	+	-	-	-
7	-	+	+	+	-	+	+	-	+	-	-
8	-	-	+	+	+	-	+	+	-	+	-
9	-	-	-	+	+	+	-	+	+	-	+
10	+	-	-	-	+	+	+	-	+	+	-
11	-	+	-	-	-	+	+	+	-	+	+
12	-	-	-	-	-	-	-	-	-	-	-

# of Main Effects	Optimal Column Selection	D_i	Est. Subsets
5	{1, 2, 3, 4, 5}	2194.037	1.0000
6	{1, 2, 3, 4, 5, 6}	9104.124	1.0000
7	{1, 2, 3, 4, 5, 6, 7}	21785.04	0.7503
8	{1, 2, 3, 4, 5, 6, 7, 8}	32262.43	0.4188

Table 4.2: 16-Run Hall's Design

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
2	-	-	-	-	-	-	-	+	+	+	+	+	+	+	+
3	-	-	-	+	+	+	+	-	-	-	-	+	+	+	+
4	-	-	-	+	+	+	+	+	+	+	+	-	-	-	-
5	-	+	+	-	-	+	+	-	-	+	+	-	-	+	+
6	-	+	+	-	-	+	+	+	+	-	-	+	+	-	-
7	-	+	+	+	+	-	-	-	+	-	+	-	+	-	+
8	-	+	+	+	+	-	-	+	-	+	-	+	-	+	-
9	+	-	+	-	+	-	+	-	-	+	+	+	+	-	-
10	+	-	+	-	+	-	+	+	+	-	-	-	-	+	+
11	+	-	+	+	-	+	-	-	+	+	-	+	-	-	+
12	+	-	+	+	-	+	-	+	-	-	+	-	+	+	-
13	+	+	-	-	+	+	-	-	+	-	+	+	-	+	-
14	+	+	-	-	+	+	-	+	-	+	-	-	+	-	+
15	+	+	-	+	-	-	+	-	+	+	-	-	+	+	-
16	+	+	-	+	-	-	+	+	-	-	+	+	-	-	+

# of Main Effects	Optimal Column Selection	D_i	Est. Subsets
6	{1, 2, 4, 8, 10, 12}	10620.22	1.0000
7	{1, 2, 4, 8, 10, 12, 15}	34106.02	0.9947
8	{1, 2, 4, 7, 8, 10, 12, 15}	90121.77	0.9603
9	{1, 2, 4, 7, 8, 9, 10, 12, 14}	166358.2	0.7559
10	{1, 2, 4, 7, 8, 9, 10, 11, 12, 14}	221737.2	0.4684
11	{1, 2, 3, 4, 5, 8, 9, 10, 11, 12, 13}	234881.2	0.2533

Table 4.3: 20-Run Plackett-Burman Design

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	+	+	-	-	+	+	+	+	-	+	-	+	-	-	-	-	+	+	-
2	-	+	+	-	-	+	+	+	+	-	+	-	+	-	-	-	-	+	+
3	+	-	+	+	-	-	+	+	+	+	-	+	-	+	-	-	-	-	+
4	+	+	-	+	+	-	-	+	+	+	+	-	+	-	+	-	-	-	-
5	-	+	+	-	+	+	-	-	+	+	+	+	-	+	-	+	-	-	-
6	-	-	+	+	-	+	+	-	-	+	+	+	+	-	+	-	+	-	-
7	-	-	-	+	+	-	+	+	-	-	+	+	+	+	-	+	-	+	-
8	-	-	-	-	+	+	-	+	+	-	-	+	+	+	+	-	+	-	+
9	+	-	-	-	-	+	+	-	+	+	-	-	+	+	+	+	-	+	-
10	-	+	-	-	-	-	+	+	-	+	+	-	-	+	+	+	+	-	+
11	+	-	+	-	-	-	-	+	+	-	+	+	-	-	+	+	+	+	-
12	-	+	-	+	-	-	-	-	+	+	-	+	+	-	-	+	+	+	+
13	+	-	+	-	+	-	-	-	-	+	+	-	+	+	-	-	+	+	+
14	+	+	-	+	-	+	-	-	-	-	+	+	-	+	+	-	-	+	+
15	+	+	+	-	+	-	+	-	-	-	-	+	+	-	+	+	-	-	+
16	+	+	+	+	-	+	-	+	-	-	-	-	+	+	-	+	+	-	-
17	-	+	+	+	+	-	+	-	+	-	-	-	-	+	+	-	+	+	-
18	-	-	+	+	+	+	-	+	-	+	-	-	-	-	+	+	-	+	+
19	+	-	-	+	+	+	+	-	+	-	+	-	-	-	-	+	+	-	+
20	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

# of Main Effects	Optimal Column Selection	D_i	Est. Subsets
9	{1 2 3 4 5 8 13 15 16}	245490.4	1.0000
10	{1 2 3 4 6 8 13 14 16 17}	525426.1	0.9848
11	{1 2 3 4 5 6 8 13 14 16 17}	1032827	0.9918
12	{1 2 3 4 5 6 8 10 13 14 16 17}	1896498	0.9177
13	{1 2 3 4 5 6 7 8 9 10 14 17 18}	3262855	0.9566
14	{1 3 4 5 6 8 9 10 11 12 15 16 18 19}	5187927	0.9035
15	{1 2 4 5 6 7 8 9 10 11 12 13 16 17 19}	7226388	0.7844

CONCLUSIONS AND FURTHER STUDY

We believe the results of this project offer good estimability for main effects and a likely number of two-factor interactions in experiments with relatively high numbers of main effects compared to the number of experimental runs. Jones and Montgomery (2010) consider 16-run designs with up to 8 main effects and show that is possible to get greater numbers of main effects with reasonable probability of not having the need to perform additional runs. The criteria proposed by Loeppky et al. (2007) have the estimability of two-factor interactions dependent on the number of main effects that are significant. The models they propose are optimized for being able to estimate all two-factor interactions associated with significant main effects up to a certain number of main potentially significant main effects. Our modified D-Optimality criteria considers only that any small subset of two-factor interactions be estimable with our main effects without performing additional runs. Considering only a small subset of two-factor interactions allows for more main effects to be significant without it altering the probable estimability of the two-factor interactions.

In this study, we considered only Plackett-Burman designs for the 12- and 20-run designs and Hall's design type V for the 16-run design. There are other designs that may result in better D_i results for a given run size and number of main effects. There is also the potential for considering designs of larger size such as a 24-run design. The problem currently is that for the 20-run designs, running the algorithm for each number of main effects took at least 24 hours, and a couple took as long as 45 hours. This makes an analysis of a particular design matrix computationally burdensome for run sizes above 16. This might be able to remedied, at least partially, through optimization. Since the subset designs are often equivelant in their D_i results, work to prescreen the designs and determine which will

produce equivalent results could potentially reduce computation time tremendously. There is nothing about the computations in this algorithm that depend on the previous iteration, so the process could also be parallelized to great effect.

It would also be interesting to explore the relationship between D_i and the proportion of estimable subsets. They don't always increase together and it's not clear what is the optimal trade off between estimability and orthogonality. A high number of estimable subsets could mean that there are a lot of highly colinear factors, whereas a large D_i signifies that the average orthogonality of the subset matrices is very high but doesn't say how many subsets are estimable.

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APPENDICES

APPENDIX A

CODE TO ANALYZE DESIGN MATRICES

```

library(BsMD)
library(R.oo)
library(FrF2)
library(xtable)
rm(list=ls())

data(PB12Des)

pb12<-PB12Des
hall5<-rbind(
c(-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1),
c(-1,-1,-1,-1,-1,-1,-1, 1, 1, 1, 1, 1, 1, 1, 1),
c(-1,-1,-1, 1, 1, 1, 1,-1,-1,-1,-1, 1, 1, 1, 1),
c(-1,-1,-1, 1, 1, 1, 1, 1, 1, 1, 1,-1,-1,-1,-1),
c(-1, 1, 1,-1,-1, 1, 1,-1,-1, 1, 1,-1,-1, 1, 1),
c(-1, 1, 1,-1,-1, 1, 1, 1, 1,-1,-1, 1, 1,-1,-1),
c(-1, 1, 1, 1, 1,-1,-1,-1, 1,-1, 1,-1, 1,-1, 1),
c(-1, 1, 1, 1, 1,-1,-1, 1,-1, 1,-1, 1,-1, 1,-1),
c( 1,-1, 1,-1, 1,-1, 1,-1,-1, 1, 1, 1, 1,-1,-1),
c( 1,-1, 1,-1, 1,-1, 1, 1, 1,-1,-1,-1,-1, 1, 1),
c( 1,-1, 1, 1,-1, 1,-1,-1, 1, 1,-1, 1,-1,-1, 1),
c( 1,-1, 1, 1,-1, 1,-1, 1,-1,-1, 1,-1, 1, 1,-1),
c( 1, 1,-1,-1, 1, 1,-1,-1, 1,-1, 1, 1,-1, 1,-1),
c( 1, 1,-1,-1, 1, 1,-1, 1,-1, 1,-1,-1, 1,-1, 1),
c( 1, 1,-1, 1,-1,-1, 1,-1, 1, 1,-1,-1, 1, 1,-1),
c( 1, 1,-1, 1,-1,-1, 1, 1,-1,-1, 1, 1,-1,-1, 1))
pb20<-rbind(
c( 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1),
c(-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1),
c( 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1),
c( 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1),
c(-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1),
c(-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1),
c(-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1),
c(-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1),
c( 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1,-1))

```

```

c(-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1, 1),
c( 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1,-1),
c(-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1, 1),
c( 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1, 1),
c( 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1, 1),
c( 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1, 1),
c( 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1,-1),
c(-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1,-1),
c(-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1, 1),
c( 1,-1,-1, 1, 1, 1, 1,-1, 1,-1, 1,-1,-1,-1,-1, 1, 1,-1, 1),
c(-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1,-1)

```

```

logsum <- function(x)
{
  sum(log(x))
}

```

```

#####
# Function : matrixEvaluation #
# Input : design matrix containing main effects only. #
# number of main effects, number of 2-FI's #
# Output : Breakdown of D_i's, estimable subsets, #
# Best columns, and time elapsed #
# Author : Kenneth Fairchild, 2011 #
#####

```

```

matrixAnalysis <- function(designmatrix,n1fi,n2fi)
{
  print(paste(nrow(designmatrix),"-run, ",n1fi," MEs and ",n2fi," 2fis",sep=""))
  ptm<-proc.time()

  X<-as.matrix(designmatrix)
  colnames(X)<-intToChar(65+0:(ncol(X)-1))

  Xf<-X
  for(i in 1:(ncol(X)-1))
  {
    for(j in (i+1):ncol(X))
    {
      Xf<-cbind(Xf,Xf[,i]*Xf[,j])
      colnames(Xf)[ncol(Xf)]<-paste(colnames(Xf)[i],colnames(Xf)[j],sep="")
    }
  }

  logsums<-rep(0,choose(ncol(X),n1fi))
  estsubsets<-rep(0,choose(ncol(X),n1fi))
}

```

```

#Combinations of "n1fi" main effects chosen from columns in the design matrix
combs<-combn(1:ncol(X),n1fi)

cnXf<-colnames(Xf)
outputdata<-NULL

bestcols<-NULL
bestdet<-0

for(i in 1:ncol(combs))
{
  #Two-Factor Interactions associated with the main effects from combination i
  itwofi <- combn(combs[,i],2)
  names2fi <- paste(colnames(X)[itwofi[1,]],colnames(X)[itwofi[2,]],sep="")

  #Ordered reference numbers for the 2-fi's associated with i
  refitwofi <- rep(0,length(names2fi))
  for(k in 1:length(names2fi))
  {
    refitwofi[k] <- which(cnXf==names2fi[k])
  }

  #Every combination of 3 2-fi's
  subcombs <- combn(refitwofi,3)

  num0det<-0
  det<-0

  for(j in 1:ncol(subcombs))
  {

    #Matrix of: Main effects from main effect combination i,
    #           and 2-fi subcombination j
    Xs<-Xf[,c(combs[,i],subcombs[1,j],subcombs[2,j],subcombs[3,j])]

    det<-log(max(det(t(Xs)%*%Xs),1))
    if(det==0)
    {
      num0det<-num0det+1
    }
    logsums[i]<-logsums[i]+det
  }
  logsums[i]<-round(logsums[i],4)
}

```

```

    estsubsets[i]<-1-num0det/ncol(subcombs)
    if(logsums[i]>bestdet)
    {
        bestdet<-logsums[i]
        bestcols<-combs[,i]
    }
}

length(logsums[which(logsums==max(logsums))])/length(logsums)
print("-----")
print(table(logsums))
print("-----")
print(table(estsubsets))
print("-----")
print("Best Columns")
print(bestcols)
print(bestdet)
print("-----")

print(proc.time()-ptm)

outputdata<-cbind(rownames(as.matrix(table(estsubsets))),as.matrix(table(logsums)))

write.csv(outputdata,paste("c:/filepath/pb",
                           nrow(designmatrix),"m",n1fi,"i",n2fi,".csv",sep=""))
return(list(logsums,bestcols))
}

pb12o6t3<-matrixAnalysis(pb12,6,3)
pb12o7t3<-matrixAnalysis(pb12,7,3)
pb12o8t3<-matrixAnalysis(pb12,8,3)
pb12o9t3<-matrixAnalysis(pb12,9,3)

pb16o6t3 <-matrixAnalysis(hall5, 6,3)
pb16o7t3 <-matrixAnalysis(hall5, 7,3)
pb16o8t3 <-matrixAnalysis(hall5, 8,3)
pb16o9t3 <-matrixAnalysis(hall5, 9,3)
pb16o10t3<-matrixAnalysis(hall5,10,3)
pb16o11t3<-matrixAnalysis(hall5,11,3)

pb20o9t3 <-matrixAnalysis(pb20, 9,3)
pb20o10t3<-matrixAnalysis(pb20,10,3)
pb20o11t3<-matrixAnalysis(pb20,11,3)
pb20o12t3<-matrixAnalysis(pb20,12,3)

```

```
pb20o13t3<-matrixAnalysis(pb20,13,3)
pb20o14t3<-matrixAnalysis(pb20,14,3)
pb20o15t3<-matrixAnalysis(pb20,15,3)
```


APPENDIX B

CODE TO EVALUATE A SPECIFIC DESIGN

```

library(R.oo)

#####
# Function : matrixEvaluation #
# Input : design matrix containing main effects only #
# Output : D_i score and proportion est. subsets #
# Author : Kenneth Fairchild, 2011 #
#####
matrixEvaluation <- function(designmatrix)
{
  X<-as.matrix(X)
  colnames(X)<-intToChar(65+0:(ncol(X)-1))

  Xf<-X
  for(i in 1:(ncol(X)-1))
  {
    for(j in (i+1):ncol(X))
    {
      Xf<-cbind(Xf,Xf[,i]*Xf[,j])
      colnames(Xf)[ncol(Xf)]<-paste(colnames(Xf)[i],colnames(Xf)[j],sep="")
    }
  }

  cnXf<-colnames(Xf)
  outputdata<-NULL

  bestcols<-NULL
  bestdet<-0

  logsum<-0
  estsubsets<-0

  #Two-Factor Interactions associated with the main effects from combination i
  itwofi <- combn(1:ncol(X),2)
  names2fi <- paste(colnames(X)[itwofi[1,]],colnames(X)[itwofi[2,]],sep="")

  #Ordered reference numbers for the 2-fi's associated with i
  refitwofi <- rep(0,length(names2fi))
  for(k in 1:length(names2fi))

```

```

{
  refitwofi[k] <- which(cnXf==names2fi[k])
}

#Every combination of 3 2-fi's
subcombs <- combn(refitwofi,3)

num0det<-0
det<-0

for(j in 1:ncol(subcombs))
{

  #Matrix of: Main effects and 2-fi subcombination j
  Xs<-Xf[,c(1:ncol(X),subcombs[1,j],subcombs[2,j],subcombs[3,j])]

  det<-log(max(det(t(Xs)%*%Xs),1))
  if(det==0)
  {
    num0det<-num0det+1
  }
  logsum<-logsum+det

}
return(list(Di = logsum, estsubsets=1-num0det/ncol(subcombs)))
}

matrixEvaluation(X)

```