Approximate Model Spaces for Model-Robust Experiment Design

Byran Smucker

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Department Seminar, VCU Department of Statistical Sciences and O.R.
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- Co-author and former graduate student Nathan Drew
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Outline

1. Introduction to Model-Robust Design
2. First Dent
3. Pushing Further
4. Latest Version
   - Approximate Model Spaces
   - Results
   - Conclusions
http://matt.might.net/articles/phd-school-in-pictures/

from Matt Might (http://matt.might.net/).
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For standard least squares regression:

\[ \text{Cov}(\hat{\beta}) = \sigma^2 (X'X)^{-1}. \]

Goal: Make \((X'X)^{-1}\) small in some way.

1. Choose a design, often via algorithm, based on a criterion that will give the design desirable properties.
   - Precise estimation (e.g. \(D\)-optimality, criterion \(|X'X|\)); or
   - Precise prediction (e.g. \(T\)-optimality).

2. Can be tailored to the design situation.
   - Constrained design space
   - Mixture of continuous and categorical factors
   - Sample size constraints
A Drawback

The form of the model between response and factors must be specified before design is constructed.
\( \mathcal{D} \)-optimal vs. Model-robust

Instead of focusing on a single model (optimal design), find design that is “good” for all models of interest, if possible.
\textbf{D-optimal vs. Model-robust}

Instead of focusing on a single model (optimal design), find design that is “good” for all models of interest, if possible.

\textit{D}-optimal design, starting with arbitrary $n$-run design $\xi_n$:

\[
\xi_n \xrightarrow{f} X(\xi_n, f) \xrightarrow{X'} M(\xi_n, f) \rightarrow \xi_n^* = \arg \max_{\xi_n} |M(\xi_n, f)|
\]
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Model-robust design with respect to a set of models $\mathcal{F} = (f_1, f_2, \ldots, f_r)$:

$$\xi_n \xrightarrow{\mathcal{F}} \{X_1, X_2, \ldots, X_r\} \rightarrow \{M_1, M_2, \ldots, M_r\} \rightarrow \xi^*_n = \arg \max_{\xi_n} g[|M_1|, |M_2|, \ldots, |M_r|]$$
Three questions with the set-of-models approach

1. What is the set of models, $\mathcal{F}$?
2. What is the function, $g$?
3. What methods can be used to find the design?
Other work

Set-of-Models Approach (not an exhaustive review)

- DuMouchel and Jones (1994); Jones et al. (2008); Jones and Nachtsheim (2011) [Bayesian approach which implicitly considers 2 models];
- Li and Nachtsheim (2000), Loeppky et al. (2007), Jones et al. (2009), Smucker et al. (2012) [two-level designs]
- Heredia-Langner et al. (2004) [genetic algorithm];
- Tsai and Gilmour (2010) [approximation of $A_s$ optimality]
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Exchange Algorithms for Constructing Model-Robust Experimental Designs

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Optimal experimental design procedures, utilizing criteria such as D-optimality, are useful for producing designs for quantitative responses, often under nonstandard conditions such as constrained design spaces. However, these methods require a priori knowledge of the exact form of the response function, an often unrealistic assumption. Model-robust designs are those that, from our perspective, are efficient with respect to a set of possible models. In this paper, we develop a model-robust technique motivated by a connection to multiresponse D-optimal design. This link spawns a generalization of the modified Fedorov exchange algorithm, which is then used to construct exact model-robust designs. We also study the effectiveness of designs robust for a small set of models compared with designs that account for much larger sets. We give several examples and compare our designs with two model-robust procedures in the literature.

Key Words: D-Optimality; Model Space; Multiresponse Design; Robust Design.
Q. What is the set of models, \( \mathcal{F} \)?

A. There were several.

1. A small set of models consisting of maximal models in specified classes.
   - e.g. \( \mathcal{F} = \{ f'_i(x), 1 \leq i \leq 3, x \in \chi \} \) where
     
     \[
     f'_1(x) = (1, x_1, x_2) \\
     f'_2(x) = (1, x_1, x_2, x_1x_2) \\
     f'_3(x) = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)
     \]

2. All possible submodels of the quadratic model.

3. All possible submodels of the quadratic model that respect strong effect heredity.
Q. What is the function, $g$?

A. Something that boiled down to

$$g(M_{\mathcal{F}}) = \prod_{\mathcal{F}} |M_f|$$  \hspace{1cm} (1)

Motivated by a connection to multiresponse $\mathcal{D}$-optimal design
Q. What method was used to find the design?

A. A modified Fedorov exchange algorithm.

From a specified candidate list, consider exchanges with design points row by row.
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Supplementary materials for this article are available online. Please go to http://www.tandfonline.com/ijr/TECH

Model-Robust Two-Level Designs Using Coordinate Exchange Algorithms and a Maximin Criterion

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We propose a candidate-list-free exchange algorithm that facilitates construction of exact, model-robust, two-level experiment designs. In particular, we investigate two model spaces previously considered in the literature. The first assumes that all main effects and an unknown subset of two-factor interactions are active, but that the experimenter knows the number of active interactions. The second assumes that an unknown subset of the main effects, and all associated two-factor interactions, are active. Previous literature uses two criteria for design construction: first, maximize the number of estimable models; then,
Q. What is the set of models, $\mathcal{F}$?

A. (1) “main effects plus $g$ interactions” (MEPI$_g$) model space [Li and Nachtsheim, 2000]; and (2) the Projective model space [Loeppky et al., 2007]. (We’ll focus on MEPI$_g$.)
Motivating MEPI: When Fractional Factorials are Inadequate

An experiment (Li and Nachtsheim 2000):
- Goal: “reduce the leakage of a clutch slave cylinder”
- Four potential factors
- Budget: 8 runs
- Engineers believe only 1 or 2 interactions will be active
Motivating MEPI: When Fractional Factorials are Inadequate

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Typical design:
- $2^{4-1}$ resolution IV design
- Only estimates 12/15 models with 2 interactions
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Model-Robust Factorial Design (MRFD) of Li and Nachtsheim estimates all 15.
Set of all models which include all main effects and $g$ two-factor interactions (2fi’s).

If there are $k$ factors, there are $t = \binom{k}{2}$ possible 2fi’s and thus the model space includes $\binom{t}{g}$ models.
Q. What is the function, $g$?

A. $g(M_F) = \min_{f \in \mathcal{F}} \left( \frac{|M_f|}{|M_f^*|} \right)^{1/p_f}$.

i.e. “maximize the minimum $\mathcal{D}$-efficiency”.

Slightly more complicated than this - before applying $g(M_F)$ as a criterion, maximize the proportion of estimable models in $\mathcal{F}$. 
Q. How to find the design?

A. Coordinate exchange (Meyer and Nachtsheim 1995).

Instead of considering exchanging a full row of the design, consider exchanges coordinate by coordinate.
Contributions

Algorithm:
Based on coordinate exchange (Meyer and Nachtsheim 1995)
– no candidate list
Sequentially maximize the number of estimable models, and
then the minimum efficiency (with respect to all models in model space)

Space of possible designs:
Li and Nachtsheim limit search to balanced designs.
Our approach removes this limitation.
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Results

Model space (Li and Nachtsheim): All \( r \) models with all \( k \) main effects and \( g \) two-factor interactions.

<table>
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<th>( k )</th>
<th>( g )</th>
<th>( r )</th>
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</table>
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“Approximate Model Spaces for Model-Robust Experiment Design”
Consider a seven-factor experiment in 16 runs.

- Full two-factor interaction model has $1 + 7 + 21 = 29$ parameters and can’t be fit.
- Assume effect sparsity: no more than $g = 4$ two-factor interactions will be active.
- There are 5,985 models which include 4 two-factor interactions.
- Strategy: Find a design algorithmically that can efficiently estimate all 5,985 models.
Advantages: More flexible and efficient compared to fractional factorial designs.

(For instance, for the example above the resolution IV FFD can estimate less than half of the 5,985 models.)

Disadvantages: Orthogonality and column-balance probably lost.
A Drawback to Set-of-Models Approach

The model spaces are too large for many experiments of interest.
The MEPI Model Space Explodes

<table>
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<tr>
<th>$k$</th>
<th>$g$</th>
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<tr>
<td>12</td>
<td>10</td>
<td>210,980,549,208</td>
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</table>
Previous methods can’t handle such large model spaces

- The largest model space Li and Nachtsheim (2000) consider includes less than 400,000 models.
- They do not give computation time for their designs for large model spaces.
Q1. What is the set of models, $\mathcal{F}$?
A1. (1) $\text{MEPl}_g$ model space; and (2) superaturated model space (Jones et al., 2009). (We’ll focus again on $\text{MEPl}_g$.)

Q2. What is the function, $g$?
A2. There’s a twist.

Q3. What methods can be used to find the design?
A3. The twist affects the answer to this question too.
**Notation/terminology**

- $\mathcal{F}$: Full set of models.
- $S_1$: Small sample of $s_1$ models chosen from $\mathcal{F}$, called the approximate model space.
- $S_2$: Larger sample of $s_2$ models chosen from $\mathcal{F}$, used to evaluate a design with respect to $\mathcal{F}$.
- A *changeable element* for a model space $\mathcal{F}$ is a model term whose presence may vary from model to model. The number of changeable elements for a model space is denoted by $c$. 
Overview of Proposed Methodology

1. Select the approximate model space $S_1$ from the full model space $F$.
2. Construct $n_t$ designs that are robust for the models in $S_1$, via algorithm.
3. Evaluate the $n_t$ designs with respect to $F$. If $F$ is too large, select a larger sample $S_2$ from $F$ and evaluate the design with respect to $S_2$.

The design that performs the best with respect to $F$ (or $S_2$) is chosen.
Ramifications of the Proposed Methodology

- Dramatically reduces computation time.
- Estimation capacity and efficiency of designs may be (slightly) inferior.
Step 1: Selecting the Approximate Model Space $S_1$

Intuition:

1. Choose $S_1$ so that the total number of times that each changeable element appears in $S_1$ is approximately equal.

2. Choose $S_1$ so that each pair of changeable elements appears together in a model $f \in S_1$ roughly the same number of times.
Step 1 (cont.): Analogy to BIBDs

Make an analogy to balanced incomplete block designs (BIBDs):

1. The number of changeable elements, \( c \), is analogous to the number of treatments in a BIBD.
2. The number of models in \( S_1, s_1 \), is analogous to the number of blocks in a BIBD.
3. The number of changeable elements in each model, \( g \), is analogous to the size of the blocks in a BIBD.

Call the choice of \( S_1 \) - the design - the meta-design to distinguish it from the original factorial-type design we want to construct.
Step 1 (cont.): Near BIBDs

For most combinations of $c$, $s_1$, and $g$ of interest will not admit a BIBD.

But because BIBD are $D$-optimal, we can use an algorithm to find a $D$-optimal block meta-design for a given $c$, $s_1$, and $g$ and this design will be near BIBD.

We constructed these near BIBD’s using SAS software’s PROC OPTEX.
Step 2: Constructing Designs

Once $S_1$ is selected, use standard algorithms to construct a design that maximizes

$$EC_{S_1} = \frac{\text{Number of estimable models in } S_1}{\text{Number of models in } S_1}$$

and

$$IC_{S_1} = \sum_{i=1}^{s_1} \frac{E_i}{s_1},$$

where $E_i = \frac{|M_i|^p_i}{n}$. 
Step 2 (cont.): Constructing Designs

We will focus on a procedure based on the restricted columnwise-pairwise (RCP) algorithm of Li and Nachtsheim (2000).

This algorithm proceeds column by column through the design, considering exchanges within a column.

Estimation capacity is the primary criterion; information capacity is used to break ties.

As with heuristic algorithms of this type, many algorithm tries should be run in order to obtain near-optimality. We use $n_t = 100$ in our work.
Step 3: Evaluating the Designs with respect to $\mathcal{F}$

- If $\mathcal{F}$ is small—say a few thousand—evaluate each design with respect to $\mathcal{F}$.
- If $\mathcal{F}$ is large, take a sample $S_2$ from $\mathcal{F}$ and evaluate each design with respect to $S_2$. 
<table>
<thead>
<tr>
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<th>$k$</th>
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* These designs are based upon 20 algorithm tries and taken from Li and Nachtsheim (2000).
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How large should $S_1$ be?

For the MEPI model space, question is complicated by a lack of monotonicity as a function of $s_1$.

In other words, in our tests a larger $s_1$ did not necessarily yield a better design than a smaller $s_1$.

However, for small and medium-sized model spaces, using

$$s_1 = \{16, 32, 64\}$$

and taking the best of the three typically gives a design close to the best observed.

For large model spaces, use

$$s_1 = \{16, 32, 64, 128\}.$$
Model-robust designs using the MEPI model space can simultaneously estimate many models that Resolution III or IV fractions cannot.

Proposed designs are competitive (and sometimes substantially superior) in terms of design efficiency, compared to designs in the literature based on $\mathcal{F}$.

Proposed designs can be constructed in a fraction of the time it takes to construct designs based upon $\mathcal{F}$.

For MEPI, use $s_1 = \{16, 32, 64\}$ for small and medium-sized model spaces; $s_1 = \{16, 32, 64, 128\}$ for large model spaces.
In addition to what has been presented, we have:

- Demonstrated method’s effectiveness for the supersaturated model space;
- Computed CIs for $EC_F$ and $IC_F$ for medium and large model spaces;
- Used coordinate exchange instead of RCP as an algorithm to construct the designs;
- Found that the designs constructed can discriminate between models as well as the designs in the literature (Li and Nachtsheim 2000; Jones et al. 2009).