Approximate Model Spaces for Model-Robust Experiment Design

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Outline

1. **Motivation**
2. Approximate Model Spaces
3. Results: MEPI
4. Size of the Approximate Model Space
5. Conclusion
6. Supplementary Slides
   - Model Discrimination
   - Supersaturated Model Space
Optimal Design

Facilitates:

- Precise estimation (e.g. $D$-optimality); or
- Precise prediction (e.g. $TV$-optimality).

Also facilitates tailor-made designs, e.g.:

- 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.
A Model-Robust Approach

Instead of focusing on a single model (optimal design), specify a set of models and find design that is “good” for all models of interest, if possible.
A Model-Robust Approach

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

\[ \mathcal{D}\text{-optimal design, starting with arbitrary } n\text{-run design } \xi_n: \]

\[ \xi_n \xrightarrow{f} \mathbf{X}(\xi_n, f) \xrightarrow{\mathbf{X}' \mathbf{X}} \mathbf{M}(\xi_n, f) \rightarrow \xi_n^* = \arg \max_{\xi_n} |\mathbf{M}(\xi_n, f)| \]
A Model-Robust Approach

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\[D\text{-optimal design, starting with arbitrary } n\text{-run design } \xi_n:\]

\[\xi_n \xrightarrow{f} X(\xi_n, f) \xrightarrow{X'} M(\xi_n, f) \rightarrow \xi_n^* = \arg \max_{\xi_n} |M(\xi_n, f)|\]

Model-robust design with respect to a set of models \(\mathcal{F} = (f_1, f_2, \ldots, f_r):\)

\[\xi_n \xrightarrow{\mathcal{F}} \{X_1, X_2, \ldots, X_r\} \rightarrow \{M_1, M_2, \ldots, M_r\} \rightarrow \xi_n^* = \arg \max_{\xi_n} g[|M_1|, |M_2|, \ldots, |M_r|]\]
Many Different Model Spaces

Main effects plus \( g \) two-factor interactions (MEPI):

- All models consisting of all \( k \) main effects and \( g \) out of \( k(k-1)/2 \) two-factor interactions

- Literature
  - Sun (1993)
  - Smucker, del Castillo, and Rosenberger, forthcoming in *Technometrics*
Many Different Model Spaces

Supersaturated (SS)

- All models consisting of $g$ out of $k$ main effects, where $k > n - 1$ and $g \leq n - 1$.
- Literature
  - Jones, Li, Nachtsheim, and Ye, *JSPI* (2009)
Other Model Spaces

Projective

- Smucker, del Castillo, and Rosenberger, forthcoming in *Technometrics*

All possible submodels of a maximal model (effect heredity can be enforced if desired)

- Tsai and Gilmour, *Technometrics* (2010)
- Smucker, del Castillo, and Rosenberger, *JQT* (2011)
Consider a five-factor experiment in 12 runs.

- Full two-factor interaction model has $1 + 5 + 10 = 16$ parameters and can’t be fit.
- Instead, assume that no more than $g = 3$ two-factor interactions will be active.
- There are 120 models which include 3 two-factor interactions.
- Design strategy: Find a design that can efficiently estimate all 120 models.

Advantage: More efficient designs in fewer runs, compared to resolution III or IV fractions.
A Drawback to Set-of-Models Approach

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

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So does the Supersaturated Model Space

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MEPI

- 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.

Supersaturated

- The largest model space Jones et al. (2009) indicate includes fewer than 40,000 models.
- They state: “... the required computing time can become prohibitively large when $n$ and $|k|$ are large ... [L]arger designs can definitely be constructed ... with more computing power.”
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Motivation
Approximate Model Spaces
Results: MEPI
Size of the Approximate Model Space
Conclusion
Supplementary Slides

Notation

- $\mathcal{F}$: 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 $\mathcal{F}$. 
Overview of Proposed Methodology

1. Select the approximate model space $S_1$ at random from the full model space $F$.
2. Construct $n_t$ designs that are robust for the models in $S_1$, via coordinate exchange.
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 $S_1$

Take a simple random sample from $\mathcal{F}$.

- An empirical study suggests $s_1 = 64$ is adequate, regardless of the size of $\mathcal{F}$.
- An alternative would be to choose the models in $S_1$ systematically.
  - We tried this, using a maximin criterion.
  - It didn’t show clear improvement, and increased the complexity of the procedure.
Step 2: Constructing Designs

Optimize the design with respect to $S_1$ via a two-step process:

1. Maximize the number of models in $S_1$ the design can estimate (i.e. maximize estimation capacity (EC)).

2. If $EC = 1$, maximize the average $D$-efficiency of the design with respect to the models in $S_1$.

This is accomplished via an algorithm that uses coordinate exchange [Meyer and Nachtsheim (1995)].
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 $S_2$.
  - Can perform inference on $EC$ and average $D$-efficiency with respect to $\mathcal{F}$. 

Smucker and Drew  Model-Robust Experiment Design
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Comparing Designs

The following designs are compared:

- $S$ designs. Designs constructed via the three step procedure described above.
  - $S$-16 designs are based on a random sample of $s_1 = 16$.
  - $S$-64 designs are based on a random sample of $s_1 = 64$.

- $\mathcal{F}$ designs. Designs constructed via the three step procedure with $S_1 = \mathcal{F}$.

- MRFD. Designs from Li and Nachtsheim (2000) for the MEPI model space. They utilize $\mathcal{F}$ and require column-balance.
MEPI: Small Experiments

![Graph showing EC and Average D-Efficiency for different designs and experiments.]

- EC (Efficiency Criterion) increasing with design F.
- Average D-Efficiency remains relatively stable across designs, with minor variations.

**Experiments**:
- \( n=12; k=5; g=4; s2=210; r=210 \)
- \( n=12; k=7; g=3; s2=1,330; r=1,330 \)
- \( n=16; k=7; g=3; s2=1,330; r=1,330 \)
- \( n=16; k=8; g=2; s2=378; r=378 \)
MEPI: Medium-sized Experiments

- Experiment:
  - $\{n=12; k=7; g=4; s2=5,985; r=5,985\}$
  - $\{n=16; k=8; g=5; s2=2,000; r=98,280\}$
  - $\{n=16; k=9; g=5; s2=2,000; r=376,992\}$
  - $\{n=16; k=10; g=3; s2=2,000; r=14,190\}$
MEPI: Large Experiments

Diagram illustrating the relationship between experiment design and average D-efficiency for different sample sizes and model sizes.
### MEPI: Design Construction Times

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</table>

Times are in minutes per algorithm try.
Since $S_1$ is chosen randomly, we wish to study the effectiveness of the procedure over multiple randomly chosen $S_1$’s. In what follows:

- 20 model sets were chosen.
- For each, $n_t = 50$ designs were constructed and the best chosen.
- The average EC and average $\overline{E_D}$ were calculated, along with standard deviations of these quantities.
MEPI: Medium-sized Experiments

- Experiment:
- \( \{n=15,k=8;q=4; \lambda_2=2.000; r=20.475\} \)
- \( \{n=16,k=9;q=5; \lambda_2=2.000; r=376.932\} \)
- \( \{n=16,k=10;q=3; \lambda_2=2.000; r=14.190\} \)

- Average EC
- Standard Deviation EC

- Average Efficiency
- Standard Deviation Efficiency

Smucker and Drew
Model-Robust Experiment Design
**Motivation**

**Approximate Model Spaces**

**Results: MEPI**

Size of the Approximate Model Space

**Conclusion**

**Supplementary Slides**

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**MEPI: Large Experiments**

[Graphs showing experimental results]
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Overall Comments

Based on the presentation:

- Proposed designs are competitive in terms of design efficiency, and constructed in fraction of the time.
- Proposed designs are more efficient than Li and Nachtsheim designs and constructed in fraction of the time.
- If at least a few degrees of freedom above saturation, larger approximate model spaces are more efficient and less variable.
- Approximate model space size of 64 seems adequate regardless of the size of $F$. 
Based on other work we have done:

- Procedure is effective for other model spaces (supersaturated; all possible submodels).
- These designs do not appear to give up a significant amount in model discriminating capabilities.
Acknowledgments

- Co-author and former graduate student Nathan Drew;
- John Bailer and Steve Wright, for their feedback;
- Miami University’s Summer Research Grant.
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Li, Sudarsanam, and Frey (Complexity, 2006) empirically examine effect sparsity.

Conclusions

- Likely between 37% and 46% (mean: 41%) of main effects will be active.
- Likely between 9% and 14% (mean: 11%) of two-factor interactions will be active.

Caveat: Only full factorial designs with 7 or fewer factors.
Model-Robust is not the same as Model-Discriminating

It is possible for two models to be estimable but indistinguishable from each other.

- One way to measure model discrimination is the subspace angle (Jones et al. 2007).
- Given a design and a pair of models, the subspace angle is the angle between the subspaces spanned by the columns of the expanded design matrices $X_1$ and $X_2$.
- If the angle is close to 90 degrees, the models are close to orthogonal.
- If the angle is close to 0, the models are close to indistinguishable (nearly aliased).

With such large model spaces, model discrimination is of concern.
Each pair of models should be compared, and when the model space is large this is computationally prohibitive.

- Thus, we again sample, this time pairs of models.
- We can sample a large enough number that inference is very sharp.
## Tabular Comparison

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<th>$g$</th>
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* If the two models to be compared were the same, this comparison was disregarded.
Graphical Comparison

**Figure:** Top row: \( \{n = 8; k = 12; g = 5\} \) supersaturated experiment with \( S_{1-64} \) design (top left) and MRSS design (top right). Bottom row: \( \{n = 24; k = 12; g = 10\} \) MEPI experiment with \( S_{1-64} \) (bottom left) and \( \{n = 28; k = 12; g = 10\} \) MEPI experiment with \( S_{1-64} \) design (bottom right).
The $S$-64 designs are competitive in terms of model discrimination (subspace angle) to designs in the literature. If the average subspace angle is too small, it can be increased by increasing the sample size.
## Supersaturated: Small Experiments

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Model-Robust Experiment Design
Supersaturated: Large Experiments

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For all designs, $EC = 1$. 
Supersaturated: Multiple Model Sets

- Smucker and Drew
- Model-Robust Experiment Design