Candidate-List-Free Exchange Algorithms for Two-Level Model-Robust Designs

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Outline

1. Background
2. Algorithm for Model-Robust Design Using the Maximin Criterion
3. Incorporating Prior Information
4. Extension: More Than Two Factor Levels
5. Computational Results
6. Conclusions

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Fractional Factorial Design FAIL: Exhibit 1

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

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- 2^{4-1} resolution IV design
- Only estimates 12/15 models with 2 interactions

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Model-Robust Design of Li and Nachtsheim estimates all 15.

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- Seven factors
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1. Minimum aberration resolution VII $2^{7-1} = 64$ fractional factorial design (too many runs)
2. Minimum aberration resolution IV $2^{7-2} = 32$ fractional factorial design (resolution too low)

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Exhibit 2 (continued)

Active Factors	*Number of Models**	*Proportion Estimable*
7	1	0
6	7	0.571
5	21	0.857
4	35	0.971

Table: Resolution IV design.

*Models with a subset of main effects and associated 2-factor interactions.

Exhibit 2 (continued)

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Table: Resolution IV design.

Active Factors	*Number of Models*	*20-run Design*	*24-run Design*
7	1	0	0
6	7	0	1
5	21	1	1
4	35	1	1

Table: Model-Robust designs (Loeppky et al.)

*Models with a subset of main effects and associated 2-factor interactions.

Model-Robustness and Two-Level Designs

Two-level experiments are typically the purview of fractional factorial designs;

- We have just seen experimental scenarios in which fractional factorial designs fail;
- Solution: Look at this design problem from a model-robustness perspective;
  - Think about the objectives of the experiment;
  - Find a design that fits those objectives.
- Model-robust designs allow as many desired models to be estimated as possible, and if all are estimable allows efficient estimation for those models.

Classical Optimal Design

Model-robust designs are the progeny of classical optimal designs, which optimize some function of the parameter estimate or prediction variance.

- Many criteria exist: $\mathcal{A}$, $\mathcal{D}$, $\mathcal{E}$, $\mathcal{G}$, $\mathcal{IV}$; which is best?

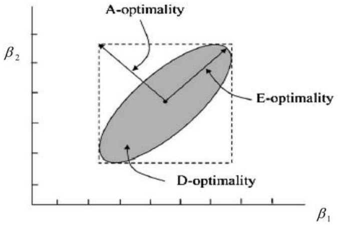

Figure: Representations of various optimality criteria[†]

[†] Atashgah & Seifi (2009) via Aspery & Macchietto (2002)

$\mathcal{D}$-optimality

Our work is based upon the $\mathcal{D}$-criterion.

- $\mathcal{D}$-optimality: $\phi(\mathbf{M}) = |\mathbf{M}|$;
- $\mathcal{D}$-optimal designs minimize the volume of confidence ellipsoid of parameters;
- Computationally simple.

Criticism of optimal design: Requires specification of the model-form before experiment is run.

Optimal Design vs. Model-Robust Design

- Instead of focusing on a single model (optimal design), find design that is "good" for all models of interest, if possible;
- "Good" first means estimable and secondly means efficiently estimated;

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$\mathcal{D}$-optimal design based on a regression model with information matrix $\mathbf{M} = \mathbf{X}'\mathbf{X}$, starting with arbitrary n-run design ξ_n:

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

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

$$\xi_n \xrightarrow{\mathcal{F}} \{\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_r\} \rightarrow \{\mathbf{M}_1, \mathbf{M}_2, \ldots, \mathbf{M}_r\} \rightarrow \xi_n^* = \arg\max_{\xi_n} g[|\mathbf{M}_1|, |\mathbf{M}_2|, \ldots, |\mathbf{M}_r|]$$

Examples of $\mathcal{F}$

Some model spaces:

- All possible submodels of a maximal model;
- All possible submodels of a maximal model, effect heredity enforced;
- All possible models having $n-1$ or fewer main effects, out of $k > n$ (**supersaturated** model space).
- All possible models with main effects plus g two-factor interactions (**MEPI** model space);
- All possible models with m out of k factors and all $\binom{m}{k}$ two-factor interactions (**projective** model space);

Our maximin approach is best suited when all $f \in \mathcal{F}$ have the same number of parameters. Thus, we focus on the last two model spaces.

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Algorithm

Definitions:

- Estimation capacity (EC) for design ξ_n and model set $\mathcal{F}$: Proportion of models ξ_n in $\mathcal{F}$ that ξ_n can estimate;
- $\mathcal{D}$-efficiency ($\mathcal{D}_{eff}$) for design ξ_n and model f_i: $(|\mathbf{M}(\xi_n, f_i)|/|\mathbf{M}(\xi_n^*, f_i)|)^{p_i}$.

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Algorithm:

1. Generate random design.
2. Use coordinate exchange to find a design which maximizes EC.
3. If $EC = 1$, use coordinate exchange to maximize $\min_{f \in \mathcal{F}} \mathcal{D}_{eff}$.

Model Spaces and Previous Work

The two model spaces we consider:

- MEPI model space (all models with all main effects and g two-factor interactions);
- Projective model space (all two-factor interaction models projecting from k to m factors).

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(Some) Previous work:

- Li and Nachtsheim (2000) studied the MEPI model space, but limited search to *balanced* designs.
- Loeppky et al. (2007) studied the projective model space, but limited search to *orthogonal* designs.
- Our approach removes these limitations.

Secondary Criterion

Not all designs with $EC = 1$ are equal.

Designs	*EC*	*Mean $\mathcal{D}$-Eff.*	*Min $\mathcal{D}$-Eff.*
1	1	.642	.494
2	1	.770	.657
3	1	.798	.598

Table: Comparison of model-robust 16-run designs with 10 factors and 2 two-factor interactions. This model space has 990 models.

Secondary criterion is necessary.

Maximin Criterion

- Li and Nachtsheim (2000) and Loeppky et al. (2007) use average $\mathcal{D}$-efficiency as secondary criterion.
- We maximize the minimum $\mathcal{D}$-efficiency over all models.
  - $\max_{\xi_n} \min_{f \in \mathcal{F}} \mathcal{D}_{eff}(\xi_n, f) = (|\mathbf{M}(\xi_n f)|/|\mathbf{M}(\xi_n, f)|)^{1/p}$;
  - Worst-case protection.
  - $\mathcal{D}$-efficiencies tend to be less variable.
  - Flexible in admitting *a priori* information.

Results I

MEPI Model space: All r models with all k main effects and g two-factor interactions.

n	k	g	r	*Designs*	*EC*	*Mean $\mathcal{D}$-Eff.*	*Min $\mathcal{D}$-Eff.*
12	5	4	210	CLF-EC	1	.888	.720
				CLF-Maximin	1	.867	.741
				L&N	.995	-	-
12	9	2	630	CLF-EC	.994	.672	.411
				L&N	.986	-	-
16	7	3	1330	CLF-EC	1	.753	.636
				CLF-Maximin	1	.878	.788
				L&N	1	.865	.723
				FFD	.771	-	-
16	10	2	990	CLF-EC	1	.642	.494
				CLF-Maximin	1	.770	.657
				L&N	1	.798	.598

Results II

Projective model space: All r models with m of the k main effects and all associated 2fi's.

n	k	m	r	*Designs*	*EC*	*Mean $\mathcal{D}$-Eff.*	*Min $\mathcal{D}$-Eff.*
20	8	5	56	CLF-EC	1	.700	.5355
				CLF-Maximin	1	.771	.667
				Loeppky et al.‡	.929	-	-
20	12	5	792	CLF-EC	.95	.735	.5355
				Loeppky et al.	.825	-	-
28	8	6	28	CLF-EC	1	.592	.447
				CLF-Maximin	1	.837	.808
				Loeppky et al.	1	.807	.678
28	12	6	924	CLF-EC	1	.697	.447
				CLF-Maximin	1	.697	.544
				Loeppky et al.	1§	-	-

‡ Results reported in their paper

§ By my calculation, less than one.

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Unequally Weighted Models

Models can be weighted. For instance, models might be partitioned into three groups:

- Group 1: Models including impossible/uninteresting interactions - leave them out of the model set completely;
- Group 2: Models including possible but unlikely interactions - include in the model set, but downweight;
- Group 3: Models including possible and reasonably expected interactions - include in the model set, with full weight;

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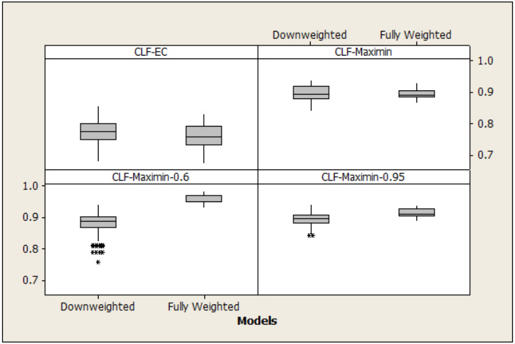
Example:

- MEPI model space;
- $\{n = 16, k = 6, g = 3\}$; 455 models;
- Group 1: No models;
- Group 2: All models with an interaction including factor 6;
- Group 3: The rest of the models in the model space.

Unequally Weighted Models (continued)



Assuming a MEPI model space, the comparison of various designs for a $\{n = 16, k = 6, g = 3\}$ *experiment, with respect to models which include 2fi's involving the sixth factor ("downweighted" models) as well as models which do not ("fully weighted" models).*

Unequally Weighted Models (continued)

Design	*Models*	$\overline{E}_{\mathcal{D}}$	min $E_{\mathcal{D}}$
CLF-EC	Downweighted	.774	.679
	Fully Weighted	.758	.671
CLF-Maximin	Downweighted	.898	.840
	Fully Weighted	.897	.865
CLF-Maximin-0.6	Downweighted	.881	.758
	Fully Weighted	.954	.930
CLF-Maximin-0.95	Downweighted	.895	.844
	Fully Weighted	.915	.888

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Two Optimizations

The approach outlined above requires two optimizations:

1. First, maximize the estimation capacity;
2. Then, if $EC = 1$, maximize the minimum efficiency.

Trade-off:

- If the run size is large enough, the first optimization tends to be fast.
  - The algorithm quickly finds a design with 100% estimation capacity;
  - Most of the computational energy is expended on the maximin part;
- If run size isn't large enough to allow all models to be estimated, all computation is expended on the estimation capacity optimization (the maximin portion is omitted).

More than Two Factor Levels

Multiple optimizations can be eliminated if we allow the factors to have more than two levels:

- Then, a quickly (and/or randomly) generated initial design will have 100% estimation capacity;
- The algorithm can focus on the maximin portion;
- Computation trade-off:
  - No estimation capacity optimization - less computation;
  - Search is more focused (more levels for coordinate exchange to consider) - more computation;

More than Two Levels: Results for MEPI Model Space

n	k	g	r	*Designs*	*EC*	$\overline{E}_{\mathcal{D}}$	*min* $E_{\mathcal{D}}$	Time
12	5	2	45	2-level	1	.983	.970	.061
				3-level	1	.983	.970	.171
12	7	3	1330	2-level	.995	n/a	n/a	6.814
				3-level	1	.545	.356	2.811
12	9	2	630	2-level	.992	n/a	n/a	4.569
				3-level	1	.422	.229	1.205
16	7	4	5985	2-level	1	.772	.619	42.467
				3-level	1	.771	.659	56.597

- The "Time" column is in the units of minutes/algorithm try.
- The two-level result for $\{n = 12, k = 9, g = 2\}$ is different than the previous result because a different set of algorithm tries and individually optimal designs were used.

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Computational Results: MEPI Model Space

n	k	g	r	Method	Minutes/Algorithm Try
12	5	2	45	CLF-Maximin	.103
				L&N[1]	.034
12	9	2	210	CLF-Maximin	8.195
				L&N	2.334
16	7	2	210	CLF-Maximin	.866
				L&N	.833
16	8	2	378	CLF-Maximin	.898
				L&N	2.125
16	9	2	630	CLF-Maximin	3.347
				L&N	4.818

A comparison of computation times for MEPI model spaces for our procedure and that of Li and Nachtsheim.

Computational Results: Projective Model Space

n	k	r	Minutes/Algorithm Try
16	10	252	7.891
16	14	2002	121.735
20	8	56	0.459
20	10	252	7.127
20	12	792	37.856
24	8	28	0.334
24	10	210	8.796
24	12	924	78.495

Assuming the projective model space, these are computation times for our procedure for a variety of experiments.

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Contributions

- We have developed a procedure to construct designs that are robust for specified model spaces;
- Our model-robust exchange algorithm has no candidate list;
- For the MEPI and projective model spaces, we allow nonorthogonal and unbalanced designs, which results in generally equal or higher proportions of estimable models than designs in the literature;
- When all models are estimable, our designs give worst-case protection (better minimum $\mathcal{D}$-efficiencies);
- This method readily and ably admits prior information.

Limitations

- The maximin criterion is not effective for model spaces in which the number of parameters varies significantly in the models composing the model set;
- The method is limited to small/medium-sized problems;
- We have implemented this method in Matlab. A fast compiled language and a better programmer could speed things up considerable, but large problems still pose a problem.

Future Work

1. The fundamental limiting factor for the model set approach is that the size of the model sets explode exponentially in the number of model parameters.
   - Thus, current research efforts are focused on developing ways to tame the huge model spaces;
2. These model-robust ideas can be translated to split-plot designs and other experimental scenarios.

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- Anonymous reviewers

[Li and Nachtsheim (2000)] Model Robust Factorial Designs. Technometrics, 42(4), 345-352.

[Loeppky, Sitter, and Tang (2007)] Nonregular Designs with Desirable Projection Properties. Technometrics, 49(4), 454-467.

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