Exchange Algorithms for Model-Robust, Exact Experimental Designs

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Miami University at Oxford, March 18, 2010

One of Your Department's Strongest Students

Prototypical Example

Plastic formulation (Snee 1985)

- Suppose you must study the effect of five mixture factors on the hardness of a plastic product using 25 runs
- Mixture constraint, other single-factor and multi-factor constraints
- The form of the regression model is unknown; main effects? quadratic? cubic terms?

Figure: Manufactured Plastics[a]

[a] www.plastipak.com.pe/empresa_ingles.htm

Outline

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Experimental Design

Definition

An **experiment** is a "test or series of tests in which *purposeful changes* are made to the input variables of a process or system so that we may observe and identify the reasons for changes that may be observed in the output response." (Montgomery 1991, emphasis added)

Standard Designs

i.e. factorial, fractional factorial, Box-Behnken, central composite

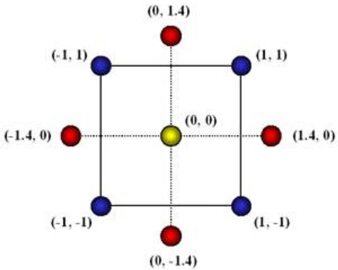

Figure: Central composite design for two factors[1]

[1] http://www.smallprecisiontools.com/Image/products/bonding/capillaries/Capillary_DOE_Matrix_1_320x240_col.jpg

Inadequacy of Standard Designs

Standard designs are often sufficient, but not always

- Design space constrained (e.g. mixture experiments)
- Categorical factors
- Nonstandard sample sizes required

In such cases, it is natural to choose a design based on a criterion of "design goodness."

Optimal Designs

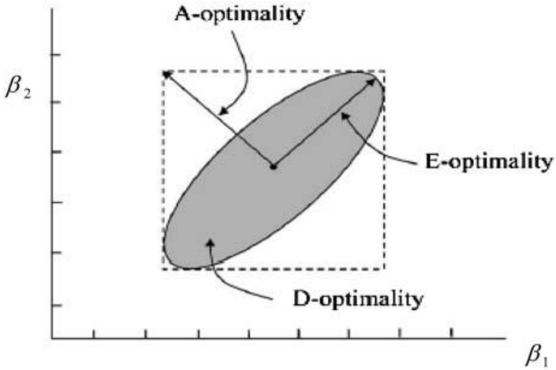

Figure: Representations of various optimality criteria[2]

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

$\mathcal{D}$-Optimality

- Most popular design criterion
- Computationally convenient
- Maximizes determinant of information matrix
- Minimizes volume of confidence ellipsoid for parameters

Criticism: Requires complete specification of the model-form, which is usually unknown at design stage.

The Problem at Hand: Model-Robust Design

Goal: construct a design which has optimal design-like qualities but which is robust to model misspecification. Our approach:

- Allow experimenters to specify a class of models
- Use as criteria some function of the determinants of the information matrices for each model (a lot more on that later)
- Develop algorithms which optimize these criteria and produce exact designs
- Investigate the properties of these model-robust designs to provide justification and understanding

Model-robust Literature

Theory: Large amount of work; practically difficult to use

- Simple cases (e.g. Box and Draper 1959)
- Continuous design theory (e.g. Läuter 1974; Dette 1995, 2000, 2001)
- Other unrealistic assumptions (e.g. "unknown contamination function with certain properties...", for instance Fang and Wiens 2003)

Practice: Smaller literature

- Bayesian approach (DuMouchel and Jones 1994)
- Model-robustness for factorial designs (Li and Nachtsheim 2000)
- Genetic algorithm as the optimization tool (Heredia-Langner et al. 2004)
- MSE prediction-type criterion (Welch 1983)

The Divide in Optimal Design

Theory (continuous designs)

- Jack Kiefer was early proponent
- Mathematically rigorous and tractable (convex optimization)
- Focus on complete solution to specific problems
- Produced myriad insights, but lacks flexibility
  - Assumes asymptotic run sizes
  - Assumes standard design regions

Practice (exact designs)

- Algorithms grew alongside theory (e.g. Fedorov's exchange algorithm)
- Heuristic (nonconvex optimization)
- Algorithms widely used by practitioners
  - Uses finite run sizes
  - Allows irregularly-shaped design regions

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My Perspective

For experimental design, theory produces insight but practical algorithms get the job done. Consequently, our approach:

1. is user-focused
2. leads to development for exact designs
3. relies on and develops theory to provide insight

This will be demonstrated, particularly in the second part of the talk.

Outline

Setting

Consider the univariate regression model of response y on factors $\mathbf{x}$:

$$\mathbf{y} = \mathbf{X}\beta + \epsilon$$

- $\mathbf{X}$ is the expanded design matrix
- OLS estimators are $\hat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$
- Assume $\epsilon \sim N(0, \sigma^2\mathbf{I})$, so $Var(\hat{\beta}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$
- Information matrix: $\frac{\mathbf{X}'\mathbf{X}}{\sigma^2} \propto \mathbf{X}'\mathbf{X} = \mathbf{M}$

$\mathcal{D}$-optimal vs. Model-robust problem

$\mathcal{D}$-optimal design:

Assume $f \rightarrow$ **Expand to X** $\rightarrow$ **Choose** ξ_n **to maximize** $|\mathbf{M}|$

Model-robust design:

Assume $\mathcal{F} \rightarrow$ **Expand each to** $\mathbf{X}_i \rightarrow$ **Choose** ξ_n **to maximize** $g(\mathbf{M}_{\mathcal{F}})$

where $g(\mathbf{M}_{\mathcal{F}}) = g(\mathbf{M}_1, \ldots, \mathbf{M}_r)$. We present two approaches:

1. $g_1(\mathbf{M}_{\mathcal{F}}(\xi_n)) = \prod_f |\mathbf{M}_f(\xi_n)|$
2. $g_2(\mathbf{M}_{\mathcal{F}}(\xi_n)) = \min_{f \in \mathcal{F}} \left(|\mathbf{M}_f(\xi_n)|/|\mathbf{M}_f^*|\right)^{1/p_f} = \min_{f \in \mathcal{F}} E_f(\xi_n)$

Outline

Multiresponse/Model Average

First model-robust criterion:

$$g_1(\mathbf{M}_{\mathcal{F}}(\xi_n)) = \prod_f |\mathbf{M}_f(\xi_n)|$$

- Find design which maximizes $g_1(\mathbf{M}_{\mathcal{F}}(\xi_n))$
- Each model $f \in \mathcal{F}$ has a "say" in the design
- Multiresponse optimal design justification

Motivation: Multiresponse $\mathcal{D}$-optimal Design

Seemingly unrelated regression model (Zellner 1962)

- $\mathbf{M}_m = \mathbf{Z}'(\boldsymbol{\Sigma} \otimes \mathbf{I})^{-1}\mathbf{Z}$ where

$$\mathbf{Z} = \begin{pmatrix} \mathbf{X}_1 & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_2 & \dots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \dots & \mathbf{X}_r \end{pmatrix}$$

- Multiresponse $\mathcal{D}$-optimal design seeks to maximize $|\mathbf{M}_m|$.
- Multiresponse designs and model-robust single response designs have roughly the same goals
- Thus, put "models" in the place of "responses" and solve multiresponse design problem to get model-robust design

- If response model forms are nested, multiresponse $\mathcal{D}$-optimal design is invariant to $\mathbf{\Sigma}$ (Krafft and Scheaffer 1992; Bischoff 1993)
- So, find design that maximizes $\left|\mathbf{Z}'(\mathbf{I} \otimes \mathbf{I})^{-1}\mathbf{Z}\right| = \prod_f |\mathbf{M}_f(\xi_n)|$
  - If $\mathcal{F}$ nested, this design is $\mathcal{D}$-optimal for the associated multiresponse model
  - Interpretation: The estimates of parameters for all models simultaneously give the minimum volume of the confidence ellipsoid of the parameters
- Generalize modified Fedorov exchange algorithm to find model-robust, modified Fedorov (MRMF) design

Small Example: Constrained Response Surface

Small design ($n = 6$) with design region

$$\chi = \{\mathbf{x} = (x_1, x_2) : -1 \leq x_1, x_2 \leq 1$$
$$x_1 + x_2 \leq 1$$
$$-0.5 \leq x_1 + x_2\}$$

with $\mathcal{F} = \{f_i^{'}(\mathbf{x})\beta_i, 1 \leq i \leq 3, \mathbf{x} \in \chi\}$ where

$$f_1^{'}(\mathbf{x}) = (1, x_1, x_2) \quad (1)$$
$$f_2^{'}(\mathbf{x}) = (1, x_1, x_2, x_1x_2) \quad (2)$$
$$f_3^{'}(\mathbf{x}) = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2) \quad (3)$$

Small Example: Results

	Model		
Design	(1)	(2)	(3)
MRMF/Model-averaging	.810	.907	.995
Design Optimal for (3)	.853	.737	1

Table: $\mathcal{D}$-efficiencies for small example with $n = 6$, protecting against three models.

Small Example: Design Optimal for Quadratic Model

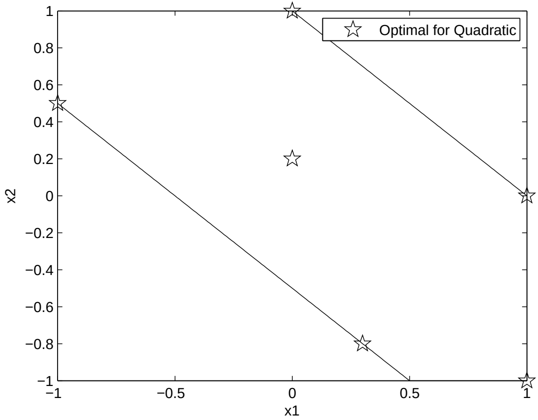

Figure: Design optimal for quadratic model, for Example 1

Small Example: Model-averaged Design

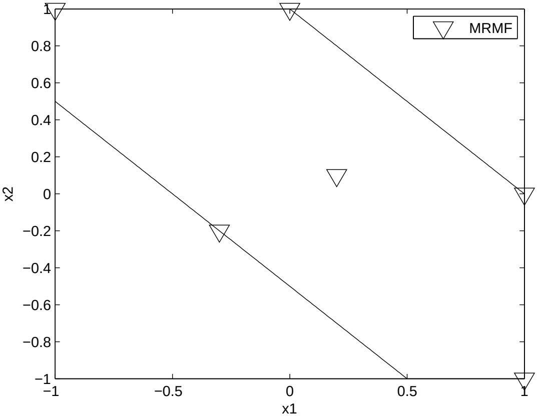

Figure: MRMF design for Example 1

Outline

Maximin Criterion

- The model-averaged designs tend to be unbalanced with respect to $\mathcal{D}$-efficiencies
- To address this problem, maximize:

$$g_2(\mathbf{M}_{\mathcal{F}}(\xi_n)) = \min_{f \in \mathcal{F}} \left(|\mathbf{M}_f(\xi_n)|/|\mathbf{M}_f^*|\right)^{1/p_f} = \min_{f \in \mathcal{F}} E_f$$

- A generalization allows the user to specify interest in each model, $\mathbf{v} = (v_1, \ldots, v_r)$, $v_i \in (0, 1]$:

$$g_3(\mathbf{M}_{\mathcal{F}}(\xi_n)) = \min_{f \in \mathcal{F}} (E_f / v_f) = \min_{f \in \mathcal{F}} G_f$$

- For example, take $\mathcal{F} = (f_1, f_2)$ with $\mathbf{v} = (1, .6)$
  - Criterion g_3 gives a design for which the second model has roughly 60% $\mathcal{D}$-efficiency of the first

Small Example, Results Revisited

	Model		
Design	(1)	(2)	(3)
$\mathcal{D}$-Maximin	.889	.894	.888
$(1,1,.6)$-$\mathcal{D}$-Maximin	.951	.959	.721
MRMF/Model-averaging	.810	.907	.995
Design Optimal for (3)	.853	.737	1

Table: $\mathcal{D}$-efficiencies for small example with $n = 6$, protecting against three models.

- $\mathcal{D}$-Maximin design is very close to balanced in terms of $\mathcal{D}$-efficiencies
- $(1,1,.6)$-$\mathcal{D}$-Maximin has $G_{f_1} = .951$, $G_{f_2} = .959$, and $G_{f_3} = .721/.6 = 1.20$, so models f_1 and f_2 are balanced

Asymptotic Properties of Maximin Criterion

Definition

Given a design, ξ, along with a set of models, $\mathcal{F}$, *generalized efficiency balance* (GEB) is achieved for a subset of models $\mathcal{F}^{'} \subseteq \mathcal{F}$ if

$$G_{f_{max}}(\xi) - G_{f_{min}}(\xi) < \epsilon$$

where $f_{min} = \arg\min_{f \in \mathcal{F}'} G_f(\xi)$, $f_{max} = \arg\max_{f \in \mathcal{F}'} G_f(\xi)$, and ϵ is an arbitrarily small positive constant. If GEB holds for $\mathcal{F}$, *complete generalized efficiency balance* (CGEB) is achieved.

- Can we guarantee GEB for some nontrivial $\mathcal{F}^{'} \subseteq \mathcal{F}$? Yes!
- Can we guarantee CGEB? No ... I mean, sort of
- Following results hold only for *asymptotically large* sample sizes

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Generalized Efficiency Balance is Guaranteed

Theorem

Assume $\mathcal{F}$ has r elements and let $\xi^* = \arg\max_{\xi \in \Xi} \min_{f \in \mathcal{F}} G_f(\xi)$ and $f_{min} = \arg\min_{f \in \mathcal{F}} G_f(\xi^*)$. Also, assume that ξ^* is not optimal for any $f \in \mathcal{F}$ individually. Then, $G_f(\xi^*) - G_{f_{min}}(\xi^*) < \epsilon$ for at least one $f \in \mathcal{F} \backslash f_{min}$.

Bottom line: For a given $\mathcal{F}$, some set of at least two models will achieve GEB.

Complete Generalized Efficiency Balance May Happen

Theorem

Assume $\mathcal{F}$ has r elements with arbitrary $\mathcal{F}' \subset \mathcal{F}$. Let $\xi^* = \arg\max_\xi \min_{f\in\mathcal{F}} G_f(\xi)$, and $\xi^{'} = \arg\max_\xi \min_{f\in\mathcal{F}'} G_f(\xi)$. If $\min_{f\in\mathcal{F}'} G_f(\xi^{'}) > \min_{f\in\mathcal{F}'} G_f(\xi^*)$, then

$$G_f(\xi^*) - G_{f_{min}}(\xi^*) < \epsilon \ \forall f \in \mathcal{F}$$

where ϵ is arbitrarily small and $f_{min} = \arg\min_{f\in\mathcal{F}} G_f(\xi^*)$.

Bottom line: If we can do better than ξ^* for all $\mathcal{F}^{'} \subset \mathcal{F}$, we will achieve CGEB

Small Example, Results Once Again

	Model		
Design	(1)	(2)	(3)
$\mathcal{D}$-Maximin	.889	.894	.888
$(1, 1, .6)$-$\mathcal{D}$-Maximin	.951	.959	.721
MRMF/Model-averaging	.810	.907	.995
Design Optimal for (3)	.853	.737	1

Table: $\mathcal{D}$-efficiencies for small example with $n = 6$, protecting against three models.

- $\mathcal{D}$-Maximin design is essentially CGEB
- $(1, 1, .6)$-$\mathcal{D}$-Maximin has $G_{f_1} = .951$, $G_{f_2} = .959$, and $G_{f_3} = .721/.6 = 1.20$, so $\mathcal{F}' = (f_1, f_2)$ is balanced

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Small Example: Model-averaged Design

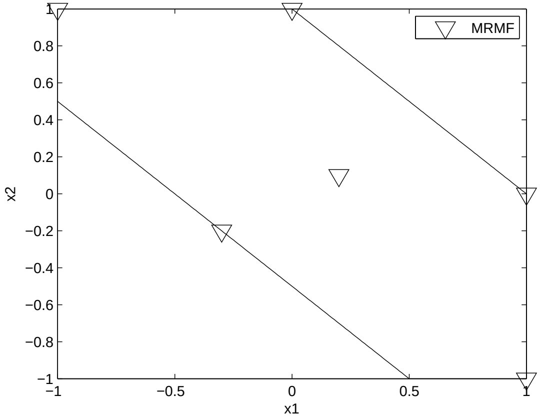

Figure: MRMF design for Example 1

Small Example: Maximin Design

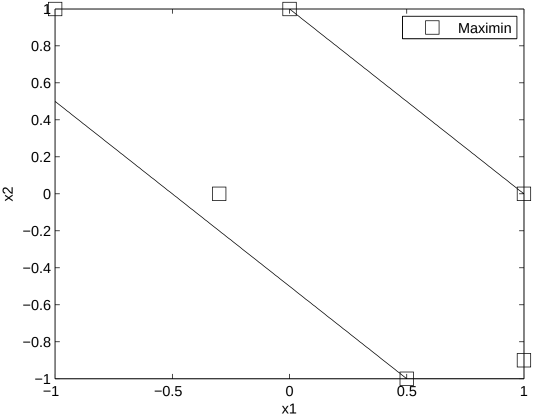

Figure: Maximin design for Example 1

Small Example: (1,1,.6)-Maximin Design

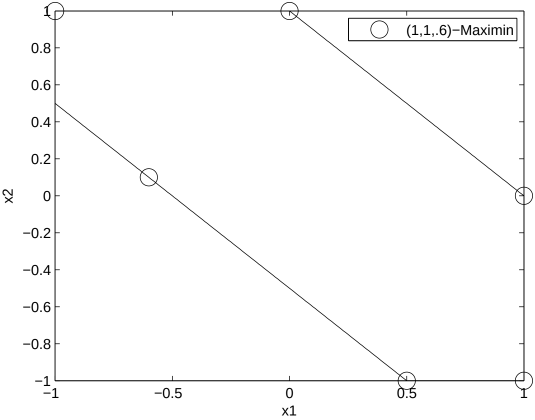

Figure: (1,1,.6)-Maximin design for Example 1

Example 1: All designs

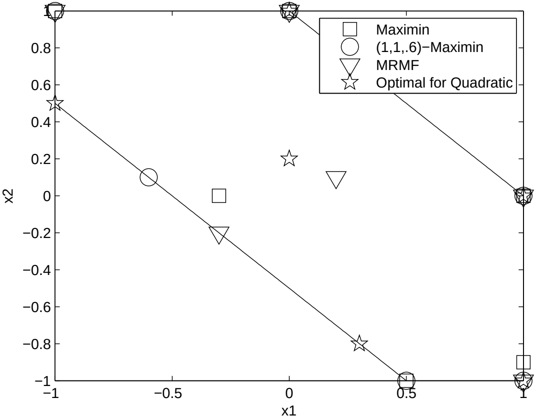

Figure: Designs for Example 1

Outline

Exchange Algorithms

The exact $\mathcal{D}$-optimal design problem is nonconvex. Thus, most commonly used method to solve them is an exchange algorithm:

- Computationally intensive procedure: Evaluate the effect of exchanging a current design point with many other points
- Made computationally tractable by determinant-updating shortcut formulae

$$|\mathbf{M}(\tilde{\xi}_n)| = |\mathbf{M}(\xi_n)| \left(1 + \Delta(\mathbf{x}_j, \mathbf{x}, \xi_n)\right)$$

- Many variations have been proposed, including
  - Fedorov exchange (Fedorov 1972)
  - Modified Fedorov (Cook and Nachtscheim 1980)
  - Coordinate Exchange (Meyer and Nachtsheim 1995)

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Modified Fedorov Exchange Algorithm

1. Begin with a nonsingular design and construct grid of points, $\mathcal{G}$, over design space
2. For a given design point, consider exchanges with all $\mathbf{x} \in \mathcal{G}$.
3. For each potential exchange, evaluate change in determinant via updating formula
4. Choose the exchange which increases the determinant the most
5. Repeat this process for each design point
6. Continue until convergence to a local optimum

Model Averaging Exchange Algorithm

Updating formula for model-robust criterion:

$$|\mathbf{M}_m(\tilde{\xi}_n)| = \prod_{i=1}^{r} |\tilde{\mathbf{X}}_i'\tilde{\mathbf{X}}_i|$$
$$= \prod_{i=1}^{r} \left|\mathbf{X}_i'\mathbf{X}_i\right| (1 + \Delta_i(\mathbf{x}_j, \mathbf{x}))$$

To prevent the algorithm from choosing a really bad exchange, take as the criterion:

$$\prod_{i=1}^{r}(1 + \Delta_i(\mathbf{x}_j, \mathbf{x}))\mathbb{I}((1 + \Delta_i(\mathbf{x}_j, \mathbf{x})) > 0)$$

Then, use the modified Fedorov algorithm, except with the model-robust criterion as standard for choosing exchanges.

Generalized Maximin Model-robust Exchange Algorithm

Requires: Set of models $\mathcal{F}$; model interest vector $\mathbf{v}$; for each model, optimal information matrix determinants;

- Start with nonsingular design, and find the efficiencies with respect to each model $f \in \mathcal{F}$
- Adjust each efficiency to account for the model interest (calculate $G_f \ \forall f \in \mathcal{F}$)
- For a given design point, consider exchanges with all points in candidate list and choose the one which results in the greatest increase in the minimum generalized efficiency
- Continue until convergence

Outline

Plastic Formulation Example

- Mixture experiment with $n = 25$
- Response is hardness of plastic
- Five factors were a binder (x_1), cobinder (x_2), plasticizer (x_3), and two monomers (x_4 and x_5)
- Design region includes mixture constraint and many single- and multi-factor constraints
- $\mathcal{F} = \{f_i^{'}(\mathbf{x})\beta_i, 1 \leq i \leq 4, \mathbf{x} \in \chi\}$ with

$$f_1^{'}(\mathbf{x}) = (\{x_i, i = 1, \ldots, 5\}) \quad (4)$$

$$f_2^{'}(\mathbf{x}) = (f_1^{'}, \{x_i x_j, i < j \leq 5\}) \quad (5)$$

$$f_3^{'}(\mathbf{x}) = (f_2^{'}, \{x_i x_j x_k, i < j < k \leq 5\}) \quad (6)$$

- Used as candidate list the extreme vertices and approximate centroids found using code by Piepel (1988)

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Results

	Model		
Design	(4)	(5)	(6)
$\mathcal{D}$-Maximin	.869	.903	.868
$(.9, 1, 1)$-$\mathcal{D}$-Maximin	.844	.934	.933
$(.9, 1, .5)$-$\mathcal{D}$-Maximin	.882	.979	.507
MRMF/Model-averaging	.822	.955	.950
Bayesian	.805	.940	.965
Optimal for (6)	.800	.924	1

Table: $\mathcal{D}$-efficiencies for constrained mixture example with $n = 25$, protecting against three models.

Outline

Future Work

1. Explore larger model sets
   - Since number of models grows exponentially, take a subset that "spans" the model space and is "symmetric"
   - Or, use a prior on model space developed by Bingham and Chipman (2007)
2. Extend to other models
   - Multiresponse (thesis)
   - Split-plot (thesis)
   - Blocked
   - Nonlinear (i.e. discrete choice designs)
3. Develop faster algorithm
   - Eliminate candidate list
   - Allow for irregularly-shaped design regions
   - Piepel, Cooley, and Jones (2005) claim such an algorithm, without adequate documentation

Contributions

- Used an intuitive, practical model-robust framework: Choose r models and use them to relax model form assumption
- Developed algorithms to find exact, model-robust designs
- Model-averaging approach
  - Maximize $\prod_{i=1}^{r} |\mathbf{M}_i|$
  - If possible models are nested, the model-robust design is the same as the associated multiresponse $\mathcal{D}$-optimal design
  - Minimizes volume of the confidence ellipsoid of parameters
- Maximin approach
  - Maximize the smallest efficiency with respect to the r models
  - Designs more balanced in terms of efficiencies than previous approaches
  - Easily admits prior information that affords the experimenter additional control over efficiencies

This presentation describes research in two papers:

- Smucker, B., del Castillo, E., and Rosenberger, J. L. (2010). Exchange Algorithms for Constructing Model-Robust Experimental Designs. *Journal of Quality Technology*. In Revision.
- Smucker, B., del Castillo, E., and Rosenberger, J. L. (2010). A Maximin Model-Robust Exchange Algorithm and its Generalization. Submitted to *Technometrics*

We are also working on two papers addressing model-robustness for multiresponse and split-plot designs.