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Title: Choosing Good Designed Experiments based on Multiple Optimization Criteria

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Choosing Good Designed Experiments based on Multiple Optimization Criteria

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When selecting which designed experiment to run, there are often multiple competing objectives of interest which we wish to simultaneously consider. Using the Pareto front approach, better alternatives for designs can be constructed and compared. The talk will give background on the Pareto front approach to multiple criteria optimization for the general scenarios, and then describe how this approach has been adapted for design of experiments applications. The approach is very flexible and any set of user-specified objectives can be used in the optimization. Several examples of different experiment design scenarios will be illustrated.

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Christine Anderson-Cook, PhD
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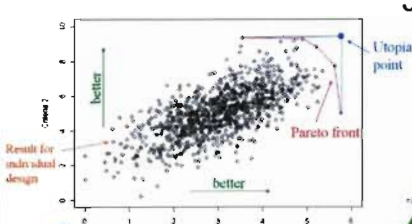
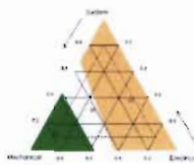
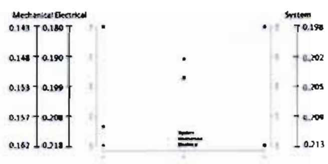
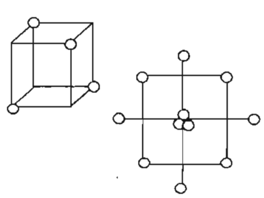
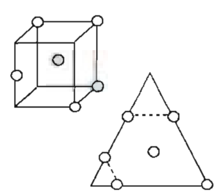


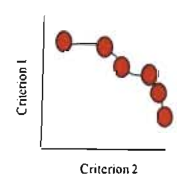




A Very Brief History of Design of Experiments







Textbook designs
- only some N
- regular regions
- good general performance

"Optimal" designs
- flexible N, region, criterion

"Multiple Criteria" designs
- flexible N, region
- consider multiple objectives
- Pareto front based

Computer Power increasing dramatically

A Non-Standard Design Problem

- Problem : Resources to run a 14-run designed experiment to estimate the model:

$$Y = \beta_0 + \beta_A A + \beta_B B + \beta_C C + \beta_D D + \beta_E E + \beta_{AB} AB + \beta_{AC} AC + \beta_{BD} BD + \beta_{CE} CE + \varepsilon \qquad \varepsilon \sim N(0,\sigma^2)$$

We are worried that some of the other 2-factor interactions (AD,AE,BC,BE,CD,DE) might be active

- What design should we run?
- What basis should we use for choosing?

Outline

1. Motivation – why should we consider more than one objective during design construction and selection?
2. Basics of Pareto front approach (2 criteria)
3. Example revisited

Initial designs ⇨ Pareto front ⇨ Reducing number of choices ⇨ Final choice

4. Conclusions

Metrics for Good Designs

1. Result in good fit of the model to the data
2. Provide good model parameter estimates
3. Provide good prediction throughout the design space.
4. Provide an estimate of "pure" experimental error.

Good estimation and prediction for chosen model

5. Give sufficient information to allow for lack of fit test.
6. Provide a check on the homogeneous variance assumption.

Ability to test various aspects of the model

7. Be insensitive (robust) to the presence of outliers in the data.
8. Be robust to to errors in the control of design levels.

Protection if things go wrong

9. Allow models of increasing order to be constructed sequentially.
10. Allow for experiments to be done in blocks.

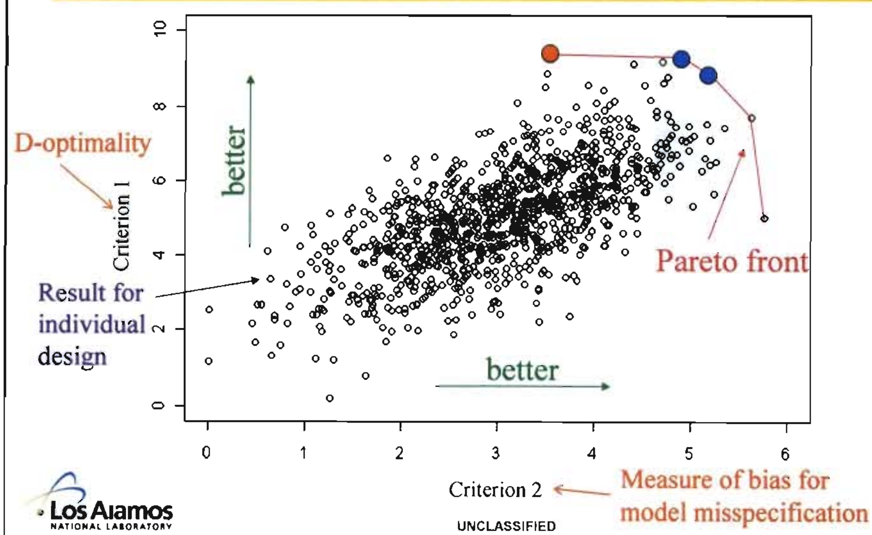
Flexibility to run and expand experiment

11. Be cost-effective.

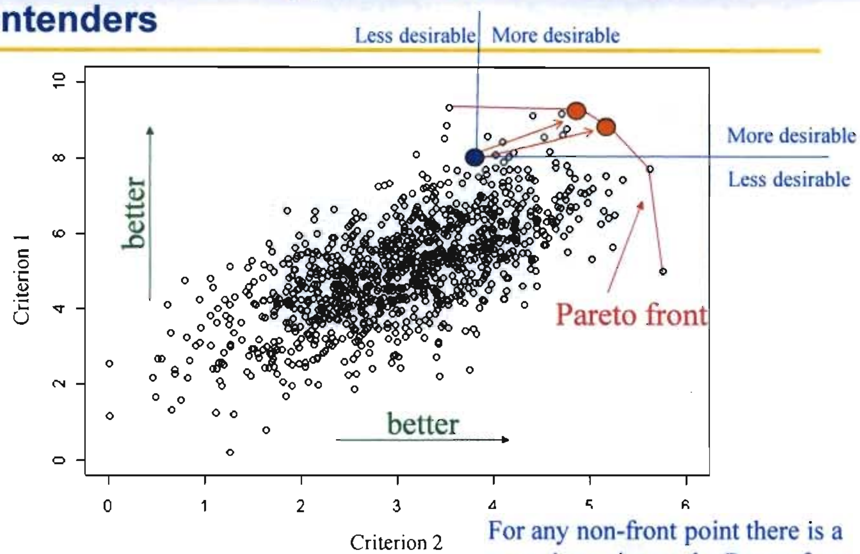
Cost

Myers, Montgomery, Anderson-Cook RSM (2009) p. 282

The Weakness of Single Criterion Optimization

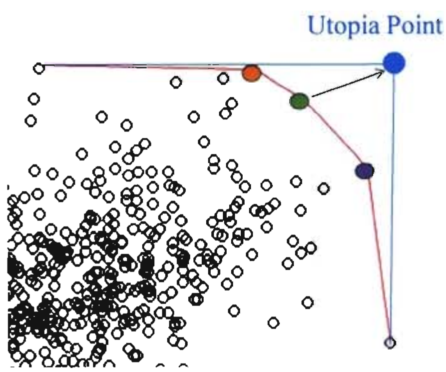


The Pareto Front Approach to Eliminate Non-Contenders



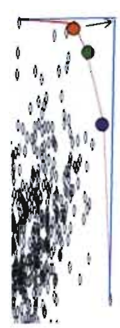
For any non-front point there is a **superior** point on the Pareto front

Deciding Between Points on the Pareto Front



Traditional Strategy:
Choose point closest to Utopia Point

But this depends on scaling!



This reflects how much we weight each objective (stretching makes more important)

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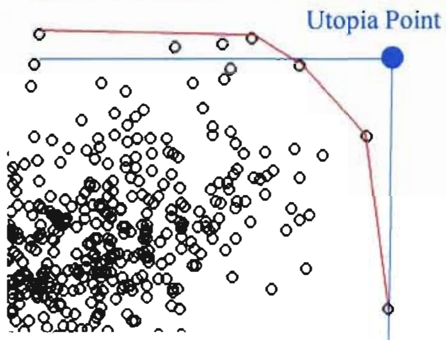
Connecting the Utopia Point Approach to Statistical Approaches to Multiple Objective Optimization



Desirability function:

$$\sum w_i C_i \qquad C_i \in [0,1]$$

(Popularized by Derringer & Suich, 1980)

Stretch of axis ⇔ Larger weight to criterion

Transform each criterion to log scale ⇔ Multiplicative form:

$$\prod (C_i)^{w_i} \qquad C_i \in [0,1]$$

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For the Example – A Screening Design

- If the model is correct:
  - Good estimation of model parameters
- If the model is incorrect (some of AD,AE,BC,BE,CD,DE active)
  - Estimates for terms in model minimally affected
  - Estimation of variance minimally affected

How do we quantify this?

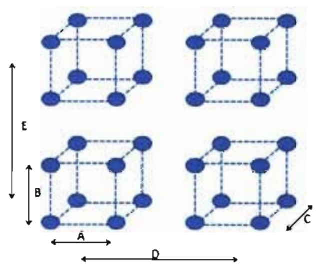
Example – Choosing a "Best" Screening Design Based on Multiple Criteria

Design requirements:

- N = 14 runs
- 5 factors
- possible factor levels (-1, +1)
- estimate all 5 main effects (A – E)
- estimate the following interactions: AB, AC, BD, CE

experts suggest that remaining interactions unlikely

32 possible design points: $(\pm 1, \pm 1, \pm 1, \pm 1, \pm 1)$



Criterion to Consider – (1) D-Optimality

Quantifies how well model parameters are estimated for the model

$$Y_i = \beta_0 + \beta_A A + \beta_B B + \beta_C C + \beta_D D + \beta_E E + \beta_{AB} AB + \beta_{AC} AC + \beta_{BD} BD + \beta_{CE} CE + \varepsilon \qquad \varepsilon \overset{i.i.d.}{\sim} N(0, \sigma^2)$$

D-criterion

maximize $|\mathbf{M}| = |\mathbf{X}'\mathbf{X}| / N^p$ p = # parameters

design matrix expanded to model form

*inversely proportional to the square of the volume of the confidence region on the regression coefficients

Criterion to Consider – (2) Bias on Model Terms

Assumed model: $\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \boldsymbol{\varepsilon}$

$X_1 \in \{A, B, C, D, E, AB, AC, BD, CE\}$

Model to protect against: $\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\varepsilon}$

$X_2 \in \{AD, AE, BC, BE, CD, DE\}$

Bias if model incorrect: $E(\hat{\boldsymbol{\beta}}_1) - E(\boldsymbol{\beta}_1) = [\boldsymbol{\beta}_1 + (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2\boldsymbol{\beta}_2] - \boldsymbol{\beta}_1$

$= \mathbf{A}\boldsymbol{\beta}_2$

If these exist, then size unknown

$$\begin{aligned} \mathrm{E}(\mathrm{SS}_{bias}) &= \mathrm{E}(\boldsymbol{\beta}_2'\mathbf{A}'\mathbf{A}\boldsymbol{\beta}_2) \\ &= \mathrm{E}(\mathrm{tr}(\mathbf{A}'\mathbf{A}\boldsymbol{\beta}_2\boldsymbol{\beta}_2')) \\ &= \sigma^2_{\beta_2}\mathrm{tr}(\mathbf{AA}'). \end{aligned}$$

Therefore, minimize $\mathrm{tr}(\mathbf{AA}')$

Criterion to Consider – (3) Bias on Error Estimate

For same $X_1 \in \{A, B, C, D, E, AB, AC, BD, CE\}$

$X_2 \in \{AD, AE, BC, BE, CD, DE\}$

Bias on estimate of error,

$$\begin{aligned} E(\mathrm{MSE}_{\mathrm{user}}) - \sigma^2 &= \boldsymbol{\beta}_2'[\mathbf{X}_1\mathbf{A} - \mathbf{X}_2]'[\mathbf{X}_1\mathbf{A} - \mathbf{X}_2]\boldsymbol{\beta}_2 / p_1 \\ &= \boldsymbol{\beta}_2'\mathbf{R}'\mathbf{R}\boldsymbol{\beta}_2 / p_1 \end{aligned}$$

Therefore, minimize $\mathrm{tr}(R'R)$

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Process for Selecting a Best Design

- The process for finding a best design for our specific goals can be summarized by a multi-stage algorithm:

1. Create designs, and measure the criteria for all designs.
2. Construct the Pareto front, which consists of all designs which are not inferior to (*Pareto dominated* by) any other designs [OBJECTIVE]
3. Select a best design from the Pareto front which best suits the needs of the experimenter [SUBJECTIVE].

Pareto Aggregating Point Exchange (PAPE) Algorithm: efficiently creates designs and builds Pareto front

Lu, Anderson-Cook, Robinson (2011 Technometrics)

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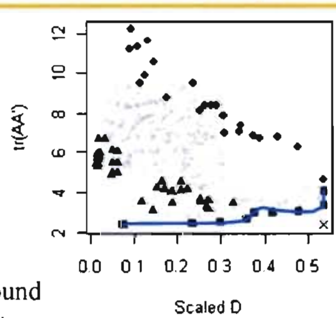
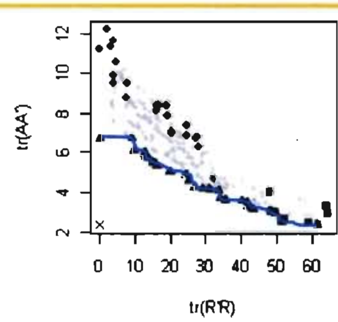
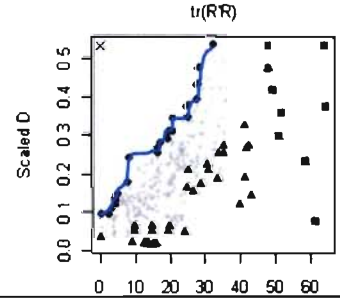
Pareto Front for Example 1





333 designs found on Pareto front (6.5 hours of run time on desktop)



■ D & tr(AA')
◆ D & tr(R'R)
▲ tr(AA') & tr(R'R)
× Utopia Point

Desirability function:

$\sum w_i C_i \qquad C_i \in [0,1]$

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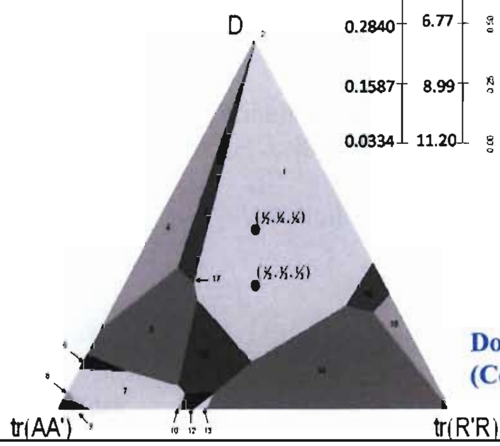
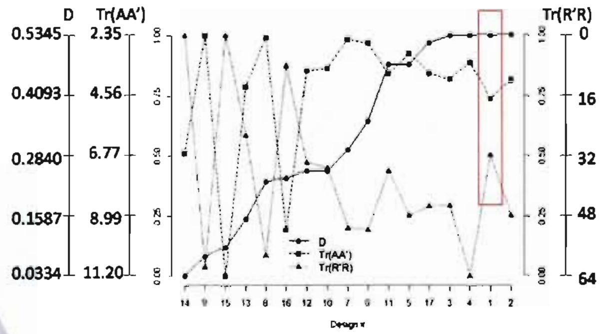
Comparing Designs

Desirability function:

$$\sum w_i C_i \qquad C_i \in [0,1]$$





Desirability function:

$$\prod (C_i)^{w_i} \qquad C_i \in [0,1]$$

Does not require new search for front! (Computationally very quick)

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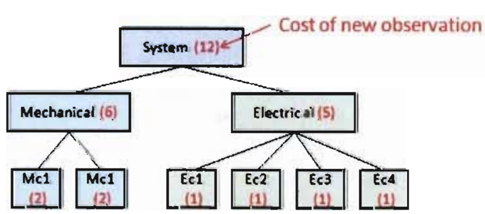
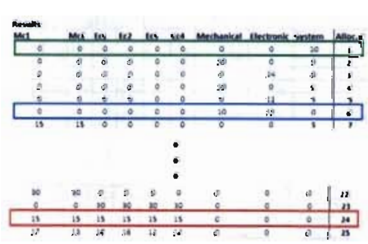
Other Applications of Pareto Front Approach for Design (in various publications)

- Example 2 (Screening Experiment):
  - D-optimality [maximize |X'X|]
  - Good estimation of pure error [maximize df_{PE}]
  - Good estimation of lack of fit [maximize tr(R'R) /(m-p)]
- Example 3 (Reliability Estimation of Complex System):
  - Good precision of system estimate
  - Good precision of sub-system estimates





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Examples (continued)

- Example 4 (Robust Parameter Design Experiment):
  - Good estimation of mean model [max D_s-mean]
  - Good estimation of variance model [max D_s-variance]
  - Size of experiment [min N]
- Example 5 (Split Plot Design):
  - Good estimation of terms when WP to SP variance ratio is unknown [max D(1), max D(10)]
  - Size of experiment [min N]
  - Number of Whole Plots [min #WP]

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\delta} + \varepsilon \qquad \varepsilon \sim N(\mathbf{0}, \sigma^2 \mathbf{I}_{N \times N}) \qquad \boldsymbol{\delta} \sim N(\mathbf{0}, \sigma_\delta^2 \mathbf{I}_{a \times a}) \qquad d = \frac{\sigma_\delta^2}{\sigma^2}$$

Conclusions

- Looking at multiple characteristics can lead to better choices of which design to run (do well for several priorities – not just one!)
- Different designs have different advantages and risks – select criteria to consider which best capture the important considerations for your experiment. It is now possible to focus on what is most important to the experimenter – and do well on those objectives.
- The Pareto front approach can divide possible designs into (1) those consider further and (2) those to eliminate, because they are dominated by other better choices. This objective step selects which designs are sensible to consider.
- Once the Pareto front has been selected, there are multiple ways of selecting the final design – but the key is to examine and understand the trade-offs between the choices. This subjective phase allows experimenter needs to be emphasized.

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