Practical Aspects of Algorithmic Design of Physical Experiments

from an Engineer’s perspective

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Objectives:

- Understand why and when to use algorithmic design.
- Know the difference between D and IV optimality and when to use one or the other.
- Position choice of optimality in the larger framework of what is require for a good (successful) DOE.
- Present an illustrative example.
- Provide working recommendations.
Agenda

Practical Aspects of Algorithmic Design of Physical Experiments:

- What’s required for a good design.
- Optimal point selection (IV versus D optimality).
- Practical aspects algorithmic design.
- Optimal design example.
- Conclusion and recommendations.

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Study Considerations

1. What is the objective of the study?
2. State the objective in terms of measured responses:
   - How will the responses be measured?
   - What precision is required?
3. Which factors will be studied?
4. What are the regions of interest and operability?
5. What order polynomial will adequately model response behavior?
6. What design should we use?

Use first principles and experience!
“Good” Response Surface Designs
Important Properties

1. Allow the polynomial chosen by the experimenter to be estimated well.

2. Give sufficient information to allow a test for lack of fit.
   - Have more unique design points than coefficients in model.
   - Provide an estimate of “pure” error.

3. Be insensitive (robust) to the presence of outliers in the data.

4. Be robust to errors in control of the factor levels.

5. Permit blocking and sequential experimentation.

6. Provide a check on homogeneous variance assumption and other useful model diagnostics; including deletion statistics.

7. Generate useful information throughout the region of interest, i.e., provide a good distribution of standard error of prediction.

8. Not contain an excessively large number of runs.

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Central Composite Designs: CCDs
Incorporate Important Properties

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Example of a Good Design
Std Error and FDS Graphs

The x-axis on the FDS plot is the fraction of the design space where the standard error of the predicted mean is less than or equal to the standard error on the y-axis.

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RSM Design Summary

Top DOE choices for RSM designs:

- **Central Composite**: robust, classic design to fit quadratic model. *(Axial distances can be modified.)*
- **Box-Behnken**: good alternative 3-level design.
- **Optimal**: most flexible design. Use for:
  - designs with multiple linear constraints
  - designs with categoric or discrete numeric factors
  - models other than full quadratic
  - to augment an existing design

**Always choose a design that fits the problem!**

**Size for precision!**
“Good” Algorithmic Designs

Important Properties via Design Points

**Property**

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**Design Points**

- Optimal
- LOF
- Replicates
- LOF & Replicates
- Excess
- Optimal
- Excess
- Sizing (*power*)
- **Enough** *but not too many*

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Practical Aspects of Algorithmic Design of Physical Experiments:

- What’s required for a good design.
- **Optimal point selection (IV versus D optimality).**
- Practical aspects algorithmic design.
- Optimal design example.
- Conclusion and recommendations.
Goal: **D-optimal** design minimizes the determinant of the \((X'X)^{-1}\) matrix. This minimizes the volume of the confidence ellipsoid for the coefficients and maximizes information about the polynomial coefficients.
An **IV-optimal** design seeks to minimize the integral of the prediction variance across the design space. These designs are built algorithmically to provide lower integrated prediction variance across the design space. This equates to minimizing the area under the FDS curve.
Optimal Point Selection
IV versus D Optimal Design

Compare point selection using **IV-optimal** and **D-optimal**:

- Build a one factor design.
- Design for a quadratic model.
- Choose all twelve runs using optimality as only criterion.
IV versus D Optimal Design
Optimal 12 Point Designs

IV-optimal

D-optimal

StdErr of Design

0.70

0.60

0.50

0.40

0.30

-1.00

0.00

1.00

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IV-optimal versus D-optimal
One Factor 12 Optimal Points

Fraction of Design Space Graph

IV min: 0.382
IV avg: 0.421
IV max: 0.577

D min: 0.395
D avg: 0.447
D max: 0.500
“Good” Response Surface Designs
Comments on the Checklist

“designing an experiment is not necessarily easy and should involve balancing multiple objectives, not just focusing on single characteristic.”


“Alphabetic optimality is not enough!”

Pat Whitcomb
Agenda

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- **Practical aspects algorithmic design.**
- Optimal design example.
- Conclusion and recommendations.
Compare point selection using IV-optimal and D-optimal:

- Build a one factor design.
- Design for a quadratic model.
- Choose eight of the twelve runs using optimality as the criteria.
- Choose four of the twelve runs as lack of fit (LOF) points using distance as the criteria.

(Maximize the minimum distance from an existing design points; i.e. fill the “holes”.)
Optimal Designs
8 Optimal + 4 LOF Points

IV-optimal

D-optimal

StdErr of Design

StdErr of Design

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IV-optimal versus D-optimal
8 Optimal and 4 Distance Points

FDS Graph

<table>
<thead>
<tr>
<th>Metric</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>IV min</td>
<td>0.381</td>
</tr>
<tr>
<td>IV avg</td>
<td>0.438</td>
</tr>
<tr>
<td>IV max</td>
<td>0.653</td>
</tr>
<tr>
<td>D min</td>
<td>0.395</td>
</tr>
<tr>
<td>D avg</td>
<td>0.448</td>
</tr>
<tr>
<td>D max</td>
<td>0.547</td>
</tr>
</tbody>
</table>

Fraction of Design Space

StdErr Mean

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IV-optimal versus D-optimal

12 Optimal - 8 Optimal + 4 Distance Points

FDS Graph

- **IV-optimal**
- **D-optimal**

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<th>12 optimal</th>
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Optimal Point Selection
IV versus D Optimal Design

Compare point selection for a two-factor 14-run design:

- Design for a quadratic model.

  - IV-optimal:
    - 14 optimal runs
    - 10 optimal and 4 LOF (distance)

  - D-optimal:
    - 14 optimal runs
    - 10 optimal and 4 LOF (distance)
IV-optimal Designs
14 Run Designs with 0 and 4 LOF Points
IV-optimal Designs
14 Run Designs with 0 and 4 LOF Points

FDS Graph

10 IV-optimal + 4 LOF points
- IV min: 0.435
- IV avg: 0.528
- IV max: 0.857

14 IV-optimal points
- IV min: 0.418
- IV avg: 0.515
- IV max: 0.908

Fraction of Design Space
D-optimal Designs
14 Run Designs with 0 and 4 LOF Points
D-optimal Designs
14 Run Designs with 0 and 4 LOF Points

FDS Graph

14 D-optimal points
Determinant of $(X'X)^{-1} = 3.906E-3$

10 D-optimal + 4 LOF points
Determinant of $(X'X)^{-1} = 5.313E-3$
Adding LOF points:

- The design is not as alphabetically optimal.
- LOF points fill empty spaces.
- Ability to detect lack of fit is enhanced.
- Adding LOF points is a good trade off with optimal points!
Estimating pure error:

- In physical experiments it is desirable to build in an estimate of experimental error.
- Replicates provide an estimate of experimental error independent of model assumptions.
- Adding replicates is a good trade off with optimal points!
Practical Aspects of Algorithmic Design of Physical Experiments:

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Spray Coating Problems (Constraints)

<table>
<thead>
<tr>
<th>Name</th>
<th>Units</th>
<th>−1 level</th>
<th>+1 level</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>flow rate</td>
<td>ml/min</td>
<td>10</td>
</tr>
<tr>
<td>B</td>
<td>pressure</td>
<td>kPa</td>
<td>3</td>
</tr>
<tr>
<td>C</td>
<td>linear speed</td>
<td>inch/sec</td>
<td>0.1</td>
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Problems:

- At the vertex (A = 10, B = 3 and C = 0.5) not enough coating is applied.
- At the vertex (A = 30, B = 10 and C = 0.1) too much coating is applied.
Prevent “not enough” Coating
(A = 10, B = 3 and C = 0.5)

Define constraint as points on edge of cuboidal space. Consider the setting for each factor that provides adequate coating while all other factors are at their low coating weight level.

- A (flow rate) $\geq 15$
  when $B = 3$ and $C = 0.5$  \( CP_A = 15 \)
- B (pressure) $\geq 6$
  when $A = 10$ and $C = 0.5$  \( CP_B = 6 \)
- C (linear speed) $\leq 0.3$
  when $A = 10$ and $B = 3$  \( CP_C = 0.3 \)
Prevent “too much” Coating (A = 30, B = 10 and C = 0.1)

Define constraint as points on edge of cuboidal space. Consider the setting for each factor that provides adequate coating while all other factors are at their high coating weight level.

- A (flow rate) ≤ 20 when B = 10 and C = 0.1  \( CP_A = 20 \)
- B (pressure) ≤ 6 when A = 30 and C = 0.1  \( CP_B = 6 \)
- C (linear speed) ≥ 0.3 when A = 30 and B = 10  \( CP_C = 0.3 \)

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Prevent Not enough and Too much
Multiple Linear Constraints

Not Enough
exclude (10, 3, 0.5)

4.5 \leq 0.6A+B-15C

Too Much
exclude (30, 10, 0.1)

0.8A+2B-40C \leq 32

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One Suggestion for Point Selection

Given how many factors \((k)\) you study and the number of coefficients \((p)\) in the model you select, use the following as a guide to a starting design:

- **Model**: \(p\) points using an optimality criterion
- **Lack-of-Fit**: 5 points; based on distance or estimating higher order model terms.
- **Replicates**: 5 points, using the model optimality criterion (most influential).

Evaluate precision of the starting design via the FDS plot:

- If more precision is required rebuild the design adding more runs.
Spray Coating Design
20 Points: 10 IV-optimal, 5 LOF, 5 replicates
Is the optimal design precise enough?

- Want to estimate the mean within ± 0.5.
- The estimated standard deviation is 0.30.
- FDS of approximately 91% is acceptable.

\[ d = 0.5 \]
\[ s = 0.3 \]
\[ a = 0.05 \]
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**“Good” Algorithmic Designs**

**Important Properties via Design Points**

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“Good” Algorithmic Designs
Suggestion for Point Selection

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Evaluate precision of the starting design via the FDS plot:
- If *more precision* is required rebuild the design adding more runs.
Practical Aspects of DOE
Remember what is Most Important

1. Identify opportunity and define objective.
2. State objective in terms of measurable responses.
   - Define the precision desired to predict each response.
   - Estimate experimental error (σ) for each response.
3. Select the input factors and ranges to study.
4. Select a design and:
   - Evaluate precision via the FDS plot.
   - Examine the design layout to ensure all the factor combinations are safe to run and are likely to result in meaningful information (no disasters).
Should I use a D-optimal or IV-optimal design?

- IV-optimal - precise estimation of the predictions
  Best for empirical response surface design

- D-optimal - precise estimation of model coefficients
  Best for screening and mechanistic models
No alphabetic optimality or sophisticated statistical analysis can make up for:

- Studying the wrong problem.
- Measuring the wrong response.
- Not having adequate precision.
- Studying the wrong factors.
- Having too many runs outside the region of operability.

Use first principles and experience!
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