Strategies for Sequential Experimentation

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Outline

• Introduction and Motivation
• Sequential DOE Strategies
• An Example
• Conclusion
Introduction and Motivation

Sequential DOE Strategies

An Example

Conclusion

Traditional Experimentation

Traditional Experimentation is often taught as a one-shot approach.

Here is a typical textbook example:

- Choose factors and define the low/high values of each
- Choose an appropriate experimental design
- Compute the expected power (or precision) of the experimental design
- Add or subtract runs needed to achieve the target power (or precision)
- Perform experiment and analyze data
- Optimize to find factor settings that achieve experimental targets
- Confirm the results of the analysis
Introduction

Zoom In

• Most textbooks offer no practical advice on these two steps:
  • Compute the expected power (or precision) of the experimental design
  • Add or subtract runs needed to achieve the target power (or precision)
• In my experience, experimenters usually do not have an unlimited budget of runs available. They usually must settle for power or precision lower than “what the textbook says” which is often around 80%.
• This usually means that whatever run budget is available will be spent in a single execution of the experiment.
• In my experience, this is often wasteful, and experimenters sell themselves short because experimentation is taught as a “one-shot” approach.

Real Life DOE

The One-Shot Approach

• Here’s a situation I run into all the time.
• Suppose you have a 3-component mixture experiment and a run budget of 14 runs.
• The component ranges are
  • $0.2 \leq x_1 \leq 0.6$
  • $0.2 \leq x_2 \leq 0.6$
  • $0.2 \leq x_3 \leq 0.6$ \hspace{1cm} x_1 + x_2 + x_3 = 1.0
• An experimenter, following standard textbook advice, would likely build an optimal design with 14 runs that may look something like…
14-Run Optimal Experimental Design

What’s the Problem??

- In theory, there is no problem. Because in textbooks the final result of the analysis always looks like this:
Real Life DOE

What Usually Happens

• More often that not, this is what happens in real problems:

![Component Diagram]

 Sequential DOE

What Now?

• We had a run budget of 14 runs. We performed a 14-run experiment.
• The results show that we may not have fully optimized our process, because the maximum occurs at an edge of the design space.
• So where do we go now?
  • Accept the results as “good enough” and move on?
  • Extrapolate outside of the original design space?
  • Throw away the data and start over?
• Could we have done something else to avoid this situation?
• Introduction and Motivation
• **Sequential DOE Strategies**
• An Example
• Conclusion

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**Design Space Strategies**

**An Alternative Approach**

• Instead of using the entire run budget to do a one-shot experiment, why not use 75% of the run budget on a first experiment, and then allocate the remaining 25% of the run budget based on the results of the first pass?

• In the previous example, we could do a **10**-run experiment first to get a sense of what’s going on.

• Based on the results of the first **10**-run experiment, we would then allocate the remaining **4** runs.

• If an optimum occurs along an edge, we can reshape the design space before allocating our remaining **4** runs to fill in the additional space.

• If the optimum occurs inside of the original design space, we can allocate the remaining **4** runs within the original design space.
Design Space Strategies

An Alternative Approach

• Start with a 10-run design:

Two Things Can Happen

Case 1:

Case 2:
**The Next Step**

**Case 1: Optimum at an Edge or Vertex**

- In this case, the optimum lies along an edge. It's unclear whether this region is the true optimum – perhaps the process can be further optimized.
- Perhaps the red region is “good enough” and we can stop there.
- In my experience, many experimenters will either stop because the run budget has been depleted, or throw away this data and start over.
- We performed 10 runs – we still have a budget of 4 runs left! Is there a way to solve this problem without having to start over or settle for the sub-par results?
- Yes! We can **augment** the original design space and perform the remaining 4 runs in the larger experimental design space!

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**The Augmented Design Space**

The optimum occurs at the edge of the design space, so we expand the space.
The Next Step

The Augmented Design Space

The green space is added to the original design space to try to capture the optimum.

Sequential DOE

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The Next Step

The Augmented Design Space

- After we augment our original design space, we add additional runs into the larger design space to try to capture the optimum.

You don’t need to throw away the original data!

Sequential DOE

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Take Home Message

Some Key Points:

• If we use our entire run budget in the original design space, then we cannot adapt to unexpected results, such as optima at the extremes.
• By keeping some runs in reserve, we can change the shape of the experimental design space as needed.
• You can sequentially expand the space several times as needed!

Mixture Example

Returning to the Mixture Example

• Recall the 10-run mixture example (14 run budget) with the following result. How can we use the Design-Expert software to experiment sequentially?
Use the Software!

How to Expand the Design Space?

Sequential DOE

Enter the New Ranges:

Sequential DOE
The Expanded Design Space

Now we have expanded the ranges of two components. We need to add some additional runs to fill the space.

Sequential DOE

Now Fill the Augmented Space

Sequential DOE
Use the Software!

The Augmented Experimental Design

To Finish: perform an additional 4 runs, analyze the data, and re-optimize.

Consider Blocking!

Another Case

What if Everything is Okay?

- Remember, there is a chance that everything goes right!
The Next Step

What's Next?

- Let's say you do only 75% of your run budget and everything goes well, like in the picture on the previous slide.
- The question then becomes: what to do if you don’t need to augment the original design space?
- How do you allocate the remaining runs?
- **Strategy:** allocate the remaining runs in a region around the optimum of the first experiment. Don’t allocate the runs as if though you had no prior information.
- **Why?** Adding additional runs near a potential optimum will improve the precision of the design in the area where it matters most.

The New Region

Notice the triangle inscribed within the original space. We’ll put the 4 additional points inside of that triangle.

The black triangle is defined as:

- $0.25 \leq x_1 \leq 0.50$
- $0.25 \leq x_2 \leq 0.50$
- $0.25 \leq x_3 \leq 0.50$
The Next Step

Compare Approaches

Original Design
SE = 0.50

4 Runs in Original Space
SE = 0.43

4 Runs in Region of Interest
SE = 0.40

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A 7-component mixture experiment was performed to try to formulate an SPF40 and SPF70 sunscreen. Three components, along with water, were varied. Three components were held fixed (invariant).

The overall run budget was 30 sunscreen formulations, but only 20 were performed in the first pass of the experiment.
After the experiment was performed, the model was optimized to find the formulation that achieves an SPF40 formulation:

Can the data collected under this design produce a sunscreen that’s SPF70?

Answer: No!

We can get about as high as SPF48. Clearly some components need to go beyond their original lows/highs.
An Example

Expand the Space

Add Runs to the Augmented Space
An Example

Sequential DOE

New high limits are highlighted

An Example

Re-analyze, Re-Optimize

We can now achieve an SPF70 formulations as well with only 7 additional runs.
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Follow Up

Benefits of Sequential DOE

• Allows for simultaneous exploration of the design space while maximizing the information that each run provides.
• Avoids situations where you are stuck with suboptimal results and have no budget left for further experimentation.
• Increases precision in regions of high interest.
• In my experience, very little research has been done in this area of DOE, and the few experimenters that are aware of this approach usually do it in an ad-hoc manner.
• Most research on sequential experimentation deals with screening, augmenting to increase the model order, adding/dropping factors.
• Caveat: This approach assumes you can change the lows/highs of your factors without great difficulty.
Consequence

**Take Home Points**

- The major point of this presentation is to encourage you to think about DOE as a sequential strategy with regards to the design space, not a one-shot experiment. Even just being aware of this technique can be a huge advantage.
- We generally recommend starting, with 60-75% of your run budget if possible. If there are issues with the experiment, the design space can be re-shaped and the remaining runs can be allocated in the new space.
- If there are no issues with the experiment, the remaining runs can be allocated in a smaller region of interest, or back in the original space.
- Design-Expert 13 will allow for factor and mixture component ranges to be changed after a design has been created. It will also include a Design Space Augment wizard that guides users through this entire process.

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