Sizing Mixture (RSM) Designs for Adequate Precision via Fraction of Design Space (FDS)

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Review – Power to size factorial designs

- Precision in place of power
  - Introduce FDS

- Sizing designs for precision
  - Two component mixture
  - Three component constrained mixture

- Sizing designs to detect a difference

Summary
Sizing Factorial Designs

During screening and characterization the emphasis is on identifying factor effects.

What are the important design factors?

For this purpose power is an ideal metric to evaluate design suitability.

Factorial Design – Power

2^3 Full Factorial $\Delta=2$ and $\sigma=1$
Factorial Design – Power

$2^3$ Full Factorial $\Delta=2$ and $\sigma=1$

<table>
<thead>
<tr>
<th>Name</th>
<th>Units</th>
<th>Diff to Detect</th>
<th>Est. Std. Dev.</th>
<th>Delta/Sigma</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td></td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
</tbody>
</table>

Power is reported at a 5.0% alpha level to detect the specified signal/noise ratio. Recommended power is at least 80%.

R1
Signal (delta) = 2.00  Noise (sigma) = 1.00  Signal/Noise (delta/sigma) = 2.00

A 57.2 %  B 57.2 %  C 57.2 %

The following three slides dig into how power is computed.

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One Replicate of $2^3$ Full Factorial

$C = (X^T X)^{-1}$ matrix

The design determines the standard error of the coefficient:

$$C = \begin{pmatrix}
0.125 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.125 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.125 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.125 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.125 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.125 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.125
\end{pmatrix}$$

$$t-value_i = \frac{\beta_i}{SE(\beta_i)} = \frac{\beta_i}{\sqrt{C_{ii}\sigma^2}} = \frac{\beta_i}{\sqrt{(0.125)\sigma^2}}$$
NonCentrality Parameter

$2^3$ Full Factorial $\Delta=2$ and $\sigma=1$

The reference $t$ distribution assumes the null hypothesis of $\Delta = 0$. The noncentrality parameter (2.828) defines the $t$ distribution under the alternate hypothesis of $\Delta = 2$.

$$\text{noncentrality}_i = \frac{\beta_i}{\sqrt{c_i\hat{\sigma}^2}} = \frac{\Delta_i}{\sqrt{c_i\hat{\sigma}^2}}$$

$$= \frac{1}{\sqrt{(0.125)(1)^2}}$$

$$= \frac{1}{0.3536} = 2.828$$

Factorial Design – Power

$2^3$ Full Factorial $\Delta=2$ and $\sigma=1$

noncentral $t_{\alpha=0.05, df=4}$ with noncentrality parameter of 2.828

Power = 57.2%
Factorial Design – Power
Two Replicates of $2^3$ Full Factorial $\Delta=2$ and $\sigma=1$

Power is reported at a 5.0% alpha level to detect the specified signal/noise ratio. Recommended power is at least 80%.

<table>
<thead>
<tr>
<th>Name</th>
<th>Units</th>
<th>Diff (to detect) Delta (Signal)</th>
<th>Est. Std. Dev. Delta (Noise)</th>
<th>Delta/Noise Signal/Noise (delta/sigma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

R1
Signal (delta) = 2.00 Noise (sigma) = 1.00 Signal/Noise (delta/sigma) = 2.00

A 95.6 %  B 95.6 %  C 95.6 %

Sizing Mixture (RSM) Designs

Two Replicates of $2^3$ Full Factorial
$C = (X^T X)^{-1}$ matrix

The design determines the standard error of the coefficient:

$$C = \begin{pmatrix}
0.0625 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.0625 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.0625 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0.0625 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.0625 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0.0625 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0.0625 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.0625
\end{pmatrix}$$

$$t\text{-value}_i = \frac{\beta_i}{\text{SE}(\beta_i)} = \frac{\beta_i}{\sqrt{c_i \sigma^2}} = \frac{\beta_i}{\sqrt{(0.0625) \sigma^2}}$$
NonCentrality Parameter

Two Replicates of $2^3$ Full Factorial $\Delta = 2$ and $\sigma = 1$

\[
\text{noncentrality}_i = \frac{\beta_i}{\sqrt{c_i \sigma^2}} = \frac{\Delta_i}{\sqrt{c_i \sigma^2}}
\]
\[
= \frac{1}{\sqrt{(0.0625)(1)^2}}
\]
\[
= \frac{1}{0.25} = 4.0
\]

Factorial Design – Power

Two Replicates of $2^3$ Full Factorial $\Delta = 2$ and $\sigma = 1$

noncentral $t_{\alpha=0.05, df=12}$ with noncentrality parameter of 4.0

Power = 95.6%
Conclusions

Factorial DOE

During screening and characterization (factorials) emphasis is on identifying factor effects.

What are the important design factors?

For this purpose power is an ideal metric to evaluate design suitability.

Sizing Mixture (RSM) Designs

Review – Power to size factorial designs

Precision in place of power
  - Introduce FDS

Sizing designs for precision
  - Two component mixture
  - Three component constrained mixture

Sizing designs to detect a difference

Summary

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Sizing Response Surface Designs

When the goal is optimization emphasis is the fitted surface.
How well does the surface represent true behavior?
For this purpose precision (FDS) is a good metric to evaluate design suitability.
(assuming model adequacy; i.e. insignificant lack of fit.)

Design Properties

1. Estimate the designed for polynomial well.
2. Give sufficient information to allow a test for lack of fit.
   ✓ Have more unique design points than coefficients in the model.
   ✓ Provide an estimate of “pure” error.
3. Remain insensitive to outliers, influential values and bias from model misspecification.
4. Be robust to errors in control of the component levels.
5. Provide a check on model assumptions, e.g., normality of errors.
6. Generate useful information throughout the region of interest, i.e., provide a good distribution of $\sqrt{\text{Var}(\hat{Y})}/\sigma^2$.
7. Do not contain an excessively large number of trials.
FDS
Fraction of Design Space

**Fraction of Design Space:**
- Calculates the volume of the design space having a prediction variance (PV) less than or equal to a specified value.
- The ratio of this volume to the total volume of the design volume is the fraction of design space.
- Produces a single plot showing the cumulative fraction of the design space on the x-axis (from zero to one) versus the PV on the y-axis.

Sizing Mixture (RSM) Designs

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Predicted Variance:

\[
PV(x_0) = \frac{\text{var}(\hat{y}_0)}{s^2} = x_0^T (X^T X)^{-1} x_0
\]

PV is a function of:

- \( x_0 \) – the location in the design space (i.e. the x coordinates for all model terms).
- \( X \) – the experimental design (i.e. where the runs are in the design space).
Prediction standard error of the expected value:

\[ PV(x_0) = \frac{\text{var}(\hat{y}_0)}{s^2} = x_0^T(X^TX)^{-1}x_0 \]

\[ \text{StdErr}(x_0) = \frac{s_{\hat{y}_0}}{s} = \sqrt{PV(x_0)} \]

1. Pick random points in the design space.
2. Calculate the standard error of the expected value
   \[ \frac{SE_{\hat{y}_0}}{s} = \sqrt{x_0^T(X^TX)^{-1}x_0} \]
3. Plot the standard error as a fraction of the design space.
Simplex-Lattice
Augmented and 4 Replicates

Sizing Mixture (RSM) Designs

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- Summary
Two Component Mixture Linear Model

The solid center line is the fitted model; \( \hat{y} \) is the expected value or mean prediction.

The curved dotted lines are the computer generated confidence limits, or the actual precision.

d Is the half-width of the desired confidence interval, or the desired precision. It is used to create the outer straight lines.

Note: The actual precision of the fitted value depends on where we are predicting.
Two Component Mixture
Linear Model

Evaluate the standard error as a fraction of design space for this design.

Two Component Mix

Click on “Evaluate” and then “Graphs”:

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Two Component Mixture
Linear Model

- Want a linear surface to represent the true response value within ± 0.64 with 95% confidence.
- The overall standard deviation for this response is 0.55.

Enter:

\[ d = 0.64 \]
\[ s = 0.55 \]
\[ \alpha (\alpha) = 1 - 0.95 = 0.05 \]

Two Component Mixture
Linear Model

Only 53% of the design space is precise enough to predict the mean within ± 0.64.
Define Precision
Half Width of the Confidence Interval

Confidence interval on the expected value:

The mean response is estimated and the precision of the estimate is quantified by a confidence interval:

\[ \hat{y} \pm t_{\alpha/2, df} \left( s_\hat{y} \right) \]

We will use the half-width of the confidence interval (d) to define the precision desired:

\[ d = t_{\alpha/2, df} \left( s_\hat{y} \right) \quad \text{or} \quad s_\hat{y} = \frac{d}{t_{\alpha/2, df}} \]

What Precision is Needed?
Mean Confidence Interval Half-Width

Input
- Half-width of confidence interval: \( d \)
- Estimate of standard deviation: \( s \)

\[ \hat{y} \pm d \]

\[ d = t_{\alpha/2, df} \left( s_\hat{y} \right) \]

\[ s_\hat{y} = s \sqrt{x_0^T \left( X^T X \right)^{-1} x_0} \]

\[ \text{StdErr Mean (FDS)} = \frac{s_\hat{y}}{s} = \sqrt{x_0^T \left( X^T X \right)^{-1} x_0} \]
Two Component Mixture
Linear Model

- Want a linear surface to represent the true response value within $\pm 0.64$ with 95% confidence.
- The overall standard deviation for this response is 0.55.

For 95% confidence $t_{0.05/2,5} = 2.571$, $d = 0.64$ & $s = 0.55$

\[
S_{\hat{y}} = \frac{d}{t_{a/2,df}} = \frac{0.64}{2.571} = 0.25
\]

\[
\text{StdErr Mean (FDS)} = \frac{S_{\hat{y}}}{s} = \frac{0.25}{0.55} = 0.45
\]

Mix section 4

FDS – StdErr Mean Plot
Fraction of Design Space

1. Pick random points in the design space.
2. Calculate the standard error of the expected value
\[
\frac{SE_{\hat{y}}}{S} = \sqrt{x_0^T (X^T X)^{-1} x_0}
\]
3. Plot the standard error as a fraction of the design space.

Mix section 4
Two Component Mixture
Linear Model

53% is precise enough, i.e. 53% has a StdErr ≤ 0.45

Two Component Mixture
Linear Model

53% of the design space has the desired precision, i.e. is inside the solid straight (red) lines.

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Sizing for Precision
FDS ≥ ?

How good is good enough? Rules of thumb:
• For exploration want FDS ≥ 80%
• For verification want FDS ≥ 90% or higher!

What can be done to improve precision?
• Manage expectations; i.e. increase d
• Decrease noise; i.e. decrease s
• Increase risk of Type I error; i.e. increase alpha
• Increase the number of runs in the design

Review – Power to size factorial designs
Precision in place of power
• Introduce FDS

Sizing designs for precision
• Two component mixture
  • Three component constrained mixture

Sizing designs to detect a difference
Summary
\[ \hat{y} = 4A + 4B + 8C + 16AC \]

Most of the action occurs on the A-C edge because of the AC coefficient of 16. The quadratic coefficient of 16 means that the response is 4 units higher at A=0.5, C=0.5 than one would expect with linear blending.

This illustrates the quadratic blending along the A-C edge as C increases from zero to one.
Power at 5% alpha level for effect of

<table>
<thead>
<tr>
<th>Term</th>
<th>StdErr*</th>
<th>VIF</th>
<th>R²-Squared</th>
<th>1 s</th>
<th>2 s</th>
<th>3 s</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.87</td>
<td>3.44</td>
<td>0.7094</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
<td>B</td>
<td>0.87</td>
<td>3.44</td>
<td>0.7094</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
<td>C</td>
<td>233.34</td>
<td>2722.29</td>
<td>0.9996</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
<td>AB</td>
<td>2.86</td>
<td>2.19</td>
<td>0.5442</td>
<td>22.9%</td>
<td>67.3%</td>
<td>94.7%</td>
</tr>
<tr>
<td>AC</td>
<td>258.98</td>
<td>1092.98</td>
<td>0.9991</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
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<td>5.0%</td>
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<td>5.0%</td>
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</table>

*Basis Std. Dev. = 1.0

Power is bottomed out at alpha!
Define Precision
Half Width of the Confidence Interval

6. Generate useful information throughout the region of interest.

Question: Will predictions, using the quadratic model from this design, be precise enough for our purposes?

- To know the truth requires an infinite number of runs; most likely this will exceed our budget.
- So the question is how precisely do we need to estimate the response?
- The trade off is more precision requires more runs.

Confidence interval on the expected value:

The mean response is estimated and the precision of the estimate is quantified by a confidence interval:

$$\hat{Y} \pm t_{\alpha/2, df} \left( s_\hat{Y} \right)$$

We will use half-width of the confidence interval ($d$) to define the precision desired:

$$d = t_{\alpha/2, df} \left( s_\hat{Y} \right) \quad \text{or} \quad s_\hat{Y} = \frac{d}{t_{\alpha/2, df}}$$
What Precision is Needed?
Confidence Interval Half-Width

Input
- Half-width of confidence interval: \( d \)
- Estimate of standard deviation: \( s \)

\[
\hat{S}_x = \frac{d}{t_{\frac{\alpha}{2}, \text{df}}} \\
S_x = s\sqrt{x_0^T (X^T X)^{-1} x_0}
\]

\[
\text{StdErr Mean (FDS)} = \frac{\hat{S}_x}{s} = \sqrt{x_0^T (X^T X)^{-1} x_0}
\]

Mixture Constrained
Quadratic Model (1 replicate)

- Want quadratic surface to represent the true response value within \( \pm 10 \) with 95% confidence.
- The standard deviation for this response is 7.8.

For 95% confidence \( t_{0.025, \text{df}} = 2.365 \), \( d = 10 \) & \( s = 7.8 \)

\[
\hat{S}_x = \frac{d}{t_{\frac{\alpha}{2}, \text{df}}} = \frac{10}{2.365} = 4.23
\]

\[
\text{StdErr Mean (FDS)} = \frac{\hat{S}_x}{s} = \frac{4.23}{7.8} = 0.54
\]

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Mixture Constrained Quadratic Model (1 replicate)

Only 58% of the design space has StdErr ≤ 0.54

Sizing Mixture (RSM) Designs

Mixture Constrained Quadratic Model (2 replicates)

Power at 5 % alpha level for effect of

<table>
<thead>
<tr>
<th>Term</th>
<th>StdErr*</th>
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<th>3 s</th>
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<td>3.44</td>
<td>0.7094</td>
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<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
<td>B</td>
<td>0.62</td>
<td>3.44</td>
<td>0.7094</td>
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<td>5.0%</td>
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<td>0.9996</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
<td>AB</td>
<td>2.02</td>
<td>2.19</td>
<td>0.5442</td>
<td>47.1%</td>
<td>96.5%</td>
<td>99.9%</td>
</tr>
<tr>
<td>AC</td>
<td>183.12</td>
<td>1092.98</td>
<td>0.9991</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
<tr>
<td>BC</td>
<td>183.12</td>
<td>1092.98</td>
<td>0.9991</td>
<td>5.0%</td>
<td>5.0%</td>
<td>5.0%</td>
</tr>
</tbody>
</table>

*Basis Std. Dev. = 1.0

Adding a replicate does little to increase power!
Mixture Constrained
Why Does Power Not Increase?

Quadratic, linear or combinations of them model response.
Model Coefficients are Correlated!

Individual coefficients can not be resolved!

Sizing Mixture (RSM) Designs

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Mixture Constrained
Quadratic Model (2 replicates)

- Want quadratic surface to represent the true response value within ± 10 with 95% confidence.
- The overall standard deviation for this response is 7.8.

For 95% confidence $t_{0.05/20} = 2.086$, $d = 10$ & $s = 7.8$

$$s_{\bar{y}} = \frac{d}{t_{\alpha/2,df}} = \frac{10}{2.086} = 4.79$$

$$\text{StdErr Mean (FDS)} = \frac{s_{\bar{y}}}{s} = \frac{4.79}{7.8} = 0.61$$

Sizing Mixture (RSM) Designs

Mixture Constrained Quadratic Model (2 replicates)

100% of the design space has StdErr ≤ 0.61

Sizing Mixture (RSM) Designs

Precision Depends On

- The size of the confidence interval half-width (d):
  A larger half-width (d) increases the FDS.
- The size of the experimental error $\sigma$:
  A smaller $\sigma$ increases the FDS.
- The $\alpha$ risk chosen:
  A larger $\alpha$ increases the FDS.
- Choose design appropriate to the problem:
  Size the design for the precision required.

Sizing Mixture (RSM) Designs
Conclusions

<table>
<thead>
<tr>
<th>Factorial DOE</th>
<th>Mixture Design and Response Surface Methods</th>
</tr>
</thead>
<tbody>
<tr>
<td>During screening and characterization (factorials) emphasis is on identifying factor effects.</td>
<td>When the goal is optimization (usually the case for mixture design &amp; RSM) emphasis is on the fitted surface.</td>
</tr>
<tr>
<td>What are the important design factors?</td>
<td>How well does the surface represent true behavior?</td>
</tr>
<tr>
<td>For this purpose power is an ideal metric to evaluate design suitability.</td>
<td>For this purpose precision (FDS) is a good metric to evaluate design suitability.</td>
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</table>

Sizing Mixture (RSM) Designs

- Review – Power to size factorial designs
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- Sizing designs for precision
  - Two component mixture
  - Three component constrained mixture
- **Sizing designs to detect a difference**
- Summary

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Detecting a Difference of $\Delta$
wherever it may occur

What is the probability of finding a difference $\geq \Delta$
if it occurs between any two points in the design space?

1. Pick random pairs of points in the design space.
2. Calculate the standard error of the difference

$$\text{SE}_{\hat{\gamma}_1 - \hat{\gamma}_2} = \sqrt{\frac{x_1^T (X^T X)^{-1} x_1 + x_2^T (X^T X)^{-1} x_2 - 2 x_1^T (X^T X)^{-1} x_2}{s}}$$
3. Plot the standard error as a fraction of the design space.
Revisit – Mixture Constrained Design for Quadratic Model

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th></th>
<th>B</th>
<th></th>
<th>C</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>≤</td>
<td>A</td>
<td>≤</td>
<td>1.0</td>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td>0.0</td>
<td>≤</td>
<td>B</td>
<td>≤</td>
<td>1.0</td>
<td></td>
<td>1.0</td>
</tr>
<tr>
<td>0.0</td>
<td>≤</td>
<td>C</td>
<td>≤</td>
<td>0.1</td>
<td></td>
<td>0.1</td>
</tr>
</tbody>
</table>

Total = 1.0

Want to detect a difference of 10 on a quadratic surface with 95% confidence. The overall standard deviation this for response is 7.8.

For 95% confidence \( t_{0.05/2,df} = 2.365 \), \( \Delta = 10 \) & \( s = 7.8 \)

\[
s_A = \frac{\Delta}{t_{0.05/2,df}} = \frac{10}{2.365} = 4.23
\]

\[
StdErr Diff (FPDS) = \frac{s_A}{s} = \frac{4.23}{7.8} = 0.54
\]
Mixture Constrained
Quadratic Model (1 replicate)

Only 37% of the design space has StdErr ≤ 0.54

Want to detect a difference of 10 on a quadratic surface with 95% confidence.

The overall standard deviation this for response is 7.8.

For 95% confidence $t_{0.025,20} = 2.086$, $\Delta = 10$ & $s = 7.8$

$$s_\Delta = \frac{\Delta}{t_{0.025,df}} = \frac{10}{2.086} = 4.79$$

$$\text{StdErr Diff (FPDS)} = \frac{s_\Delta}{s} = \frac{4.79}{7.8} = 0.61$$
Detecting a Difference of $\Delta$ Depends On

- The size of the difference ($\Delta$):
  A larger difference ($\Delta$) increases the FPDS.

- The size of the experimental error $\sigma$:
  A smaller $\sigma$ increases the FPDS

- The $\alpha$ risk chosen:
  A larger $\alpha$ increases the FPDS.

- Choose design appropriate to the problem:
  Size the design to detect a difference of interest.
Conclusions

Factorial DOE | Mixture Design and Response Surface Methods
---|---
During screening and characterization (factorials) emphasis is on identifying factor effects. | When the goal is to detect a change in the response emphasis is on differences over the fitted surface.
What are the important design factors? | Does a difference ≥ D occur in the design space?
For this purpose power is an ideal metric to evaluate design suitability. | For this purpose precision (FPDS) is a good metric to evaluate design suitability.

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- **Summary**

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Summary

Two criteria covered:

1. Precision of expected value, StdErr Mean:
   Use the StdErr Mean when the purpose of the DOE is to quantify shape; i.e. functional design (e.g. optimization).

2. Precision to detect a difference, StdErr Diff:
   Use the StdErr Diff when the purpose of the DOE is to detect change in the design space.

Two criteria not covered:

1. Precision of predicted value, StdErr Pred:
   Use the StdErr Pred when the purpose of the DOE is to develop a model for prediction.

2. Precision to form a tolerance interval, TI Multiplier:
   Use the TI Multiplier when the purpose of the DOE is to form a tolerance interval at a point in the design space.

   (new in Design-Expert version 8)
References


Sizing Mixture (RSM) Designs

Thank You for Attending

To obtain a copy of my slides:

- Give me your business card
- Send a request to pat@statease.com