Process Improvement: Steepest Ascent

BIOE 498/598 PJ

Spring 2021

Process Improvement

Design of Experiments is focused on **process characterization**.

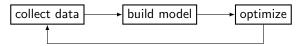
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- ► How large are the effects?

Process improvement asks "what factor settings yield the optimal response?"



Process improvement by steepest ascent

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Process improvement by steepest ascent

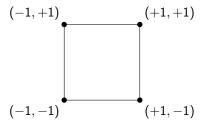
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Process improvement by steepest ascent

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- ► The **method of steepest ascent** moves us quickly toward regions of better response.
- The emphasis is on moving quickly using few runs and first order models.

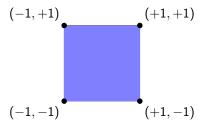
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Runs in a factorial design sample the corners of a unit cube.



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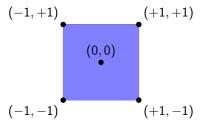
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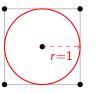
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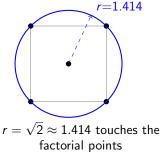


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First-order response surfaces

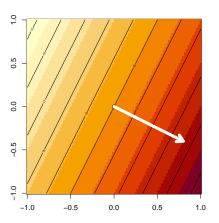
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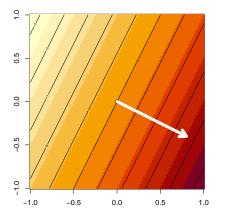
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We want to move "uphill" to improve the response using the **method of steepest ascent**.

If our goal was to minimize the response, we use *steepest descent* by

- Moving opposite of the uphill direction, or
- 2. Multiplying the response by -1.

Finding the ascent direction for first-order models

Let's compute the partial derivatives along each factor's dimension.

$$\frac{\partial y}{\partial x_1} = \frac{\partial}{\partial x_1} \left(20 + 3.6x_1 - 1.8x_2 \right) = 3.6$$

$$\frac{\partial y}{\partial x_2} = \frac{\partial}{\partial x_2} \left(20 + 3.6x_1 - 1.8x_2 \right) = -1.8$$

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Two things to note:

- 1. The rate of ascent along each direction is simply the effect size β_i .
- 2. The rate of change is different for the two dimensions. For every step of unit length along x_1 we must move 3.6/(-1.8) = -1/2 units along x_2 .

Consider the general first-order model

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_n x_n$$

- 1. Find the effect size with the largest **magnitude**. We'll call this β_j and the associated factor x_j .
- 2. Choose a step size (in coded units) along this dimension, called Δx_j .
- 3. For all other dimensions $i \neq j$, the step size is

$$\Delta x_i = \frac{\beta_i}{\beta_j} \Delta x_j$$

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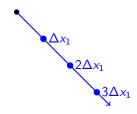
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- 2. Let $\Delta x_1 = 1$.
- 3. $\Delta x_2 = \frac{\beta_2}{\beta_1} \Delta x_1 = \frac{-1.8}{3.6} (1) = -0.5$

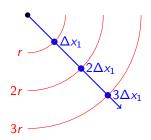
Why standardize step sizes?

Uniform steps give uniform differences in design radii.



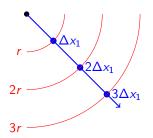
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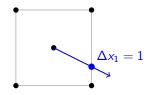


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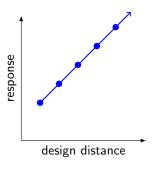
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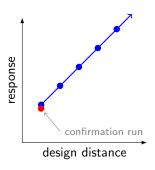
A standardized step of 1 always defines a point on the design space boundary.



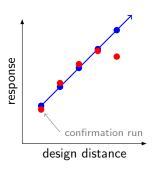
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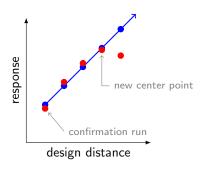
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- Eventually the actual response will stop increasing.
- When the response drifts, we use the best response location as the center for a new set of experiments.



What about interactions?

Models with interactions have curved paths of steepest ascent since the gradient changes with x.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

$$\nabla y = \begin{pmatrix} \frac{\partial y}{\partial x_1} \\ \frac{\partial y}{\partial x_2} \end{pmatrix} = \begin{pmatrix} \beta_1 + \beta_{12} x_2 \\ \beta_2 + \beta_{12} x_1 \end{pmatrix}$$

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However, in practice we usually ignore the interactions.

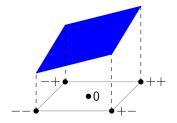
- ► The model will often break down before the curvature becomes significant.
- We rarely have enough runs in the initial design to identify interactions.

When is a first order model not good enough?

- The FF designs used for process improvement are usually augmented by **center points** repeated runs at the design center (0,0).
- Center points serve two purposes:
 - Estimate the pure error via the standard deviation of the repeated runs.
 - 2. Test for *lack of fit* to detect curvature.

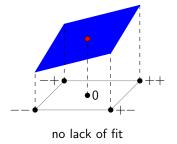
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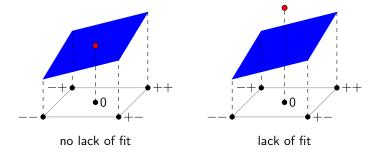
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$$F_{\text{curve}} = \frac{SS_{\text{curve}}/\text{DF}(SS_{\text{curve}})}{SS_{\text{error}}/\text{DF}(SS_{\text{error}})}$$

temp	time	yield
_	_	39.3
_	+	40.0
+	_	40.9
+	+	41.5
0	0	40.3
0	0	40.5
0	0	40.7
0	0	40.2
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pf(0.0605, 1, 4, lower.tail=FALSE) $\rightarrow p < 0.818$.

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- 4. Go to (1) and repeat using the location of maximum response as the new center point.