Process Improvement: Steepest Ascent

BIOE 498/598 PJ

Spring 2022

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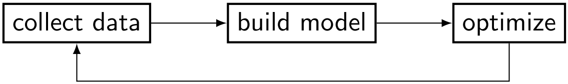
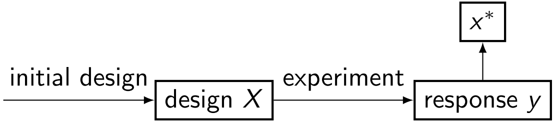
Process improvement asks "what factor settings yield the optimal response?"



Surrogate Optimization



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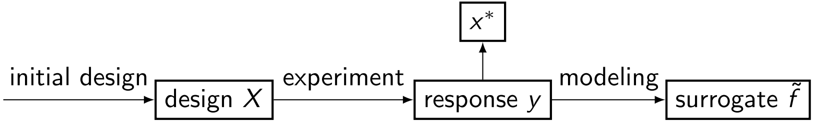

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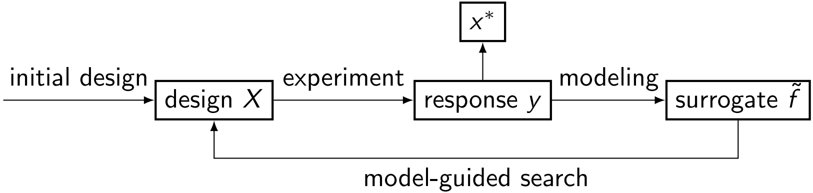

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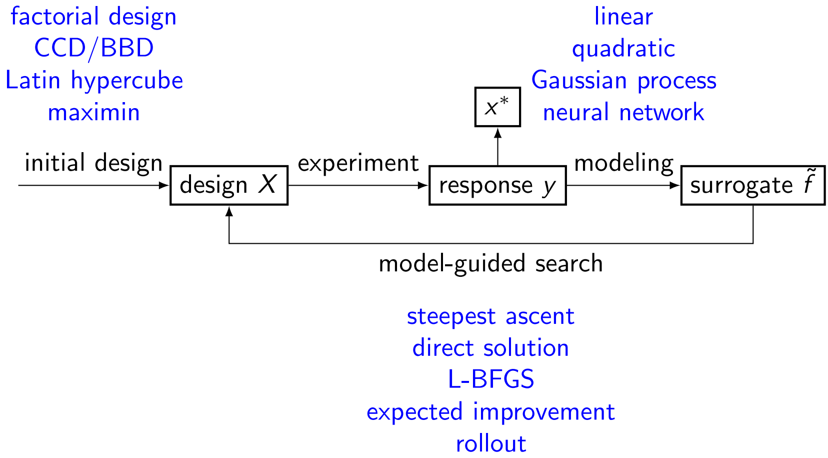

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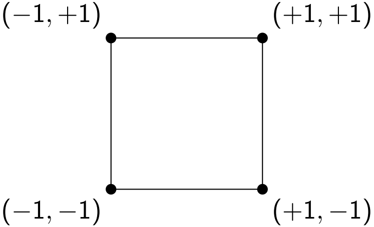
- The emphasis is on moving quickly using few runs and first order models.

The Design Space

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



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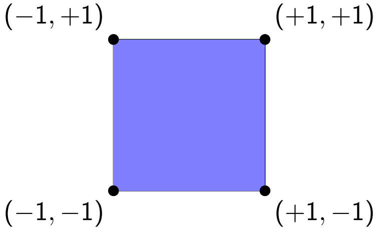

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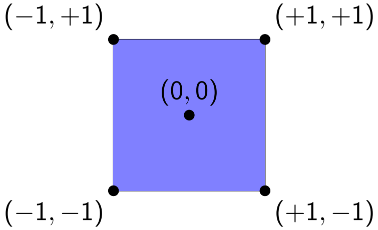

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The origin $(0, 0)$ in *coded units* is called the **center point**.

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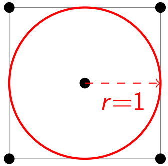

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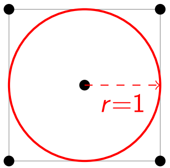

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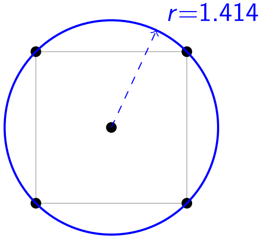

$r = \sqrt{2} \approx 1.414$ touches the factorial points

First-order response surfaces

Consider the first-order linear model (without interactions)

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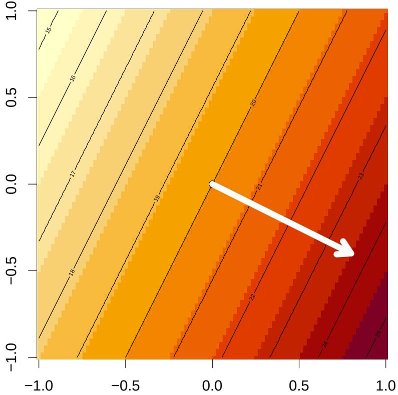

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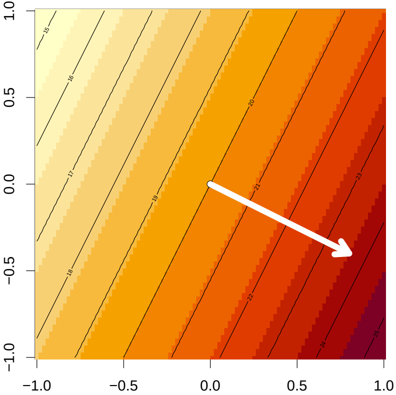

We want to move "uphill" to improve the response using the **method of steepest ascent**.

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

1. 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.

Standardized step sizes for steepest ascent

Consider the general first-order model

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

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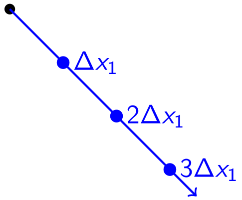
3. $\Delta x_2 = \frac{\beta_2}{\beta_1} \Delta x_1 = \frac{-1.8}{3.6}(1) = -0.5$

Why standardize step sizes?

Uniform steps give uniform differences in design radii.



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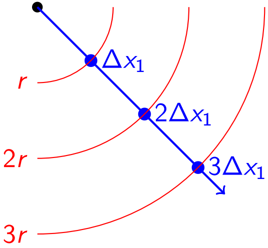

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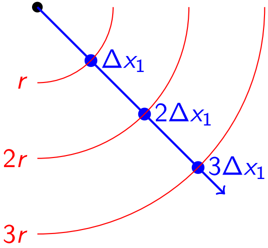
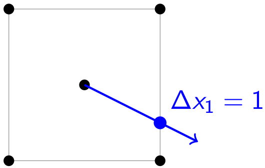


A standardized step of 1 always defines a point on the design space boundary.



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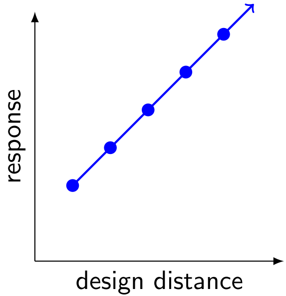
- A first order model predicts the response will increase *forever*.
- We perform additional runs at every step along the ascent path.



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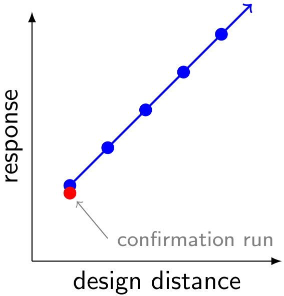

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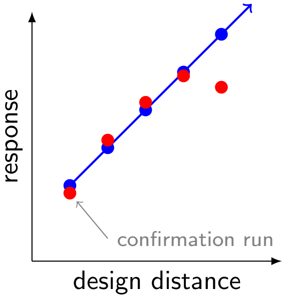

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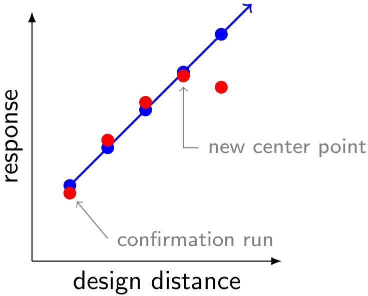
- When the response drifts, we use the best response location as the center for a new set of experiments.



What about interactions?

Models with interactions have **curved** paths of steepest ascent since the gradient changes with $\boldsymbol{x}$.

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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 $(0, 0)$.
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  1. Estimate the *pure error* via the standard deviation of the repeated runs.
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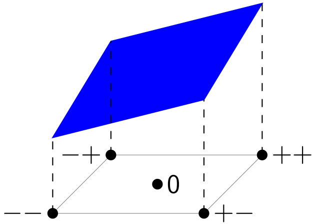

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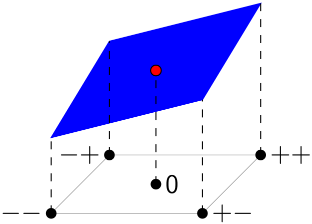

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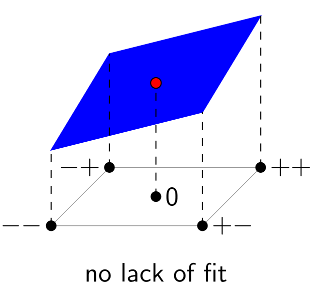

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4. $$F_{\text{curve}} = \frac{SS_{\text{curve}}/\text{DF}(SS_{\text{curve}})}{SS_{\text{error}}/\text{DF}(SS_{\text{error}})}$$

Example: Testing for curvature (Myers 2009)

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
0	0	40.6

Example: Testing for curvature (Myers 2009)

1. $\bar{y}_{\text{fact}} = (39.3 + 40.0 + 40.9 + 41.5)/4 = 40.425$
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0	0	40.5
0	0	40.7
0	0	40.2
0	0	40.6

`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.