Response Surface Methodology: Curvature

BIOE 498/598 PJ

Spring 2022

Last time: The method of steepest ascent

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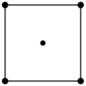

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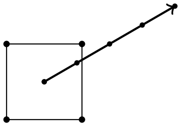

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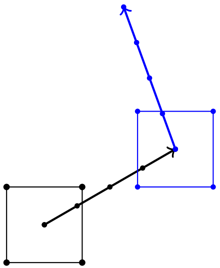

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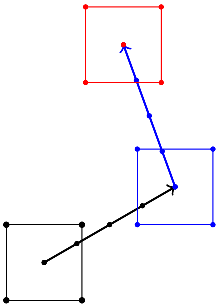

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- Begin with a FF+CP design.
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- New FF+CP; repeat steepest ascent.
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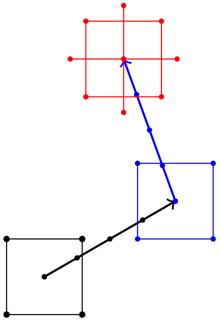
- **Today**: Fitting a model to a curved response surface.



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:
  1. Estimate the *pure error* via the standard deviation of the repeated runs.
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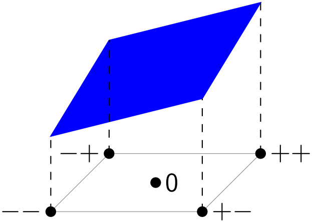

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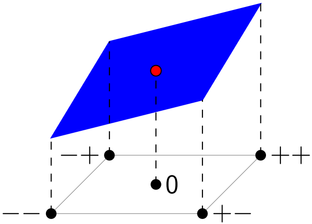

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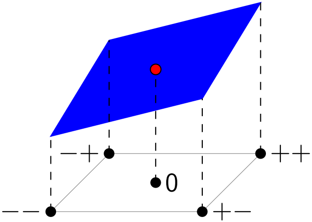

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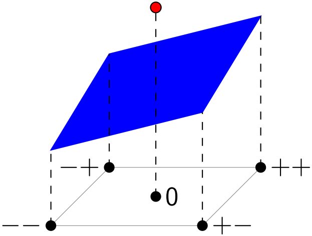

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Testing for lack of fit due to curvature

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2. $$SS_{\text{curve}} = \frac{n_{\text{fact}}\, n_{\text{center}}(\bar{y}_{\text{fact}} - \bar{y}_{\text{center}})^2}{n_{\text{fact}} + n_{\text{center}}}, \quad \text{DF}(SS_{\text{curve}}) = 1$$

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3. $$SS_{\text{error}} = \sum_{\substack{\text{center}\\ \text{points}}} (y_i - \bar{y}_{\text{center}})^2, \quad \text{DF}(SS_{\text{error}}) = n_{\text{center}} - 1$$

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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. $\bar{y}_{\text{fact}} = (39.3 + 40.0 + 40.9 + 41.5)/4 = 40.425$
   $\bar{y}_{\text{center}} = (40.3+40.5+40.7+40.2+40.6)/5 = 40.46$

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`pf(0.0605, 1, 4, lower.tail=FALSE)` $\rightarrow p < 0.818$.

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5. Switch to a **curved** model and *Response Surface Methodology* (RSM).

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$$y = 20 + 3.6x_1 - 1.8x_2 - 0.6x_1x_2$$

Set $x_2 = 0$, then $y \to \infty$ as $x_1 \to \infty$.

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- Usually we don't know f, so we approximate it with a simpler function.
- **We are not claiming that f is a particular shape.** Rather, we claim that an approximation is "good enough" over our domain of interest.

Approximating f with a general quadratic

Let's find the second-order Taylor series of $f(x_1, x_2)$ centered at zero:

$$f(x_1, x_2) \approx \ f|_0 \ + \ \left.\frac{\partial f}{\partial x_1}\right|_0 x_1 + \ \left.\frac{\partial f}{\partial x_2}\right|_0 x_2 + \ \frac{1}{2}\left.\frac{\partial^2 f}{\partial x_1^2}\right|_0 x_1^2 + \ \frac{1}{2}\left.\frac{\partial^2 f}{\partial x_2^2}\right|_0 x_2^2 + \ \frac{1}{2}\left.\frac{\partial^2 f}{\partial x_1 \partial x_2}\right|_0 x_1 x_2$$

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- In general we will have k factors and the quadratic approximation will be

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{j=1}^{k} \sum_{i=1}^{j-1} \beta_{ij} x_i x_j.$$

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- This model has $1 + 2k + k(k-1)/2$ parameters, so RSM designs must have at least this many runs.