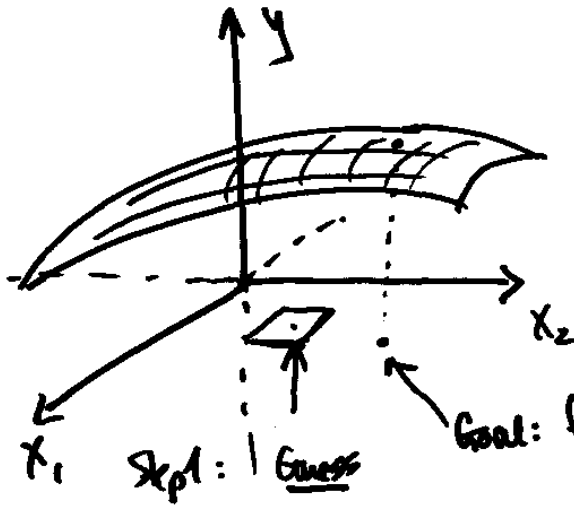
Response surface methodology

Stat 526
5-12-15

(1)



Step 1: Guess

Goal: find this point

Step 2: Construct a 2^k design centered at your initial guess. Include center points.

(2)

$$\text{Test stat} = \frac{\bar{y}_c - \bar{y}_F}{s\sqrt{\frac{1}{n_c}+\frac{1}{n_F}}} = t, \; df = df_E$$

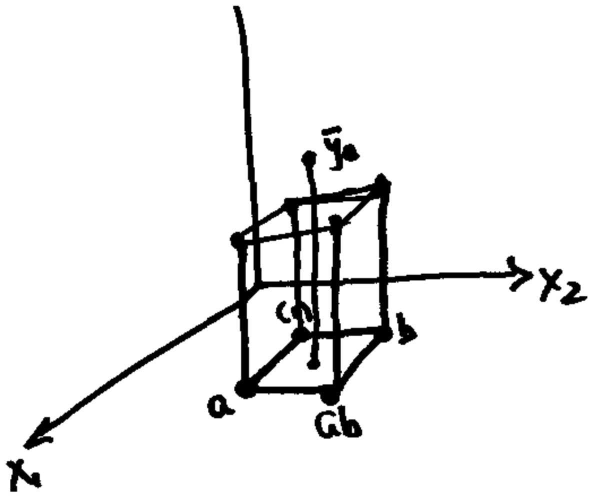
$s \leftarrow \sqrt{MSE}$

$$t^2 \sim F_{1, df_E}$$

$$t^2 = \frac{(\bar{y}_c - \bar{y}_F)^2}{MSE\left(\frac{1}{n_c}+\frac{1}{n_F}\right)} = \frac{\left[\frac{n_c n_F(\bar{y}_c - \bar{y}_F)^2}{n_c + n_F}\right]}{MSE}$$

$SS_{curv.}$

③



<u>Test for curvature</u> Compare $\bar{y}_c$ = average y-value at the center points

and $\bar{y}_F$ = average y-value at the "factorial" points

④

If H_0 is rejected, then you found curvature & skip to the final phase.

If you fail to find curvature, then guess again.

The second guess should be 1 <u>step</u> in the direction of steepest ascent.

still some guesswork here

Fit a linear model to the results of the 2^k with center points design

⑤

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \dots + \beta_k x_k + \varepsilon$$

The gradient vector is $\dfrac{dy}{d\vec{x}} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix} = \vec{\nabla}$

$$y \hat{\approx} y_0 + \underbrace{\vec{\nabla}'(\vec{x} - \vec{x}_0)}$$

maximized when $\vec{x} - \vec{x}_0$ is in the same direction as $\vec{\nabla}$

⑥

The estimated gradient vector is $\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix}$.

Take 1 step in that direction.

Our new guess is $(x_{10} + b_1 d, x_{20} + b_2 d, \dots, x_{k0} + b_k d)$

Run 1 observation. Observe y.

If y increased over the previous center point value, take another step in the same direction.

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Continue this process until you fail to see an increase in y. Go back one step. This is the new center point. Start over.

Keep going through the algorithm until the test for curvature is significant.

At this center point, we will set up a
<u>central composite design</u>

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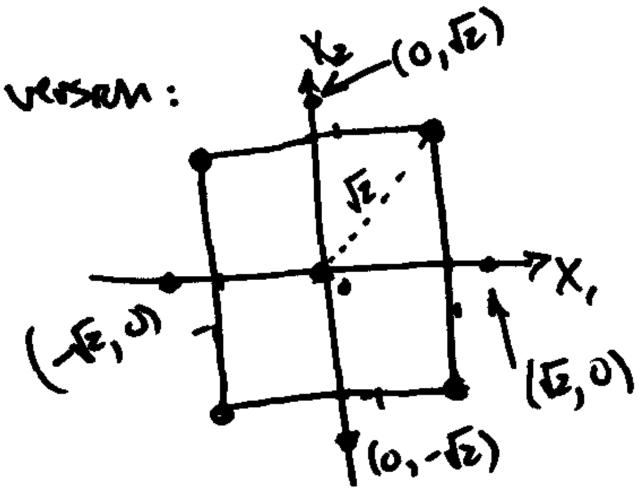
2^2 version:



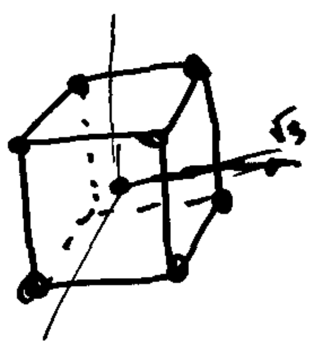
2^k version:

Corner points,

center points,

Axial points at $\pm\sqrt{k}$

2^3 version



(9)

Fit a full quadratic model

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

Write the solution as

$$\hat{y} = b_0 + \vec{x}'\vec{b} + \vec{x}' B \vec{x}, \text{ where}$$

$$\vec{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_k \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} b_{11} & & \frac{1}{2}b_{ij} \\ & b_{22} & \\ & & \ddots \\ \frac{1}{2}b_{ji} & & & b_{kk} \end{bmatrix}$$

(10)

To find the potential optimum,

$$\text{set } \frac{d\hat{y}}{d\vec{x}} = \vec{0}$$

$$\frac{d\hat{y}}{d\vec{x}} = \vec{0} + \vec{b} + 2B\vec{x} \overset{\text{set}}{=} \vec{0}$$

$$2B\vec{x} = -\vec{b}$$

$$\vec{x} = -\frac{1}{2}B^{-1}\vec{b}$$

if this exists