Ch 5: Response Surface Model (RSM)

Friday, February 11, 2022 7:14 PM

(A) Quadratic (2nd order model)

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

Ex: 3 variables x_1, x_2, x_3

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$$

- Stationary point: where a maximum or minimum response occur

Use Gradient vector to find the stationary point

$$\vec{\nabla} \hat{y} = \vec{0}$$

OR $$\frac{\partial \hat{y}}{\partial x_1} = 0, \quad \frac{\partial \hat{y}}{\partial x_2} = 0$$

Ex Given the surface: $\hat{y} = 100 + 5x_1 + 10x_2 - 8x_1^2 - 12x_2^2 - 12x_1x_2$

$$\frac{\partial \hat{y}}{\partial x_1} = 5 - 16x_1 - 12x_2 = 0$$

$$\frac{\partial \hat{y}}{\partial x_2} = +10 - 24x_2 - 12x_1 = 0$$

Solve equs: $\begin{cases} 16x_1 + 12x_2 = 5 \\ 12x_1 + 24x_2 = 10 \end{cases}$ $\quad \left\{ x_1 = 0, x_2 = \frac{5}{12} \right\}$

Response at ~~this~~ locat: $\hat{y} = 102.08$

(B) Canonical analysis of 2nd order model

$$\hat{y} = \beta_0 + \vec{x}^t \cdot \vec{b} + \vec{x}^t \cdot B \cdot \vec{x} \quad \text{where}$$

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \end{bmatrix}; \quad B = \begin{bmatrix} b_{11} & \frac{1}{2}b_{12} & \cdots & \frac{1}{2}b_{1k} \\ \cdot & b_{22} & \cdot & \end{bmatrix}; \quad \vec{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \end{bmatrix}$$

$$\vec{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} ; \quad B = \begin{bmatrix} b_{11} & \frac{1}{2}b_{12} & \cdots & \frac{1}{2}b_{1k} \\ \vdots & b_{22} & & \vdots \\ & & \ddots & \\ \frac{1}{2}b_{k1} & \cdots & & b_{kk} \end{bmatrix} ; \quad \vec{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_k \end{bmatrix}$$

Note $\vec{x}^t = [x_1 \ x_2 \ - \ x_k]$ $\quad$ B is symmetric $B^t = B$

B1 Stationary Point take partial derivatives

$$\frac{\partial \hat{y}}{\partial \vec{x}} = \vec{b} + 2 \cdot B \vec{x} = \vec{0}$$

$$\Rightarrow \boxed{\vec{x}_s = -\frac{1}{2} B^{-1} \cdot \vec{b}}$$

Response value at $\vec{x}_s$

$$\hat{y}_s = b_0 + \vec{x}_s^t \cdot \vec{b} + \vec{x}_s^t \cdot B \cdot \vec{x}_s$$

$$= b_0 + \vec{x}_s^t \cdot \vec{b} + \underbrace{-\frac{1}{2} \vec{b}^t \cdot (B^{-1})^t} \cdot B \left(-\frac{1}{2} B^{-1} \cdot \vec{b}\right)$$

Note $(B^t) = B$; $(B^{-1})^t = (B^t)^{-1} = B^{-1}$

The last part is equal $\left(\frac{1}{4} \vec{b}^t \cdot B^{-1}\right) \vec{b}$

$$\boxed{\hat{y}_s = b_0 - \frac{1}{2} \vec{x}_s^t \cdot \vec{b}}$$

X_s is called sationary point ; y_s : stationary point value

B2 Minimum or Maximum

- {Eigenvectors and eigenvalues} of matrix B are used to determine the stationary point is a Min/or Max
- The approach is to Diagonalize B using e-vectors and e-values

Let P be a matrix, whose columns are normalized eigenvectors of B. Note. if B is $k \times k$, then B has atmost k eigenvalues. For example if B is 3×3 then B has at most 3 e-values

---

Eigenvalues / Eigenvectors of a matrix

Eigenvalue: $\lambda \in \mathbb{R}$ is an eigenvalue of a matrix A if, exist a vector $\vec{x}$ such that

$$\boxed{A.\vec{x} = \lambda . \vec{x}}$$

To find eigenvalues. $A\vec{x} - \lambda\vec{x} = \vec{0}$; $(A-\lambda I).\vec{x} = \vec{0}$

$\Leftrightarrow \det(A-\lambda I) = 0$ where $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Ex: (1) $A = \begin{bmatrix} 2 & 1 \\ 4 & 2 \end{bmatrix}$

Form matrix $A - \lambda I = \begin{bmatrix} 2 & 1 \\ 4 & 2 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2-\lambda & 1 \\ 4 & 2-\lambda \end{bmatrix}$

$\det(A-\lambda I) = (2-\lambda)^2 - 4 = 0$

Solve this quadratic eqn $(2-\lambda)^2 = 4$

$2-\lambda = \pm 2$; $\lambda = \begin{cases} 0 \\ 4 \end{cases}$

(2) Now find eigenvectors for each λ. $\lambda = 0$, $\lambda = 4$

* $\lambda = 0$ Use the same equation. $(A-\lambda I)\vec{x} = \vec{0}$

$\begin{bmatrix} 2 & 1 \\ 4 & 2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$; $2x_1 + x_2 = 0$

any (x_1, x_2) satisfy this equation. Many!

Let $x_2 = s$, then $x_1 = -\frac{1}{2}s$. $\begin{bmatrix} -\frac{1}{2}s \\ s \end{bmatrix} = s\begin{bmatrix} -\frac{1}{2} \\ 1 \end{bmatrix}$

any s

$$\circledast \quad \lambda = 4 \quad \begin{bmatrix} 2-4 & 1 \\ 4 & 2-4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \vec{0}$$

$$\begin{bmatrix} -2 & 1 \\ 4 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} ; \quad -2x_1 + x_2 = 0$$

Let $t = x_2$; $x_1 = \frac{1}{2} x_2 = \frac{1}{2} t$

$$\begin{bmatrix} \frac{1}{2} t \\ t \end{bmatrix} = t \begin{bmatrix} \frac{1}{2} \\ 1 \end{bmatrix}$$

So $\lambda = 0 \quad s \begin{bmatrix} -\frac{1}{2} \\ 1 \end{bmatrix}$; $\lambda = 4 \quad t \begin{bmatrix} \frac{1}{2} \\ 1 \end{bmatrix}$

So, let $\vec{u} = \begin{bmatrix} -\frac{1}{2} \\ 1 \end{bmatrix}$ $\vec{v} = \begin{bmatrix} \frac{1}{2} \\ 1 \end{bmatrix}$

Form $P = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \\ 1 & 1 \end{bmatrix}$

Check

$$P^t \cdot A \cdot P = \begin{bmatrix} -\frac{1}{2} & 1 \\ \frac{1}{2} & 1 \end{bmatrix} \cdot A \cdot \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \\ 1 & 1 \end{bmatrix} =$$

B3 Diagonalization of B

$$P^t \cdot B \cdot P = \Lambda \doteq \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \; \lambda_k \end{bmatrix}$$

Use translation at $\vec{x}_s$. $\vec{z} = \vec{x} - \vec{x}_s$.

Rotation $\vec{w} = P^t \cdot \vec{z}$

+ Rotation $\hat{y} = \vec{y}_s + \vec{w}^t \cdot \Lambda \vec{w}$

In w-coordinates

$$\boxed{\hat{y} = \vec{y}_s + \sum^k \lambda_i \cdot w_i^2}$$

$$\boxed{\hat{y} = \vec{y}_s + \sum_{i=1}^{k} \lambda_i \cdot w_i^2}$$

Results. w_i are called canonical variables

(1) If $\lambda_1, \lambda_2, \ldots, \lambda_k$ are all negatives. $\vec{x}_s$ is a Max

(2) If $\lambda_1, \lambda_2, \ldots, \lambda_k$ are all positive. $\vec{x}_s$ is a Min

(3) If $\lambda_1, \lambda_2 \cdot \lambda_k$ mixed signs $\vec{x}_s$ is saddle