Stat 566
5-13-25

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

Write this in matrix form:

$$y = \beta_0 + \vec{x}'\vec{\beta} + \vec{x}' A \vec{x} + \vec{\varepsilon}$$

where $\vec{\beta} = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$ and $A = \begin{bmatrix} \beta_{11} & & \frac{1}{2}\beta_{ij} \\ & \beta_{22} & \\ \frac{1}{2}\beta_{ji} & & \ddots \quad \beta_{kk} \end{bmatrix}$

Solution will look like

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

Now, find the $\vec{x}$ that maximizes $\hat{y}$. ②

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

$$\frac{d\hat{y}}{d\vec{x}} = \vec{0} + \vec{b} + 2B\vec{x} \overset{set}{=} \vec{0}$$ (see 564 notes)

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

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

if this exists

③

How can we tell if $\vec{x}_M$ is a min, max, or saddle point?

Evaluate y at $\vec{x}_M$:

$$\hat{y}_M = b_0 + \vec{x}_M{}'\vec{b} + \vec{x}_M{}' B \vec{x}_M$$

$$= b_0 + \left(-\tfrac{1}{2}\right)\vec{b}' B^{-1}\vec{b} + \left(-\tfrac{1}{2}\right)^2 \vec{b}' \cancel{B^{-1} B} B^{-1}\vec{b}$$

$$= b_0 - \tfrac{1}{2}\vec{b}' B^{-1}\vec{b} + \tfrac{1}{4}\vec{b}' B^{-1}\vec{b}$$

$$= b_0 - \tfrac{1}{4}\vec{b}' B^{-1}\vec{b}$$

④

Let $\vec{x}$ be a value close to $\vec{x}_M$

and let $\hat{y}$ be the corresponding y-value

Write $\hat{y} = \hat{y}_M + (\hat{y} - \hat{y}_M)$

$$= \hat{y}_M + \Big(\cancel{b_0} + \vec{x}'\vec{b} + \vec{x}' B \vec{x} - \big(\cancel{b_0} - \tfrac{1}{4}\vec{b}' B^{-1}\vec{b}\big)\Big)$$

$$= \hat{y}_M + \Big(\vec{x}'\vec{b} + \underbrace{\tfrac{1}{4}\vec{b}' B^{-1}\vec{b}}_{-\frac{1}{2}\vec{b}'\vec{x}_M} + \vec{x}' B \vec{x}\Big)$$

⑤

$$\hat{y} = \hat{y}_m + \left(\vec{x}' - \tfrac{1}{2}\vec{x}_m'\right)\vec{b} + \vec{x}'B\vec{x}$$

$$= \hat{y}_m + \left(\vec{x}' - \tfrac{1}{2}\vec{x}_m'\right)\vec{b} + (\vec{x}-\vec{x}_m)'B(\vec{x}-\vec{x}_m)$$
$$+ \vec{x}'B\vec{x}_m + \vec{x}_m'B\vec{x} - \vec{x}_m'B\vec{x}_m$$

$$= \hat{y}_m + \left(\vec{x}' - \tfrac{1}{2}\vec{x}_m'\right)\vec{b} + (\vec{x}-\vec{x}_m)'B(\vec{x}-\vec{x}_m)$$
$$+ \vec{x}'B\left(-\tfrac{1}{2}B^{-1}\vec{b}\right) + \left(-\tfrac{1}{2}B^{-1}\vec{b}\right)'B\vec{x}$$
$$- \left(-\tfrac{1}{2}B^{-1}\vec{b}\right)'B\left(-\tfrac{1}{2}B^{-1}\vec{b}\right)$$

⑥

$$= \hat{y}_m + \left(\cancel{\vec{x}'} - \tfrac{1}{2}\vec{x}_m'\right)\vec{b} + (\vec{x}-\vec{x}_m)'B(\vec{x}-\vec{x}_m)$$
$$\cancel{-\tfrac{1}{2}\vec{x}'\vec{b}} \; \cancel{-\tfrac{1}{2}\vec{b}'\vec{x}} - \tfrac{1}{4}\vec{b}'B^{-1}\vec{b}$$

$$= \hat{y}_m - \tfrac{1}{2}\vec{x}_m'\vec{b} + (\vec{x}-\vec{x}_m)'B(\vec{x}-\vec{x}_m)$$
$$- \tfrac{1}{4}\vec{b}'B^{-1}\vec{b}$$

$$= \hat{y}_m \cancel{- \tfrac{1}{2}\left(-\tfrac{1}{2}B^{-1}\vec{b}\right)'\vec{b}} + (\vec{x}-\vec{x}_m)'B(\vec{x}-\vec{x}_m)$$
$$\cancel{-\tfrac{1}{4}\vec{b}'B^{-1}\vec{b}}$$

$$\hat{y} = \hat{y}_m + (\vec{x}-\vec{x}_m)'B(\vec{x}-\vec{x}_m)$$

(7)

Write $B = P \Lambda P^{-1}$ spectral decomposition

diagonal matrix of eigenvalues

its columns are the eigenvectors

Since B is also symmetric,

$$B = P \Lambda P'$$

Now, $\hat{y} = \hat{y}_m + \underbrace{(\vec{x} - \vec{x}_m)'}_{\vec{w}\,'} P \Lambda \underbrace{P'(\vec{x} - \vec{x}_m)}_{\vec{w}}$

(8)

$$\hat{y} = \hat{y}_m + \vec{w}\,' \Lambda \vec{w}$$

$$= \hat{y}_m + [w_1 \; w_2 \; \cdots \; w_k] \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & \ddots & \lambda_k \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_k \end{bmatrix}$$

$$\hat{y} = \hat{y}_m + \lambda_1 w_1^2 + \lambda_2 w_2^2 + \ldots + \lambda_k w_k^2$$

$\Rightarrow$ If B is <u>pos. def.</u>, then $\lambda_i > 0 \; \forall i$

and $\hat{y} > \hat{y}_m$, so $\hat{y}_m$ is a <u>minimum</u>

$\Rightarrow$ If B is <u>neg. def.</u>, then $\lambda_i < 0 \; \forall i$

and $\hat{y} < \hat{y}_m$, so $\hat{y}_m$ is a **maximum**

$\Rightarrow$ If B is neither pos. def. nor neg. def.,
then $\hat{y}_m$ is a saddle point.