Quadratic Forms and Extrema of Functions of Many Variables
ChE641, IIT Kanpur

<u>Part 10</u>

$$\underline{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix}$$

Quadratic form $\xrightarrow{}$ scalar $\quad Q = \langle \underline{x} | \underset{\text{real lin. operator}}{\mathcal{M}} \underline{x} \rangle$

In a given basis, $Q(\underline{x}) = \underline{x}^T \cdot \underset{\text{real matrix}}{\underline{\underline{M}}} \cdot \underline{x}$

$$\underset{\text{real matrix}}{\mathcal{M}} = \underset{\text{Symm}}{\mathcal{A}} + \underset{\text{anti-Symm.}}{\mathcal{B}}$$

$$\mathcal{A} = \frac{\mathcal{M} + \mathcal{M}^T}{2} ; \quad \mathcal{B} = \frac{\mathcal{M} - \mathcal{M}^T}{2}$$

$$Q = \underline{x}^T \underline{\underline{M}}\, \underline{x} = \underline{x}^T \underline{\underline{A}}\, \underline{x} + \underline{x}^T \underline{\underline{B}}\, \underline{x}$$

$Q = Q^T$ Because Q is scalar

$$Q^T = (x^T A x)^T + (x^T \underline{\underline{B}} x)^T$$

$$= x^T A^T x + x^T B^T x$$

$$Q^T = x^T A x - x^T B x$$

$$Q = x^T A x + x^T B x$$

$$(ABC)^T = C^T B^T A^T$$

$$\boxed{x^T \underset{\text{antisymm.}}{B} x = 0}$$

$$Q = x^T \underset{\text{symm.}}{A} x$$

$$Q = (x_1 \;\; x_2 \;\; x_3) \begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{array}{l} x_1^2 + x_2^2 - 3x_3^2 \\ + 2x_1x_2 + 6x_1x_3 \\ - 6x_2x_1 \end{array}$$

$$Q = \langle x | A x \rangle = \underline{x}^T \cdot \underline{\underline{A}} \cdot \underline{x}$$

$\underline{\underline{S}}^{-1} = \underline{\underline{S}}^T$ (orthogonal)

Transform: $\underline{x} = \underline{\underline{S}} \cdot \underline{x}'$ $\qquad \underline{x}' = \underline{\underline{S}}^{-1} \cdot \underline{x}$

$$\underline{x}' = \underline{\underline{S}}^T \cdot \underline{x}$$

$$Q = (\underline{\underline{S}} \cdot \underline{x}')^T \cdot \underline{\underline{A}} \cdot (\underline{\underline{S}} \cdot \underline{x}')$$

$$= (\underline{x}')^T \cdot \underline{\underline{S}}^T \cdot \underline{\underline{A}} \cdot \underline{\underline{S}} \cdot \underline{x}'$$

$$Q = (\underline{x}')^T \cdot \underline{\underline{S}}^T \cdot \underline{\underline{A}} \cdot \underline{\underline{S}} \cdot \underline{x}'$$

$$Q = (\underline{x}')^T \cdot \underline{\underline{A}}' \cdot \underline{x}' = \underline{x}^T \cdot \underline{\underline{A}} \cdot \underline{x}$$

eig vecs

$$\underline{\underline{A}}\, \underline{e}_i = \lambda_i \underline{e}_i$$

If we chose $\underline{\underline{S}}$ s.t. $\begin{pmatrix} \underline{e}_1 & \underline{e}_2 & \cdots & \underline{e}_N \end{pmatrix}$ $\rightarrow$ then $\underline{\underline{A}}' \rightarrow \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_N \end{pmatrix}$

$$Q = (x')^T \cdot \underline{\underline{A}}' \; \underline{x}'$$

$$= (x_1' \; x_2' \; \cdots \; x_N') \begin{pmatrix} \lambda_1 & 0 & 0 & 0 & \cdots \\ 0 & \lambda_2 & 0 & \cdots & \\ & & \ddots & & \\ & & & & \lambda_N \end{pmatrix} \begin{pmatrix} x_1' \\ x_2' \\ \vdots \\ x_N' \end{pmatrix}$$

$$= \lambda_1 x_1'^2 + \lambda_2 x_2'^2 + \cdots + \lambda_N x_N'^2$$

No cross term $\cancel{x_1' x_2'}$

Extrema of fn. of many variables.

$f(x_1, x_2 \dots x_N)$ $\qquad \left.\frac{\partial f}{\partial x_i}\right) = 0 \quad i = 1 \dots N \rightarrow \underline{x}_0$

$$\Delta f = f(\underline{x}) - f(\underline{x}_0) \approx \frac{1}{2} \sum_i^N \sum_j^N \boxed{\left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right)_0} \Delta x_i \Delta x_j$$

max, min or saddle.

eigvalues

$$\underline{\underline{M}} = M_{ij} = \left.\frac{\partial^2 f}{\partial x_i \partial x_j}\right)_0$$

"Hessian" Matrix.

$$\Delta f \approx \frac{1}{2} \underline{\Delta x}^T \cdot \underline{\underline{M}} \; \underline{\Delta x}$$

$\underline{\underline{M}}$ is real, Symm.

N real eig val. orthog. eig vec

eig val. for $\underline{\underline{M}}$

$\underline{\underline{M}} \, \underline{e}_i = \lambda_i \underline{e}_i$

$$\underline{\Delta x} = \sum a_i \underline{e}_i$$

$$\Delta f = \frac{1}{2} \underline{\Delta x}^T \cdot \underline{\underline{M}} \cdot \underline{\Delta x}$$

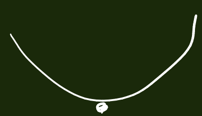
$$= \frac{1}{2} \underline{\Delta x}^T \sum a_i \underline{\underline{M}} \cdot \underline{e}_i$$

$$= \frac{1}{2} \underline{\Delta x}^T \sum a_i \lambda_i \underline{e}_i$$

$$= \frac{1}{2} \sum_j a_j \underline{e}_j^T \sum a_i \lambda_i \underline{e}_i$$

$$= \frac{1}{2} \sum_j \sum_i a_i a_j \lambda_i \, \underline{e}_j^T \underline{e}_i \qquad \delta_{ij}$$

$$\Delta f = \frac{1}{2} \sum_i a_i^2 \lambda_i$$



For Min: $\Delta f > 0 \longrightarrow \lambda_i > 0$

For Max: $\Delta f < 0 \longrightarrow \lambda_i < 0$

Saddle point $\longrightarrow$ Some λ_i's +ve $\quad \lambda_i$'s −ve