Lecture 34 : Distance Matrices, Procrustes Problem

Triangle inequality

Suppose $\|x_1 - x_2\|^2 = 1$ $\quad \|x_2 - x_3\|^2 = 1$ $\quad \|x_1 - x_3\|^2 = 6$

$$D = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 6 \\ 1 & 6 & 0 \end{bmatrix}$$

$X^T X = G$ = positive semidefinite

$G_{ij} = (x_i, x_j)$

Conclusion: G will not come out positive semidefinite if triangle inequality fails.

Procrustes problem – optimal rotation from basis 1 to basis 2

$$\begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix} Q \approx \begin{bmatrix} | & | & & | \\ y_1 & y_2 & \cdots & y_n \\ | & | & & | \end{bmatrix}$$

$$\min_{Q^TQ = I} \| YQ - X \|_F^2$$

Facts:

(i) Frobenius norm : $\|A\|_F^2 = a_{11}^2 + a_{12}^2 + \cdots + a_{1n}^2 + a_{21}^2 + \cdots \cdots + a_{nn}^2$ = trace of A^TA = $\begin{bmatrix} A \end{bmatrix}^T \begin{bmatrix} A \end{bmatrix}$

(ii) $\|QA\|_F^2 = \|A\|_F^2$

because $\|Qv\|^2 = \|v\|^2$

→ columns of A

$A = U\Sigma V^T$

$QA = \underline{\underline{QU}}\,\Sigma V^T$

↓

Singular values unchanged by Q

(iii) $\text{trace}(A^TB) = \text{trace}(B^TA) = \text{trace of } (BA^T)$

just transpose of each other, sum down the diagonal does not change

$\text{trace}(CD) = \text{trace}(DC)$

same nonzero eigenvalues

Back to $\min\limits_{Q^TQ=I} \|YQ - X\|_F^2$

$Y^TX = U\Sigma V^T$

Best $Q = UV^T$

proof is in notes