

Principal Component Analysis. PCA.

Given a dataset $X_{(N \times D)}$

N - rows - datapoints.

D - columns - dimensions.

$$x_i \in \mathbb{R}^D$$

we want to transform

$$X_{(N \times D)} \rightarrow Z_{(N \times K)}$$

such that $K \ll D$

while performing transformation, lets preserve variance in the dataset.

→ perform mean centering on the dataset

Say there is a unit vector $\hat{u}_{(D \times 1)}$ such that the variance across \hat{u} is maximum.

we want to compute \hat{u}

Variance \Rightarrow projecting x across \hat{u}

$$= \frac{1}{N} \sum_{i=1}^N (x_i^T \hat{u})^2$$

(mean centered x)

$$= \hat{u}^T \left(\frac{1}{N} \sum x_i x_i^T \right) \hat{u}$$

$\frac{1}{N} \sum_{i=1}^N x_i x_i^T = S =$ Covariance matrix of dataset x .
mean centered.

we want to maximize $\hat{u}^T S \hat{u}$ such that $\hat{u}^T \hat{u} = 1$ (unit vector).

→ adding this as Lagrangian constraint

$$\hat{u}^T S \hat{u} - \lambda (\hat{u}^T \hat{u} - 1). \quad \Rightarrow \text{maximize.}$$

∴ differentiating wrt $\hat{u} \Rightarrow$

$$2 S \hat{u} - 2 \lambda \hat{u} = 0.$$

$$S \hat{u} = \lambda \hat{u}.$$

this is of form eigen transformation analysis.

∴ \hat{u} is eigen vectors of S

eigen value = λ

$$\text{when } S \hat{u} = \lambda \hat{u}.$$

for \hat{u} that maximizes variance,

$$\begin{aligned} \text{variance} &= \hat{u}^T S \hat{u} = \hat{u}^T \lambda \hat{u} = \lambda \hat{u}^T \hat{u} \\ &= \lambda = \text{max variance across } \hat{u} \\ &\quad \text{eigen vector} \end{aligned}$$