

# PCA formulation

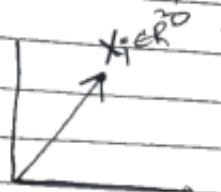
Monday, September 28, 2020

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Q. How to find the direction that preserves maximum variance?



For projecting  $\vec{x}_i$  in any other direction, we have to multiply  $\vec{x}_i$  with a unit vector in that direction so basically when we say we want the direction which preserves maximum variance we want the unit vector in that direction ( $\hat{u}$ )

$$\vec{x}_i \cdot \hat{u}$$

⇒ Norm of unit vector is one  $\|\hat{u}\| = 1$

Let's assume that our data is mean-centered. (mean of each column is zero). Subtract mean from each column and make it mean-centered.

Variance of new data along  $\hat{u} = \frac{1}{N} \sum_{i=1}^N (\vec{x}_i^T \hat{u})^2$

$$= \frac{1}{N} \sum_{i=1}^N \hat{u}^T \vec{x}_i \vec{x}_i^T \hat{u}$$

$$= \hat{u}^T \left( \frac{1}{N} \sum_{i=1}^N \vec{x}_i \vec{x}_i^T \right) \hat{u}$$

$S =$  sample covariance matrix of  $X$

covariance

$$\frac{1}{N} \sum (\vec{x}_i - \mu) (\vec{x}_i - \mu)^T$$

$\mu = 0$  in our case

$$S = \frac{1}{N} \sum_{i=1}^N \vec{x}_i \vec{x}_i^T$$

$$\sigma^2 = \hat{u}^T S \hat{u}$$

We want a  $\hat{u}$  such that the term

$\hat{u}^T S \hat{u}$  is maximized and at the same

time  $\hat{u}^T \hat{u} = 1$  i.e. it is a unit vector

Each Principal component is a weight

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Objective function of PCA.

find  $\hat{u} \rightarrow \max \hat{u}^T S \hat{u} \text{ st. } \hat{u}^T \hat{u} = 1$

Constrained optimization problem. Let's introduce a Lagrangian

$$\max_{\hat{u}, \lambda} \hat{u}^T S \hat{u} - \lambda (\hat{u}^T \hat{u} - 1) = 0$$

Derivative wrt  $u$  and  $\lambda$  & equate to 0

$$\frac{\partial \hat{u}^T S \hat{u}}{\partial \hat{u}} = 2 S \hat{u}$$

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

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

$$\frac{\partial}{\partial \lambda}$$

$$\hat{u}^T \hat{u} = 1$$

This is where we go back to Eigen vector Analysis (see  $S \hat{u} = \lambda \hat{u}$  form)

Property of eigen vector = They are unit length

Find eigen vector of  $S$ . Once we find  $S$  that will be  $\hat{u}$  then

$$\hat{u}_{\max} = \hat{u}^T S \hat{u} = \hat{u}^T \lambda \hat{u}$$

$$= \lambda \hat{u}^T \hat{u}$$

$S \hat{u}$  was the variance along  $\hat{u}$  & we see that it is  $\lambda$

$$\hat{u}_{\max} = \lambda$$

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We will get  $D$  eigen vectors which will satisfy the equation as  $S$  is a  $D \times D$  matrix

Projection in Direction  $\begin{bmatrix} \hat{u}_1 & \hat{u}_2 & \dots & \hat{u}_D \\ \lambda_1 & \lambda_2 & & \lambda_D \end{bmatrix}$

The eigen vector corresponding to the largest Eigen value gives the direction of maximal variance.

PCA is a linear algorithm.

$X_i \rightarrow Z_i$  (Dimensionality Reduction)

$$Z_i = W^T X_i$$

$L \times D \quad D \times 1$

$Z_i \rightarrow \hat{X}_i$  (Reconstruction)

$$\hat{X}_i = W Z_i$$

$D \times L \quad L \times 1$

when will Reconstruction be useful?  $\rightarrow$  Compression

How to see loss of information due to PCA? Recover the data back & check the difference (shown in lab)

$\Rightarrow$  PCA for face Recognition.

Complexity of PCA (mainly Eigen value decomposition step)  
 $= O(D^3) \Rightarrow D = \text{no. of original features}$