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TA Session : 16th October, 2020

Principal Component Analysis

(I)

What is it?

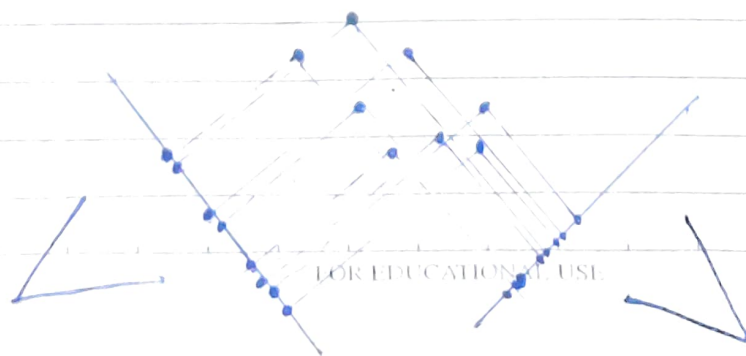
Single line : unsupervised dimensionality reduction technique

Defn : PCA is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of linearly uncorrelated variables called principal components.

Why?


- It is an important technique for visualization
- Denoising and data compression.
- Reduces training time?

Think of it as taking a picture!



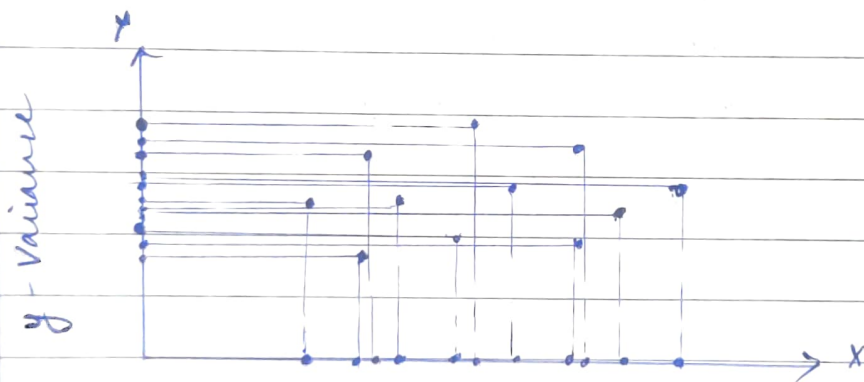
(II) Lens 1

- Mean
- Variance

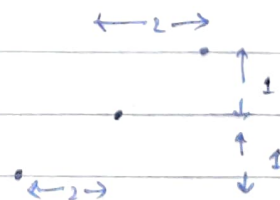
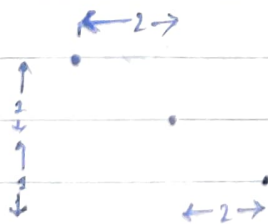

 $\frac{1^2 + 0^2 + 1^2}{3}$ How spread out?


 $\frac{5^2 + 0^2 + 5^2}{3}$

2D



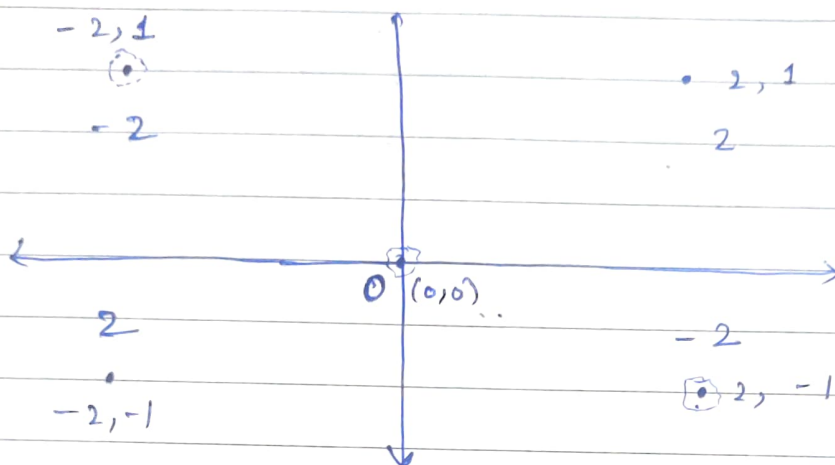
x - variance



x - variance = $\frac{2^2 + 0^2 + 2^2}{3}$

y - variance = $\frac{1^2 + 0^2 + 1^2}{3}$

Covariance



sum of product of co-ordinates

$$\text{Covariance} = \frac{2 + 0 + 2}{3} = \frac{4}{3}$$

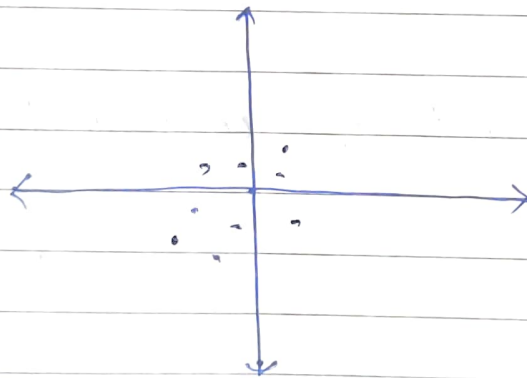
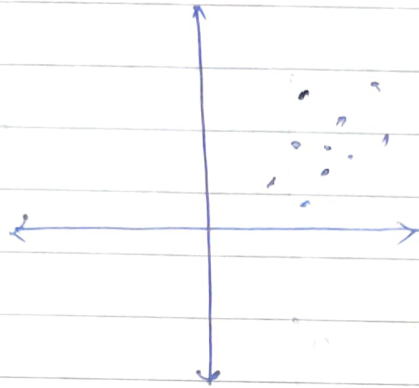
$$\text{Covariance} = \frac{(-2) + 0 + (-2)}{3} = -\frac{4}{3}$$

negative
covariance

zero
covariance

positive
covariance

PCA (2D)



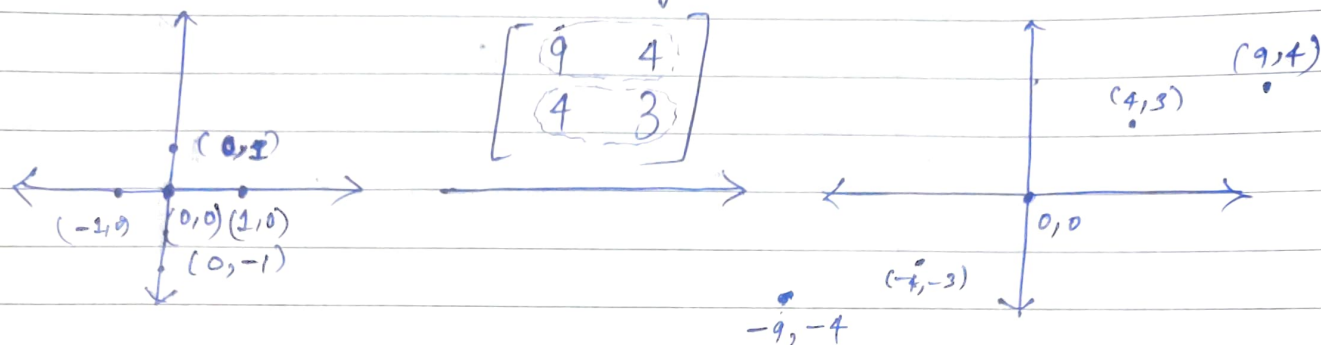
Covariance Matrix

$$2 \times 2 \quad V = \begin{bmatrix} \text{Var}(x) & \text{Cov}(x, y) \\ \text{Cov}(x, y) & \text{Var}(y) \end{bmatrix}$$

$$\left\{ \begin{bmatrix} 9 & 4 \\ 4 & 3 \end{bmatrix} \right\}$$

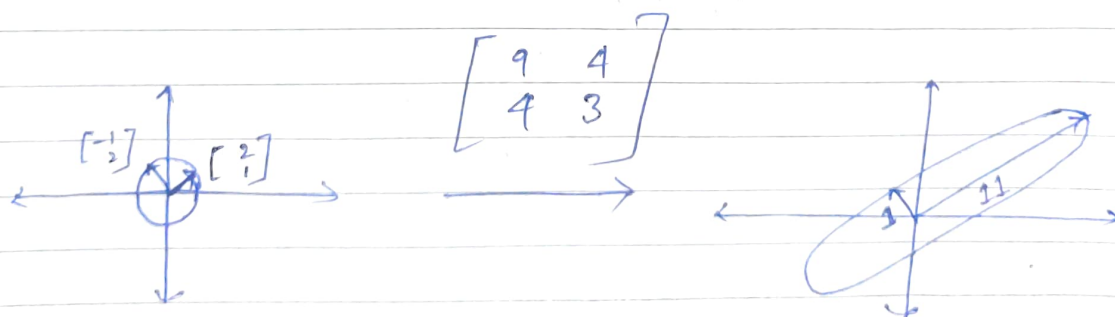
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Linear Transformation



$$(x, y) \longrightarrow (9x + 4y, 4x + 3y)$$

$(0, 0)$	\longrightarrow	$(0, 0)$
$(1, 0)$	\longrightarrow	$(9, 4)$
$(0, 1)$	\longrightarrow	$(4, 3)$
$(-1, 0)$	\longrightarrow	$(-9, -4)$
$(0, -1)$	\longrightarrow	$(-4, -3)$



Eigen vectors

$$\begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

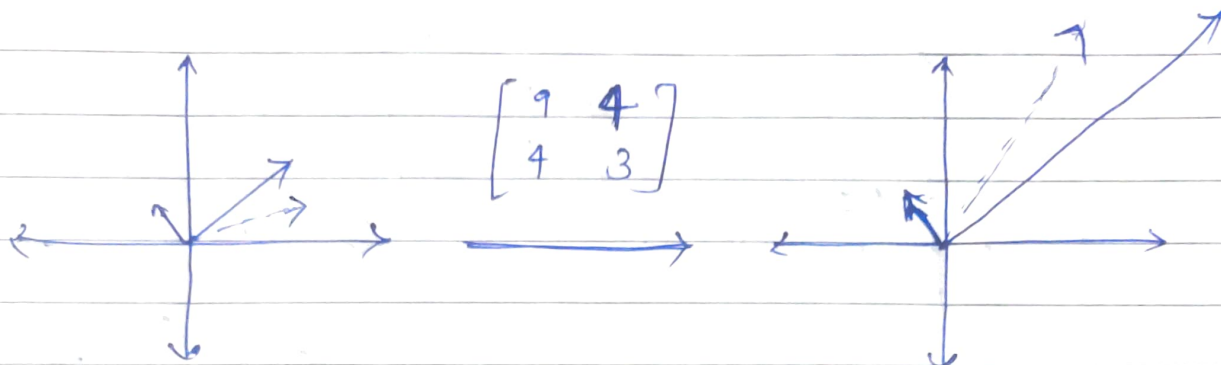
$$\begin{bmatrix} -1 \\ 2 \end{bmatrix}$$

Eigen values

1 1

1

Why eigenvectors?



$$\begin{bmatrix} 9 & 4 \\ 4 & 3 \end{bmatrix} v = \lambda v$$

\downarrow \downarrow
eigenvector eigenvalue.

How to calculate?

$$\begin{bmatrix} 9 & 4 \\ 4 & 3 \end{bmatrix}$$

Find eigenvalues

- Characteristic polynomial

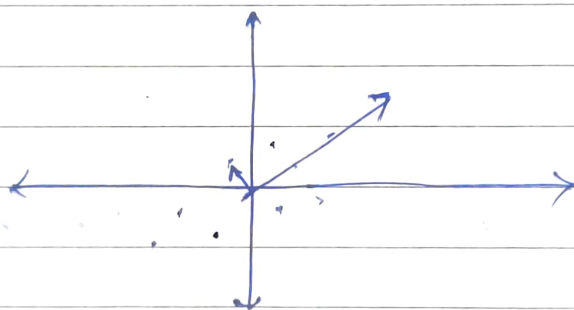
$$\begin{vmatrix} (x-9) & -4 \\ -4 & (x-3) \end{vmatrix} = (x-9)(x-3) - (-4)(-4) \\ = x^2 - 12x + 11 \\ = (x-11)(x-1)$$

Eigenvalues : 11 and 1

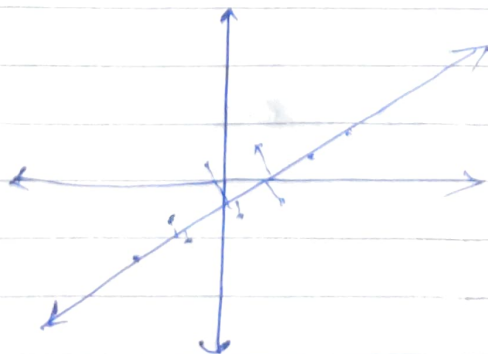
Eigenvectors

$$\begin{bmatrix} 9 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 11 \begin{bmatrix} x \\ y \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$



- Eigenvalues are real.
- The eigenvectors are perpendicular.
Why?



PCA (Multi-dimension)

	att 1	att 2	att 3	att 4	att 5
N_1					
N_2					
N_3					
.					
(
(
(

Covariance Matrix (5x5)

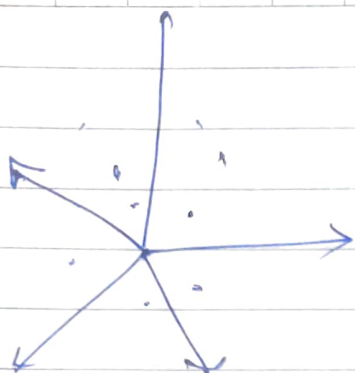
	a	b	c	d	e
x					
y					
z					
u					

5 eigenvectors & eigenvalues.

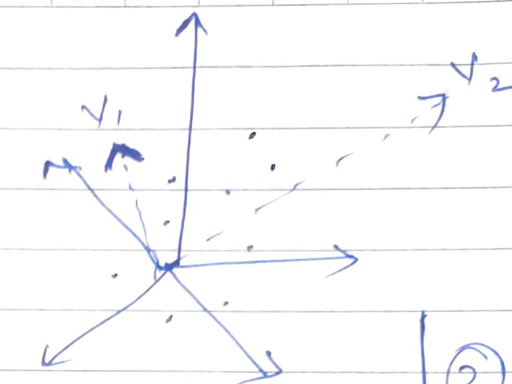
V_1	λ_1
V_2	λ_2
V_3	λ_3
V_4	λ_4
V_5	λ_5

↓
descending order

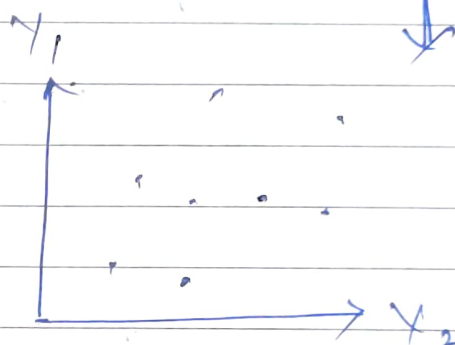
5



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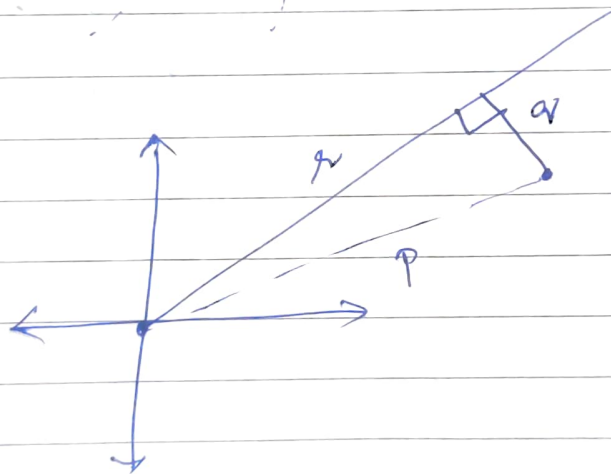
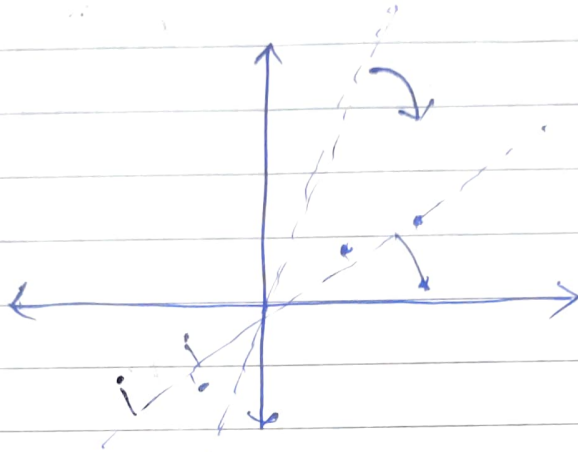


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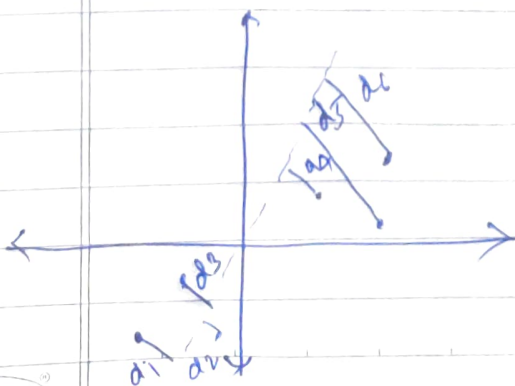
X

(III) Lens 2



$$r^2 = p^2 + q^2$$

Either minimize q
or maximize r

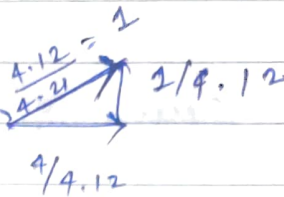
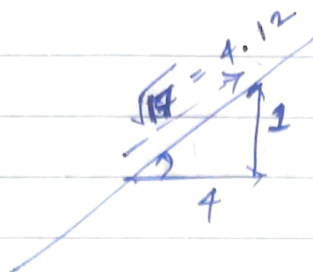


$$S = d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2$$

line $\rightarrow \max(S)$

Principal Component 1

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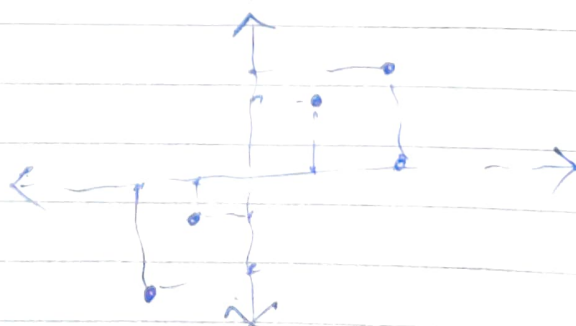
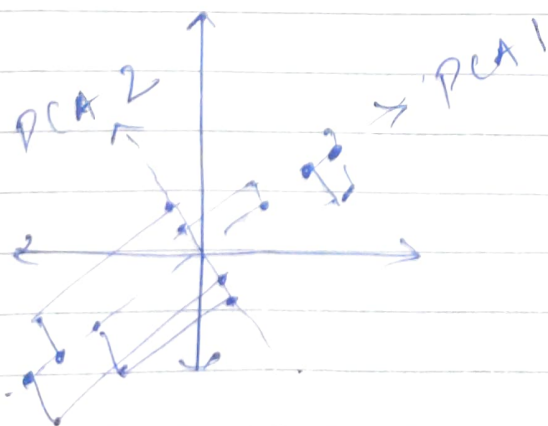
unit vector
 \Rightarrow eigenvector
 for PC1

$$d_1^2 + d_2^2 + d_3^2 + d_4^2 + d_5^2 + d_6^2$$

\Rightarrow eigenvalue for PC1

?

Variance



variation for PC1 :

sum of squared distances
 $n-1$

var 1 \rightarrow PCA 1

var 2 \rightarrow PCA 2

$$\text{PCA 1 (\%)} = \frac{\text{var 1}}{\text{var 1} + \text{var 2}}$$

(IV) Connecting the lenses

Eigenvalues of original covariance matrix is equal to the variances of the reduced space.

- Covariance of original space

$$C_X = \frac{1}{n} X^T X$$

- PCA : Eigendecomposition of covariance of the original space.

$$C_X = \frac{1}{n} X^T X = U \Lambda U^T$$

- Projected Data : $Y = XU$
(U has eigenvectors as columns)

- Covariance of the reduced space

$$C_Y = \frac{1}{n} Y^T Y$$

$$= \frac{1}{n} (XU)(XU)^T$$

$$= \frac{1}{n} U^T X^T X U$$

$$= U^T \left(\frac{1}{n} X^T X \right) U$$

$$C_y = U^T C_x U$$

$$= U^T U \Lambda U^T U$$

$$= \Lambda \rightarrow \text{which was the diagonal matrix consisting of eigenvalues}$$