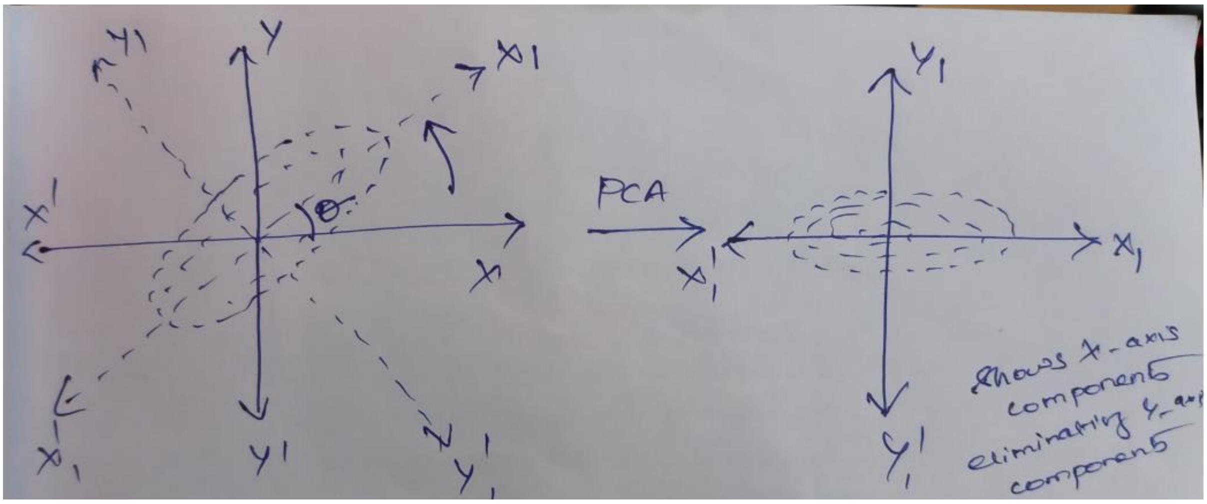
# Principal Component Analysis (PCA) in Machine Learning?

1. PCA can be abbreviated as Principal Component Analysis
2. PCA comes under the Unsupervised Machine Learning category
3. Reducing the number of variables in a data collection while retaining as much information as feasible is the main goal of PCA. PCA can be mainly used for Dimensionality Reduction and also for important feature selection.
4. Correlated features to Independent features




## Why Do We Need PCA in Machine Learning?

- Too many features (dimensions) in data can cause problems in machine learning.
- This is called the "curse of dimensionality."
- Having too many features makes it harder to learn relationships, leading to inaccurate predictions.
- PCA helps reduce features without losing significant information.
- This combats the curse of dimensionality and improves model accuracy.

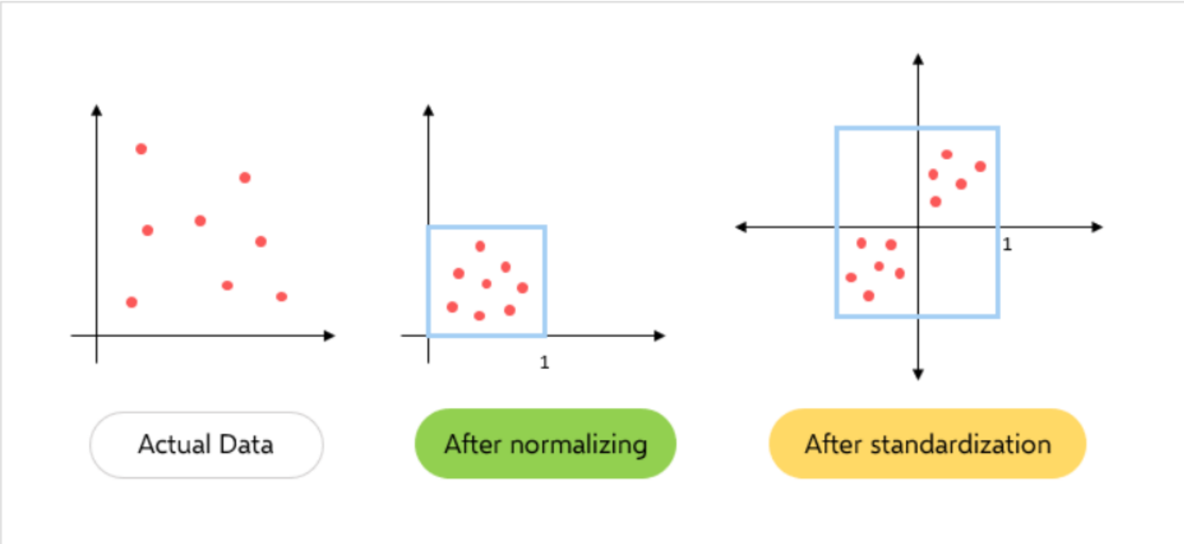
## When to use PCA?

1. Whenever we need to know our features are independent of each other
2. Whenever we need fewer features from higher features

# Basic Terminologies of PCA

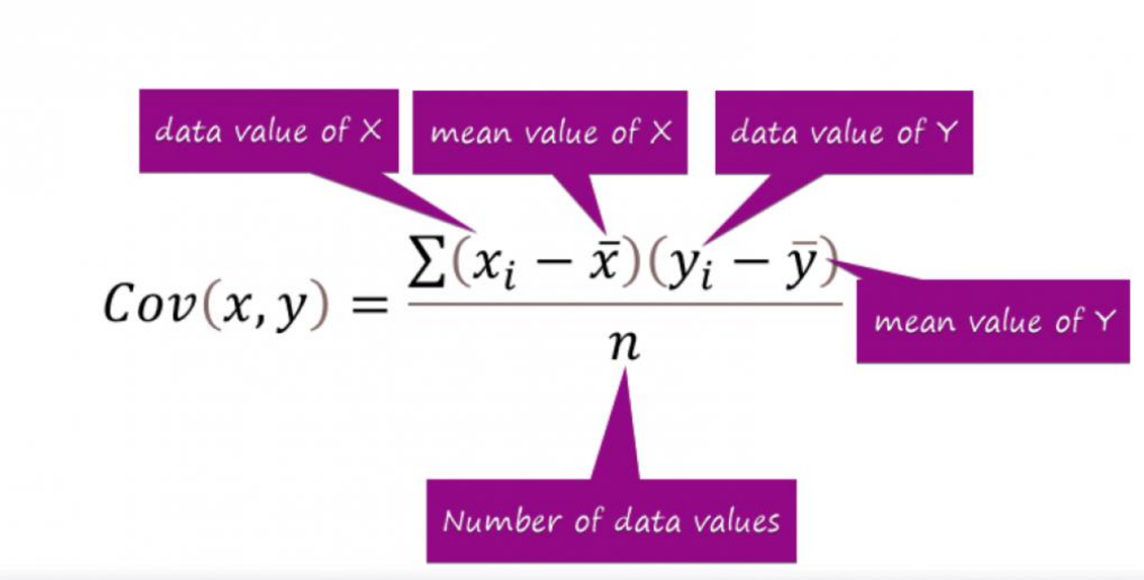
Before getting into PCA, we need to understand some basic terminologies,

- **Variance** – for calculating the variation of data distributed across dimensionality of graph
- **Covariance** – calculating dependencies and relationship between features
- **Standardizing data** – Scaling our dataset within a specific range for unbiased output



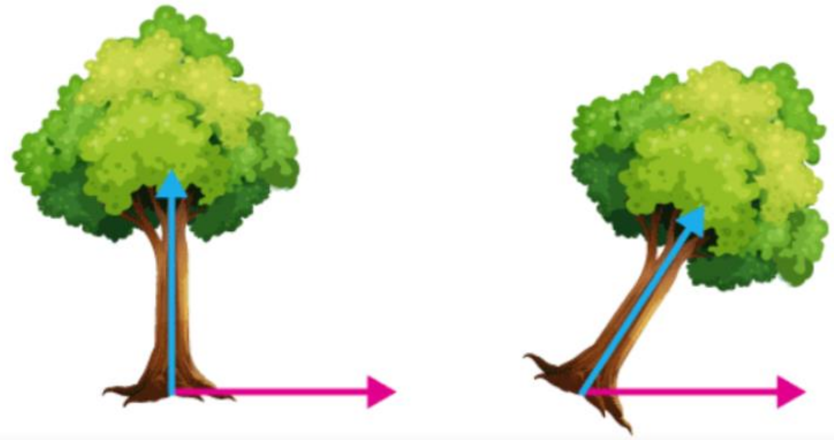

*Source: PCA Terminologies*

- **Covariance matrix** – Used for calculating interdependencies between the features or variables and also helps in reduce it to improve the performance

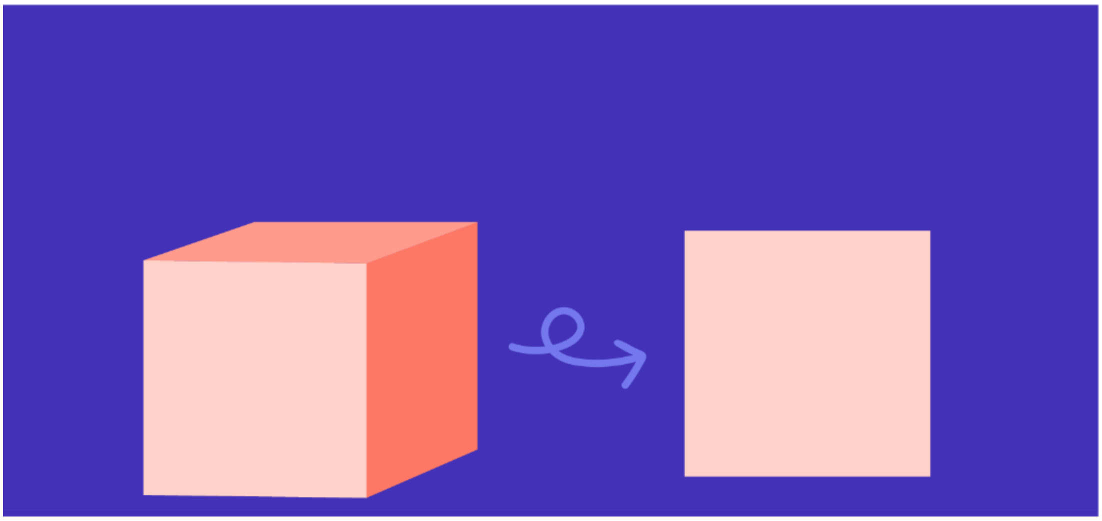



$$Cov(x,y) = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{n}$$

- **EigenValues and EigenVectors** – Eigenvectors' purpose is to find out the largest variance that exists in the dataset to calculate Principal Component. Eigenvalue means the magnitude of the Eigenvector. Eigenvalue indicates variance in a particular direction and whereas eigenvector is expanding or contracting X-Y (2D) graph without altering the direction.



- **Dimensionality Reduction –** Transpose of original data and multiply it by transposing of the derived feature vector. Reducing the features without losing information.



# How does PCA work?

The steps involved for PCA are as follows-

1. Original Data
2. Normalize the original data (mean =0, variance =1)
3. Calculating covariance matrix
4. Calculating Eigen values, Eigen vectors, and normalized Eigenvectors
5. Calculating Principal Component (PC)
6. Plot the graph for orthogonality between PCs

consider dataset,

| Feature | sample1 | Sample2 | Sample3 | Sample4 |
|---|---|---|---|---|
| a | 4 | 8 | 13 | 7 |
| b | 11 | 4 | 5 | 14 |

Step1:

No. of features, $n = 2$ (a,b)

No. of samples, $N = 4$ (sample1, sample2, sample3, sample4)

Step2:

calculating mean,

$$\bar{a} = \frac{4+8+13+7}{4} = 8$$

$$\bar{b} = \frac{11+4+5+14}{4} = 8.5$$

Step3:

calculating covariance matrix, between features,
In the given dataset, ordered features are as,
(a,a), (a,b), (b,a), (b,b)

$$\text{Cov}(a,a) = \frac{1}{N-1}\sum_{k=1}^{N}(a_i-\bar{a})(a_i-\bar{a})$$

$$= \frac{1}{N-1}\sum_{k=1}^{N}(a_i-\bar{a})^2 \longrightarrow \text{for same feature}$$

$$= \frac{1}{4-1}\left[(4-8)^2+(8-8)^2+(13-8)^2+(7-8)^2\right]$$

$$= \frac{4^2+0+5^2+1^2}{3} = \frac{\cancel{8}^{16}+0+25+1}{3}$$

$$= \frac{\cancel{2}42}{3} = \underline{\underline{14}}.$$

$$\text{cov}(a,b) = \frac{1}{N-1}\sum_{k=1}^{N}(a_i-\bar{a})(b_i-\bar{b})$$

$$= \frac{1}{4-1}\left[(4-8)(11-8.5)+(8-8)(4-8.5)+ (13-8)(5-8.5)+(7-8)(14-8.5)\right]$$

$$= \frac{1}{3}\left[(-4)(2.5)+(0)+(5)(-3.5)+(-1)(5.5)\right]$$

$$= \frac{1}{3}\left[-10-17.5-5.5\right] = \frac{-33}{3} = \underline{\underline{-11}}$$

$$\mathrm{cov}(b,a) = \frac{1}{N-1} \sum_{k=1}^{N} (b_i - \bar{b})(a_i - \bar{a})$$

$$= \mathrm{cov}(a,b)$$

$$= -11$$

$$\mathrm{cov}(b,b) = \frac{1}{N-1} \sum_{k=1}^{N} (b_i - \bar{b})(b_i - \bar{b})$$

$$= \frac{1}{N-1} \sum_{k=1}^{N} (b_i - \bar{b})^2$$

$$= \frac{1}{4-1} \left[ (11-8.5)^2 + (4-8.5)^2 + (5-8.5)^2 + (14-8.5)^2 \right]$$

$$= \frac{1}{3} \left[ (2.5)^2 + (-4.5)^2 + (-3.5)^2 + (5.5)^2 \right]$$

$$= \frac{1}{3} \left[ 6.25 + 20.25 + 12.25 + 30.25 \right]$$

$$= \frac{69}{3} = \underline{\underline{23}}$$

Hence covariance matrix can be

$$S = \begin{bmatrix} \mathrm{cov}(a,a) & \mathrm{cov}(a,b) \\ \mathrm{cov}(b,a) & \mathrm{cov}(b,b) \end{bmatrix} = \begin{bmatrix} 14 & -11 \\ -11 & 23 \end{bmatrix}$$

<u>Step4:-</u>

calculate Eigen value, Eigen vector, Normalized Eigen vector.

Inorder calculate Eigen value,

$$\det(S - \lambda I) = 0$$

$$I(\text{Identity matrix}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\lambda I = \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix}$$

$$\det\left( \begin{bmatrix} 14 & -11 \\ -11 & 23 \end{bmatrix} - \begin{bmatrix} \lambda & 0 \\ 0 & \lambda \end{bmatrix} \right) = 0$$

$$\det\begin{pmatrix} 14-\lambda & -11 \\ -11 & 23-\lambda \end{pmatrix} = 0.$$

$$(14-\lambda)(23-\lambda) - (-11 \times -11) = 0$$

$$322 - 14\lambda - 23\lambda + \lambda^2 - 121 = 0$$

$201 - 37\lambda + \lambda^2 = 0.$

After rearranging,

$$\lambda^2 - 37\lambda + 201 = 0.$$

'$\lambda$' can be calculated by quadratic equ,

$$\lambda = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \qquad a = 1,\ b = -37,\ c = 201$$

$$= \frac{-(-37) \pm \sqrt{(-37)^2 - 4(1)(201)}}{2(1)}$$

$$= \frac{37 \pm \sqrt{1369 - 804}}{2} = \frac{37 \pm \sqrt{565}}{2}$$

$$= \frac{37 \pm 23.76}{2} \Rightarrow \frac{37 + 23.76}{2}, \frac{37 - 23.76}{2}$$

$$= \frac{60.76}{2}, \frac{13.24}{2}$$

Eigen Values. $\boxed{\lambda_1 = 30.38,\ \lambda_2 = 6.62}$

So, while arranging in descending order,

$$\lambda_1 > \lambda_2 > \ldots$$

Hence, $\lambda_1 = 30.38$

$\lambda_2 = 6.62$

We are going to find out Eigenvectors for Eigen Value, $\lambda = 30.38$.

$$(S - \lambda_1 I)\, u_1 = 0$$

Covariance matrix   30.38   Identity matrix   Eigen vector of $\lambda_1$

$$\left(\begin{pmatrix} 14 & -11 \\ -11 & 23 \end{pmatrix} - 30.38 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right) u_1 = 0$$

Assume $u_1 = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$

Hence,

$$\begin{pmatrix} 14 & -11 \\ -11 & 23 \end{pmatrix} - \begin{pmatrix} 30.38 & 0 \\ 0 & 30.38 \end{pmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{pmatrix} 14-30.38 & -11 \\ -11 & 23-30.38 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{pmatrix} -16.38 & -11 \\ -11 & -7.38 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$-16.38\,u_1 - 11u_2 = 0 \rightarrow (1)$

$-11\,u_1 - 7.38u_2 = 0 \rightarrow (2)$

so, from this if we need to calculate $u_1$ & $u_2$

$(1) \times 7.38 \Rightarrow 120.88u_1 - \cancel{81.18}u_2 = 0$

$(2) \times -11. \Rightarrow +121\,u_1 + \cancel{81.18}\,u_2 = 0$

$0.12u_1 = 0$

$\boxed{u_1 = 0}$

then, apply $u_1$ in (1), then

$-16.38 \times 0 - 11u_2 = 0$

$\boxed{u_2 = 0}$

this can't be possible, hence

$$\begin{bmatrix} (14-\lambda_1) & (-11) \\ (-11) & (23-\lambda_1) \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$(14-\lambda_1)u_1 - 11u_2 = 0 \longrightarrow (a)$

$-11u_1 + (23-\lambda_1)u_2 = 0 \longrightarrow (b)$

from (a),

$(14-\lambda_1)u_1 - 11u_2 = 0$

$(14-\lambda_1)u_1 = 11u_2.$

$\frac{u_1}{11} = \frac{u_2}{14-\lambda_1} = A$ (Assigning)

Assume $\underline{A=1}$,

$\frac{u_1}{11} = \frac{u_2}{14-\lambda_1} = A = 1.$

Hence, $\frac{u_1}{11} = 1 \Rightarrow u_1 = 11.$

$\frac{u_2}{14-\lambda_1} = 1 \Rightarrow u_2 = 14-\lambda_1$

$= 14 - 30.38$

$= -16.38.$

Hence Eigen vector for $\lambda_1 \Rightarrow \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 11 \\ -16.38 \end{bmatrix}$

Then if we want to normalize the eigen vectors,

$$n_1 = \begin{bmatrix} 11/\sqrt{11^2+16.38^2} \\ -16.38/\sqrt{11^2+16.38^2} \end{bmatrix}$$ / dividing by the length.

$$= \begin{bmatrix} \frac{11}{19.73} \\ -16.38/19.73 \end{bmatrix} = \begin{bmatrix} 0.5575 \\ -0.8302 \end{bmatrix}$$

Now, calculate eigen vector for $\lambda_2 = 6.62$

$$(S - \lambda_2 I) U_2 = 0$$

$$\begin{bmatrix} (14-\lambda_2) & -11 \\ -11 & (23-\lambda_2) \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$(14-\lambda_2)U_1 - 11U_2 = 0 \rightarrow (c)$$

$$-11U_1 - (23-\lambda_2)U_2 = 0 \rightarrow (d)$$

from (c),

$$(14-\lambda_2)U_1 - 11U_2 = 0$$

$$(14-\lambda_2)U_1 = 11U_2$$

$$\frac{U_1}{11} = \frac{U_2}{14-\lambda_2} = B \text{ (Assume}$$

Assume $B = 1$,

$$\frac{U_1}{11} = \frac{U_2}{14-\lambda_2} = B = 1$$

Hence, $\frac{U_1}{11} = 1 \Rightarrow U_1 = 11$

$$\frac{U_2}{14-\lambda_2} = 1 \Rightarrow U_2 = 14-\lambda_2$$
$$= 14 - 6.62$$
$$= 7.38$$

Hence, Eigen Vector for $\lambda_2 = \begin{bmatrix} 11 \\ 7.38 \end{bmatrix}$

If we want to normalize eigen vector,

$$n_2 = \begin{bmatrix} 11/\sqrt{11^2+7.38^2} \\ 7.38/\sqrt{11^2+7.38^2} \end{bmatrix} = \begin{bmatrix} 11/13.24 \\ 7.38/13.24 \end{bmatrix}$$

$$= \begin{bmatrix} 0.8308 \\ 0.5574 \end{bmatrix}$$

Step 5: New dataset,

| Feature | sample1 | sample2 | sample3 | sample4 |
|---|---|---|---|---|
| a | 4 | 8 | 13 | 7 |
| b | 11 | 4 | 5 | 14 |

| 1st PC | $P_{11}$ | $P_{12}$ | $P_{13}$ | $P_{14}$ |
|---|---|---|---|---|
| | sample1 | sample2 | sample3 | sample4 |

$$P_{11} = n_1^T \begin{bmatrix} 4-8 \\ 11-8.5 \end{bmatrix}$$

$$= \begin{bmatrix} 0.5575 & -0.8302 \end{bmatrix} \begin{bmatrix} -4 \\ 2.5 \end{bmatrix}$$

$$= (-2.23 - 2.0755)$$

$$= -4.305$$

$$P_{12} = n_1^T \begin{bmatrix} 8-8 \\ 4-8.5 \end{bmatrix} \Rightarrow (0.5575 \; -0.8302) \begin{pmatrix} 0 \\ -4.5 \end{pmatrix}$$

$$= 0 + 3.7359 = 3.7359$$

$$P_{13} = n_1^T \begin{bmatrix} 13-8 \\ 5-8.5 \end{bmatrix} \Rightarrow (0.5575 \; -0.8302) \begin{pmatrix} 5 \\ -3.5 \end{pmatrix}$$

$$= 2.787 + 2.905 = \underline{5.692}$$

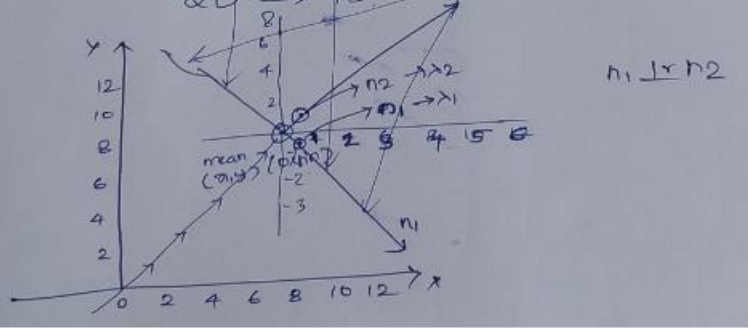
$$P_{14} = n_1^T \begin{bmatrix} 7-8 \\ 14-8.5 \end{bmatrix} = (0.5575 \; -0.8302) \begin{pmatrix} -1 \\ 5.5 \end{pmatrix}$$

$$= -0.5575 - 4.5661$$

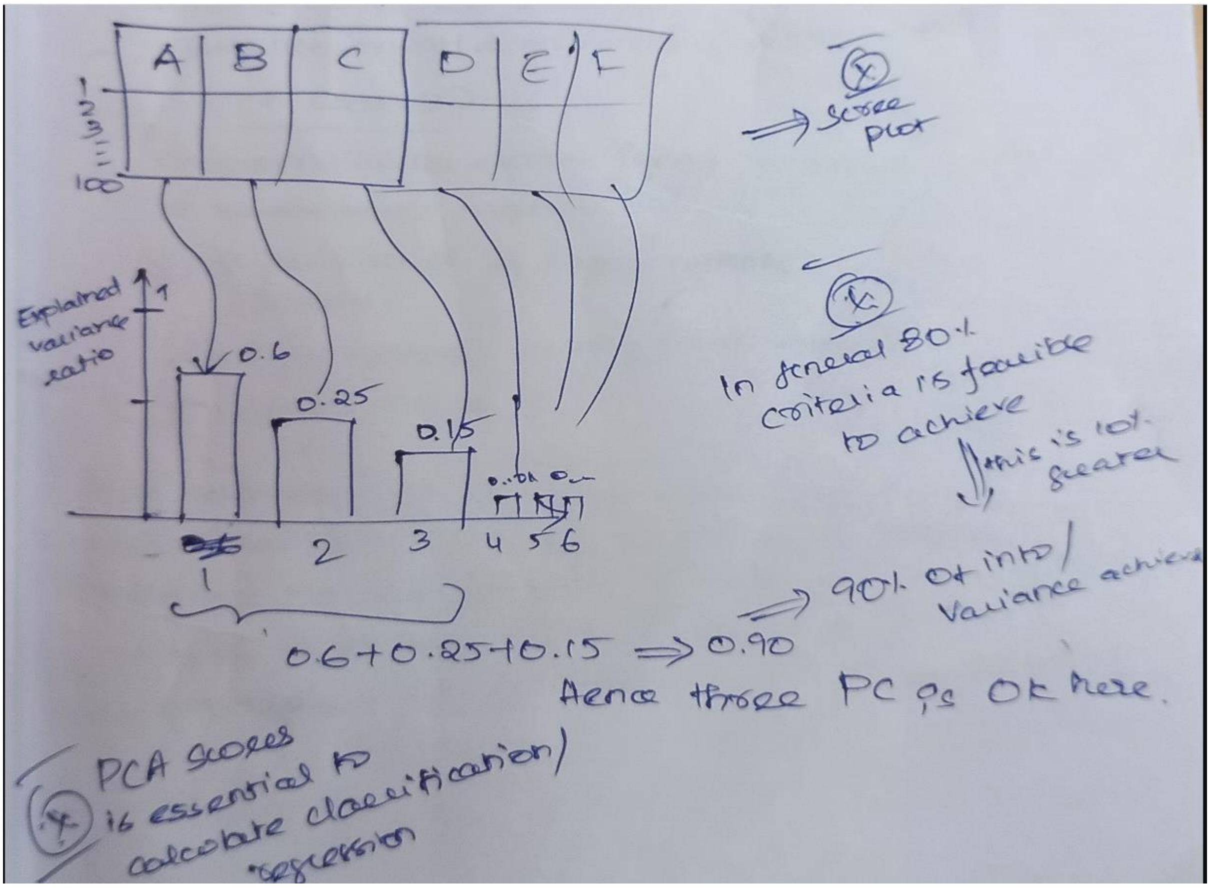
$$= -5.123$$

$$\boxed{PC1 = -4.305 \quad 3.7359 \quad 5.692 \quad -5.123}$$

$$2D \xRightarrow{PCA} 1D$$




$n_1 \perp r \; n_2$




# Advantage for Principal Component Analysis

1. Used for Dimensionality Reduction
2. PCA will assist you in eliminating all related features, sometimes referred to as multi-collinearity.
3. The time required to train your model is now substantially shorter because to PCA's reduction in the number of features.
4. PCA aids in overcoming overfitting by eliminating the extraneous features from your dataset.

# Disadvantage for Principal Component Analysis

1. Useful for quantitative data but not effective with qualitative data.
2. Interpretation of PC is difficult from original data

# Application for Principal Component Analysis

1. Computer Vision
2. Bio-informatics application
3. For compressed images or resizing of the image
4. Discovering patterns from high-dimensional data
5. Reduction of dimensions
6. Multidimensional Data – Visualization