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SNS COLLEGE OF TECHNOLOGY

Coimbatore-35
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DEPARTMENT OF ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

23AMB201 - MACHINE LEARNING

II YEAR IV SEM

UNIT IV – UNSUPERVISED LEARNING ALGORITHM

TOPIC 8 – Principal Component Analysis

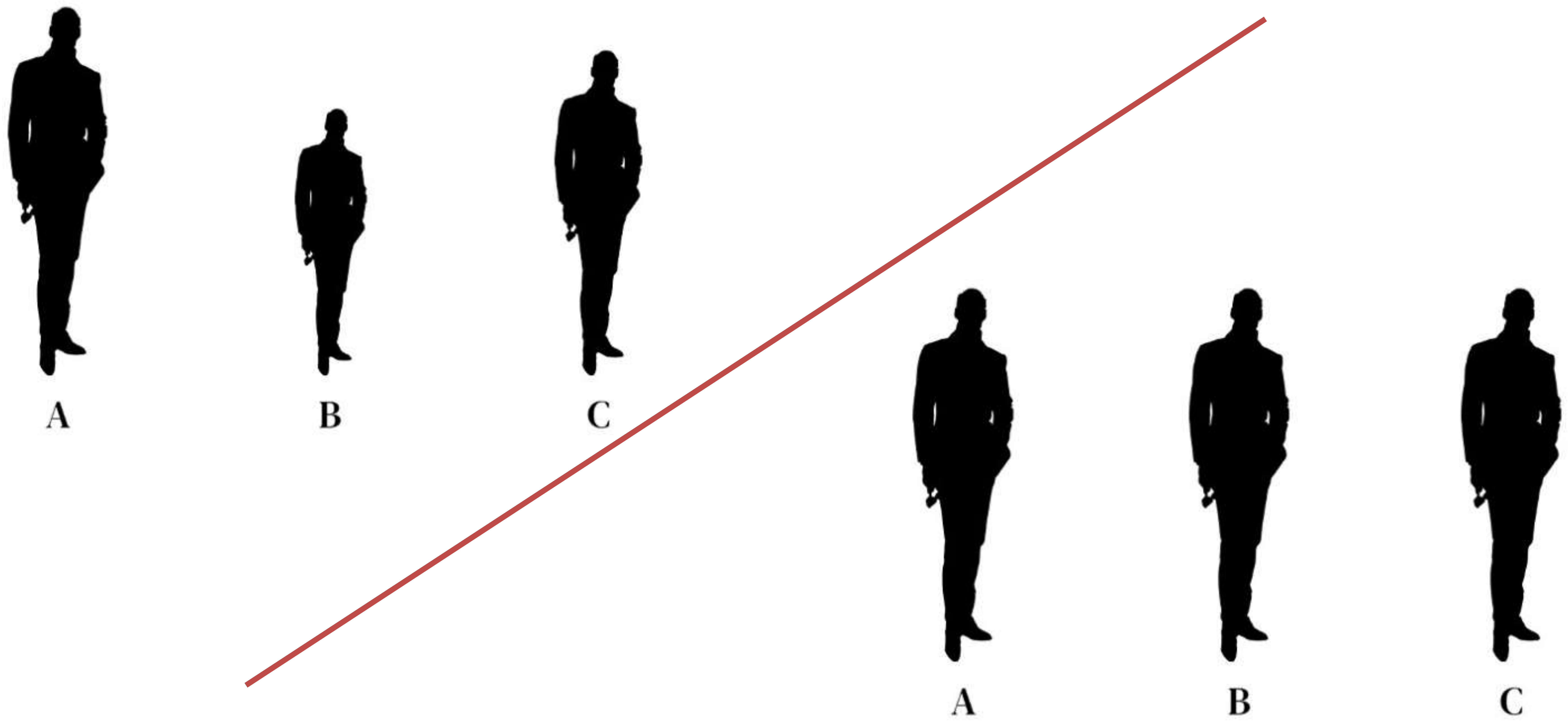
Principal Components Analysis

1. PCA comes under the Unsupervised Machine Learning category
2. The main goal of PCA is to **reduce the number of variables in a data collection while retaining as much information as feasible**. Principal component analysis in machine learning can be mainly used for Dimensionality Reduction and important feature selection.
3. Correlated features to Independent features

When should Principal Component Analysis be used in ML?

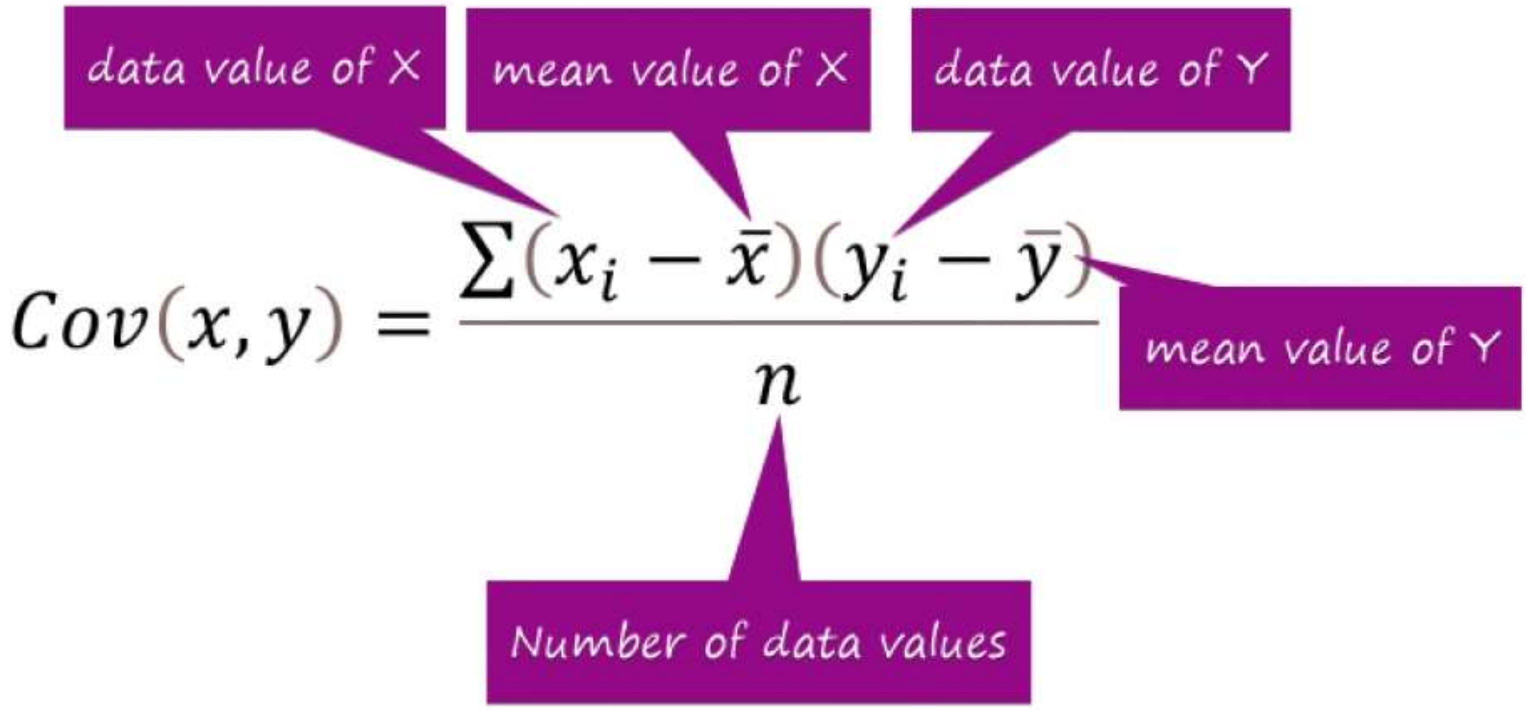
1. Whenever we need to know our features are independent of each other
2. Whenever we need fewer features from higher features

Intuition behind PCA: we need to find the tallest person

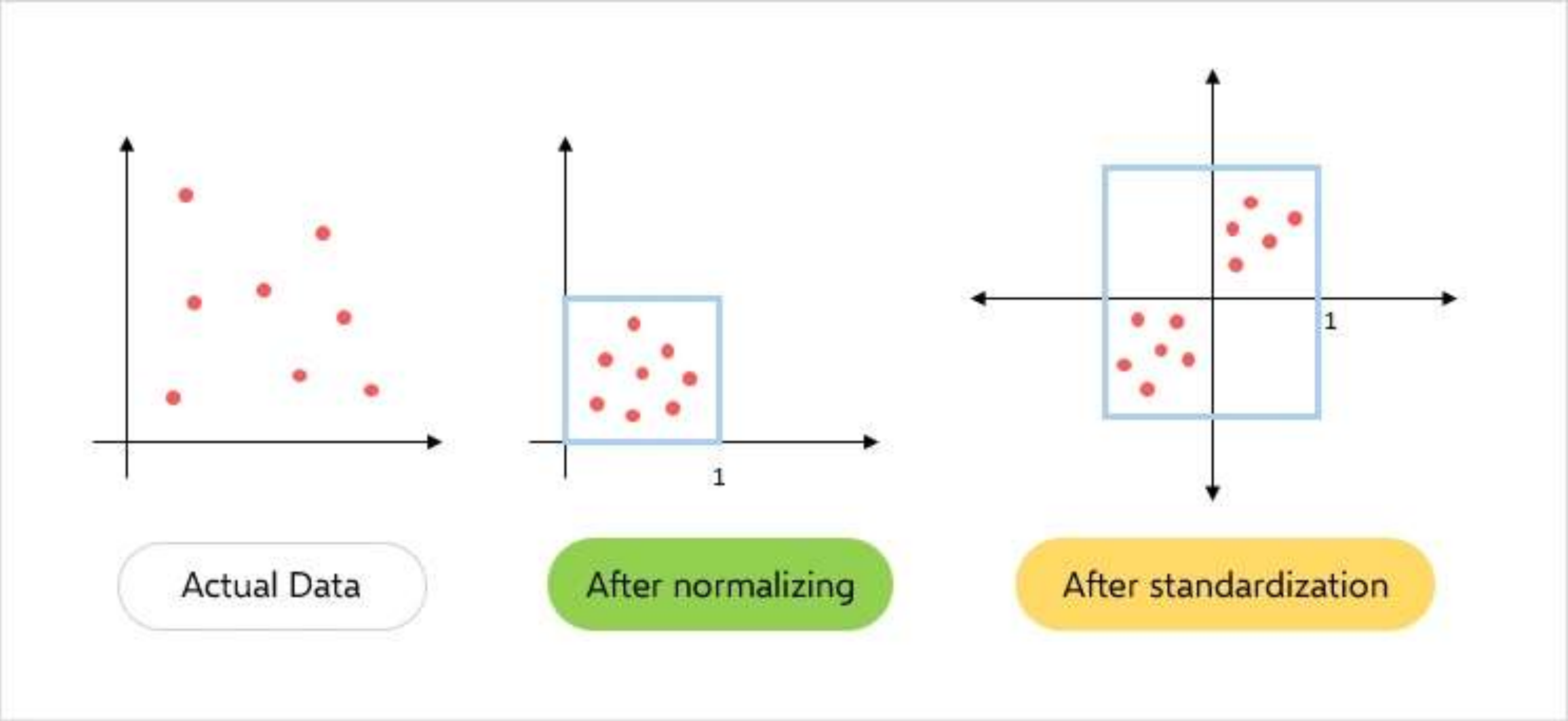


Basic Terminologies of PCA

1. **Variance**: For calculating the variation of data distributed across the dimensionality of the graph
2. **Covariance**: Calculating dependencies and relationship between features
3. **Standardizing data**: Scaling our dataset within a specific range for unbiased output
4. **Covariance matrix**: Used for calculating interdependencies between the features or variables and also helps in reducing it to improve the performance
5. **EigenVectors**: The eigenvectors aim to find the largest dataset variance to calculate the Principal Component.
6. **Eigenvalue**:The eigenvalue indicates variance in a particular direction



PCM



How Does PCA Work?

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. The eigenvectors represent the principal components, while the eigenvalues indicate the importance of each principal component.
6. Calculating Principal Component (PC)
7. Plot the graph for orthogonality between PCs

How Does PCA Work?

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,

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

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

How Does PCA Work?

Step3:

calculating covariance matrix, between features,

In the given dataset, ordered features are as,

(a,a), (a,b), (b,a), (b,b)

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

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

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

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

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

How Does PCA Work?

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

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

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

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

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

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

$$= -11$$

How Does PCA Work?

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

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

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

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

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

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

Hence covariance matrix can be

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

How Does PCA Work?

Step4:-

calculate Eigen value, Eigen vector, Normalized Eigen vector.

Inorder calculate Eigen value,

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

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

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

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

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

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

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

How Does PCA Work?

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

After rearranging,

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

'λ' can be calculated by quadratic eqn,

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

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

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

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

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

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

How Does PCA Work?

So, while arranging in descending order,

$$\lambda_1 > \lambda_2 > \dots$$

Hence, $\lambda_1 = 30.38$

$\lambda_2 = 6.62$

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

$$(\underbrace{S}_{\text{Covariance matrix}} - \underbrace{\lambda_1}_{30.38} \underbrace{I}_{\text{Identity matrix}})\, \underbrace{U_1}_{\text{Eigen vector of } \lambda_1} = 0$$

$$\left(\begin{pmatrix} 14 & -11 \\ -11 & 23 \end{pmatrix} - 30.38 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right) U_1 = 0$$

Assume $U_1 = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$

Hence,

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

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

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

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

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

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

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

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

$$0.12\,u_1 = 0$$

$$\boxed{u_1 = 0}$$

then, apply u_1 in (1), then

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

$$\boxed{u_2 = 0}$$

How Does PCA Work?

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 $\lambda_1 \Rightarrow \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 11 \\ -16.38 \end{bmatrix}$

Calculating PC

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,

$$\frac{v_1}{11} = \frac{v_2}{14-\lambda_2} = B = 1$$

Hence, $\frac{v_1}{11} = 1 \Rightarrow v_1 = 11$

$$\frac{v_2}{14-\lambda_2} = 1 \Rightarrow v_2 = 14-\lambda_2$$

$$= 14 - 6.62$$

$$= 7.38$$

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

If we want to normalize eigen vector,

$$n_2 = \begin{bmatrix} 11/\sqrt{11^2+7.38^2} \\ 7.88/\sqrt{11^2+7.38^2} \end{bmatrix} = \begin{bmatrix} 11/13.24 \\ 7.88/13.24 \end{bmatrix}$$

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

Normolized Eigen vector

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

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

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

$$= (-2.23 - 2.0755)$$

$$= -4.305$$

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

$$= 0 + 3.7359 = 3.7359$$

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

$$= 2.787 + 2.905 = 5.692$$

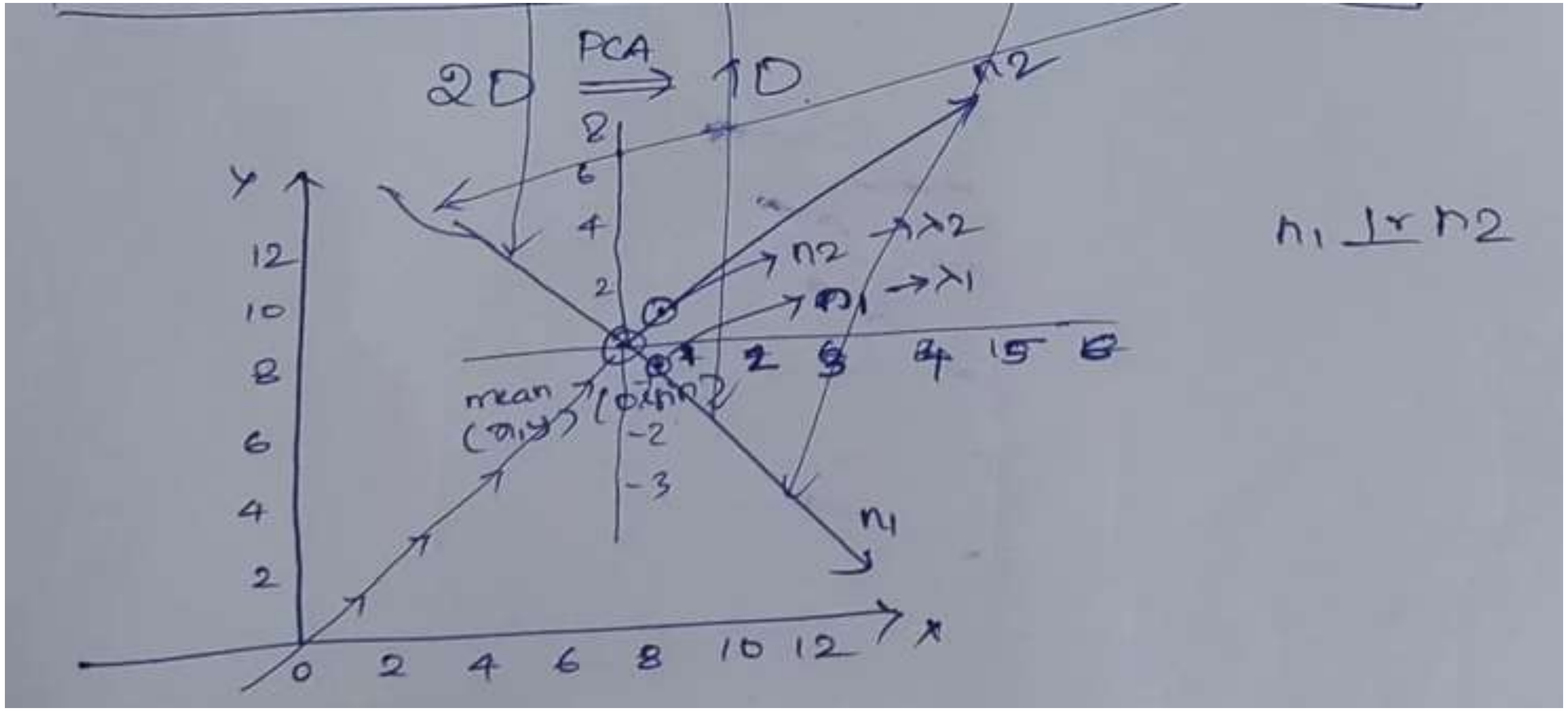
$$P_{14} = n_1^T \begin{bmatrix} 7-8 \\ 14-8.5 \end{bmatrix} = \begin{pmatrix} 0.5575 & -0.8302 \end{pmatrix} \begin{pmatrix} -1 \\ 5.5 \end{pmatrix}$$

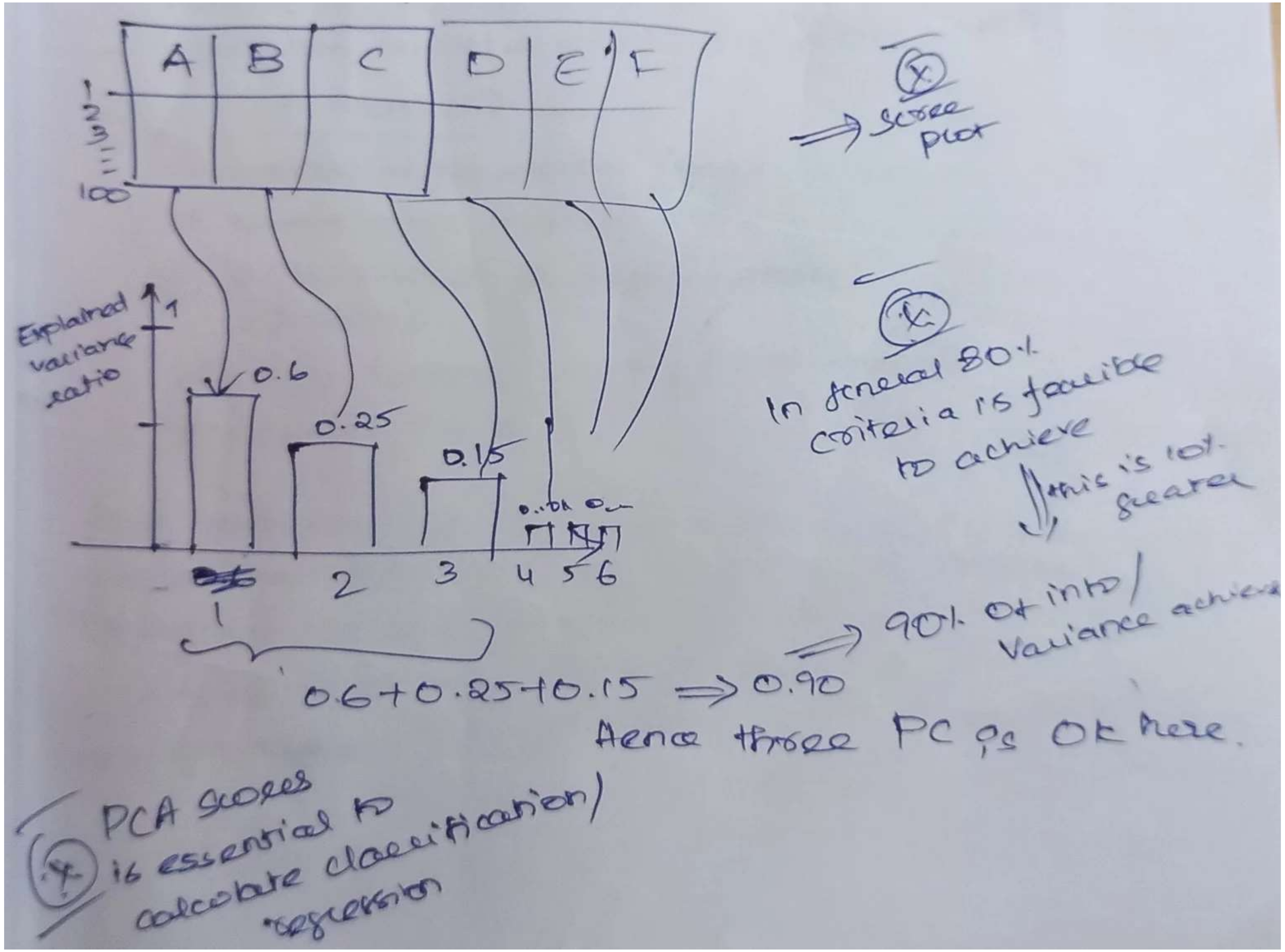
$$= -0.5575 - 4.5661$$

$$= -5.123$$

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

Normolized Eigen vector




A B C D E F
1
2
3
100
score plot
Explained variance ratio
1
0.6
0.25
0.15
1 2 3 4 5 6
In general 80% criteria is feasible to achieve
this is 10% greater
90% of info/ Variance achieved
0.6+0.25+0.15 ⇒ 0.90
Hence three PC is OK here.
PCA scores is essential to calculate classification/ regression

References

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P. Flach, ―Machine Learning: The art and science of algorithms that make sense of data‖, Cambridge University Press, 2012.

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