Unsupervised learning

Outline

- Unsupervised Learning
  - Clustering: KMeans
  - Dimensionality Reduction: PCA

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Clustering: K-Means

- Given a predefined K

1. Randomly initialize K cluster centers
2. Assign each instance to the nearest center
3. Update each center as the mean of all the instances in the cluster
4. Repeat Step 2-3 until the centers do not change anymore

K-Means

- Consider the two dimensional patterns (2, 1), (3, 5), (4, 3), (5, 6), (6, 7), (7, 8).
- Cluster them using K-Means Algorithm. Let K = 2.

K-Means

<u>Step-01:</u> Randomly initialize K cluster centers.
Let's choose:

$$Centroid\ 1 = (2,1), Centroid\ 2 = (7,8)$$

K-Means

<u>Step-02:</u> Assign each instance to the nearest center

- draw a table showing all the results.Using the table, we decide which point belongs to which cluster.
- The given point belongs to that cluster whose center is nearest to it.

Given Points	Distance to Centroid 1 (2, 1)	Distance to Centroid 2 (7, 8)	Assigned Cluster
(2,1)	0.0	8.6	1
(3,5)	4.12	5.83	1
(4,3)	2.83	6.4	1
(5,6)	5.83	3.61	2
(6,7)	7.81	1.41	2
(7,8)	8.6	0.0	2

K-Means

Step-03: Update the each center as the mean of all the instances in the cluster.

- $\boldsymbol{Cluster\ 1}:\ \boldsymbol{Points}\ =\ (\mathbf{2},\mathbf{1}),(\mathbf{3},\mathbf{5}),(\mathbf{4},\mathbf{3})$
  - $\boldsymbol{New\ Centroid\ 1}\ =\ \left(\frac{\mathbf{2+3+4}}{\mathbf{3}},\frac{\mathbf{1+5+3}}{\mathbf{3}}\right)=(\mathbf{3},\mathbf{3})$
- $\boldsymbol{Cluster\ 2}:\ \boldsymbol{Points}\ =\ (\mathbf{5},\mathbf{6}),(\mathbf{6},\mathbf{7}),(\mathbf{7},\mathbf{8})$
  - $\boldsymbol{New\ Centroid\ 2}\ =\ \left(\frac{\mathbf{5+6+7}}{\mathbf{3}},\frac{\mathbf{6+7+8}}{\mathbf{3}}\right)=(\mathbf{6},\mathbf{7})$

Step-04: the centers changed. Repeat Step-02 and Step-03

K-Means

Repeat Step-02: Assign each instance to the nearest center

Given Points	Distance to Centroid 1 (3, 3)	Distance to Centroid 2 (6, 7)	Assigned Cluster
(2,1)	2.24	7.21	1
(3,5)	2.0	4.24	1
(4,3)	1.0	5.0	1
(5,6)	3.61	1.41	2
(6,7)	5.0	0.0	2
(7,8)	6.4	1.41	2

The clusters remain the same as before:

- $Cluster\ 1\text{:}\ (2,1),(3,5),(4,3)$
- $Cluster\ 2\text{:}\ (5,6),(6,7),(7,8)$

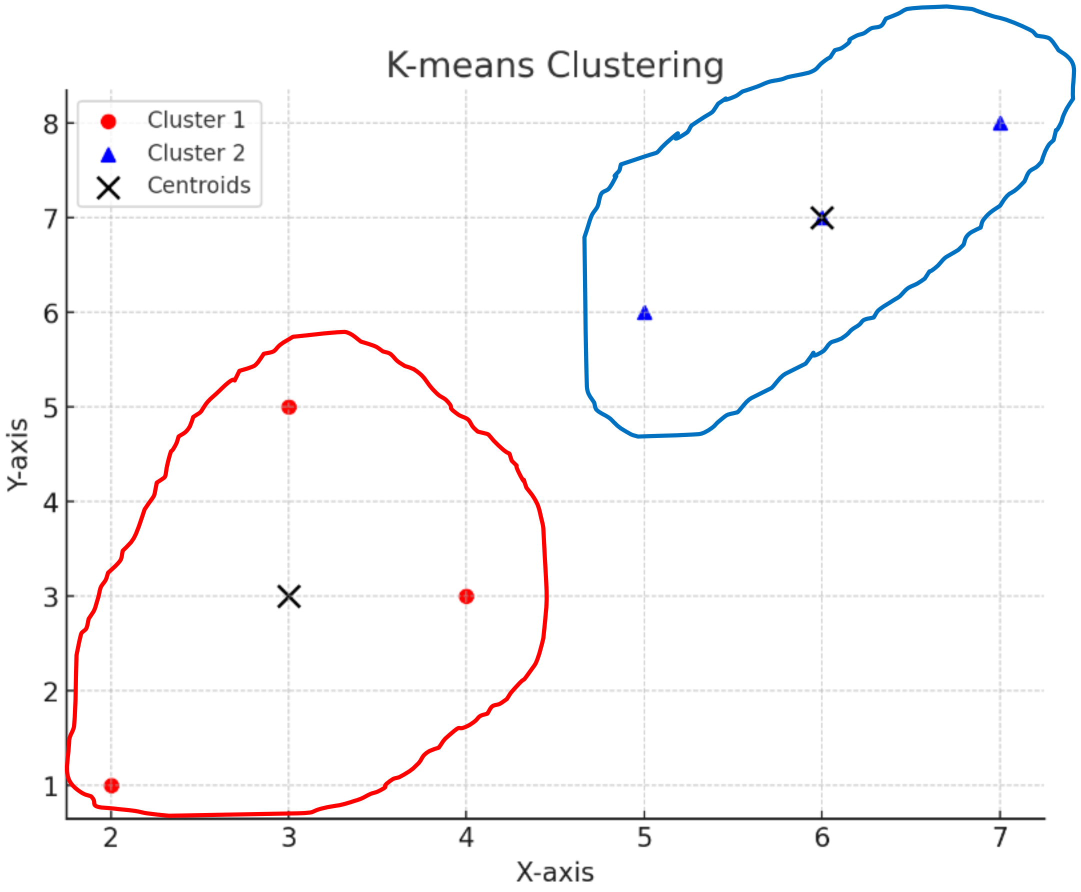
K-Means

Repeat Step-03: Update the each center as the mean of all the instances in the cluster.

- $\boldsymbol{Cluster\ 1:\ Points\ =\ (2,1),(3,5),(4,3)}$
  - $\boldsymbol{New\ Centroid\ 1\ =\left(\frac{2+3+4}{3},\frac{1+5+3}{3}\right)=(3,3)}$
- $\boldsymbol{Cluster\ 2:\ Points\ =\ (5,6),(6,7),(7,8)}$
  - $\boldsymbol{New\ Centroid\ 2\ =\left(\frac{5+6+7}{3},\frac{6+7+8}{3}\right)=(6,7)}$

Step-04: **the centers do not change anymore, stop.**

K-Means Results



Outline

- Unsupervised Learning
  - Clustering: KMeans
  - Dimensionality Reduction: PCA

PCA

- Consider the two dimensional patterns (2, 1), (3, 5), (4, 3), (5, 6), (6, 7), (7, 8).
- Compute the principal component using PCA Algorithm.

Steps of PCA Algorithm

- The steps involved in PCA Algorithm are as follows:
  - **Step-01:** Get data.
  - **Step-02:** Compute the mean vector (µ).
  - **Step-03:** Subtract mean from the given data.
  - **Step-04:** Calculate the covariance matrix.
  - **Step-05:** Calculate the eigen vectors and eigen values of the covariance matrix.
  - **Step-06:** Choosing components and forming a feature vector.
  - **Step-07:** Deriving the new data set.

PCA

Step-01:

Get data.

The given feature vectors are-

- $x_1 = (2, 1)$
- $x_2 = (3, 5)$
- $x_3 = (4, 3)$
- $x_4 = (5, 6)$
- $x_5 = (6, 7)$
- $x_6 = (7, 8)$

$$\begin{bmatrix} 2 \\ 1 \end{bmatrix} \begin{bmatrix} 3 \\ 5 \end{bmatrix} \begin{bmatrix} 4 \\ 3 \end{bmatrix} \begin{bmatrix} 5 \\ 6 \end{bmatrix} \begin{bmatrix} 6 \\ 7 \end{bmatrix} \begin{bmatrix} 7 \\ 8 \end{bmatrix}$$

PCA

<u>Step-02:</u>

Calculate the mean vector (μ).

Mean vector (μ)
= ((2 + 3 + 4 + 5 + 6 + 7) / 6, (1 + 5 + 3 + 6 + 7 + 8) / 6)
= (4.5, 5)

Thus, Mean vector (μ) = $\begin{bmatrix} 4.5 \\ 5 \end{bmatrix}$

PCA

Step-03:

Subtract mean vector (μ) from the given feature vectors.

- $x_1 - \mu = (2 - 4.5,\ 1 - 5) = (-2.5,\ -4)$
- $x_2 - \mu = (3 - 4.5,\ 5 - 5) = (-1.5,\ 0)$
- $x_3 - \mu = (4 - 4.5,\ 3 - 5) = (-0.5,\ -2)$
- $x_4 - \mu = (5 - 4.5,\ 6 - 5) = (0.5,\ 1)$
- $x_5 - \mu = (6 - 4.5,\ 7 - 5) = (1.5,\ 2)$
- $x_6 - \mu = (7 - 4.5,\ 8 - 5) = (2.5,\ 3)$

Feature vectors (x_i) after subtracting mean vector (μ) are:

$$\begin{bmatrix} -2.5 \\ -4 \end{bmatrix} \begin{bmatrix} -1.5 \\ 0 \end{bmatrix} \begin{bmatrix} -0.5 \\ -2 \end{bmatrix} \begin{bmatrix} 0.5 \\ 1 \end{bmatrix} \begin{bmatrix} 1.5 \\ 2 \end{bmatrix} \begin{bmatrix} 2.5 \\ 3 \end{bmatrix}$$

PCA

Step-04:

Calculate the covariance matrix.

Covariance matrix is given by-

$$\text{Covariance Matrix} = \frac{\Sigma(x_i - \mu)(x_i - \mu)^t}{n}$$

$$m_1 = (x_1 - \mu)(x_1 - \mu)^t = \begin{bmatrix} -2.5 \\ -4 \end{bmatrix} \begin{bmatrix} -2.5 & -4 \end{bmatrix} = \begin{bmatrix} 6.25 & 10 \\ 10 & 16 \end{bmatrix}$$

$$m_2 = (x_2 - \mu)(x_2 - \mu)^t = \begin{bmatrix} -1.5 \\ 0 \end{bmatrix} \begin{bmatrix} -1.5 & 0 \end{bmatrix} = \begin{bmatrix} 2.25 & 0 \\ 0 & 0 \end{bmatrix}$$

$$m_3 = (x_3 - \mu)(x_3 - \mu)^t = \begin{bmatrix} -0.5 \\ -2 \end{bmatrix} \begin{bmatrix} -0.5 & -2 \end{bmatrix} = \begin{bmatrix} 0.25 & 1 \\ 1 & 4 \end{bmatrix}$$

$$m_4 = (x_4 - \mu)(x_4 - \mu)^t = \begin{bmatrix} 0.5 \\ 1 \end{bmatrix} \begin{bmatrix} 0.5 & 1 \end{bmatrix} = \begin{bmatrix} 0.25 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$

$$m_5 = (x_5 - \mu)(x_5 - \mu)^t = \begin{bmatrix} 1.5 \\ 2 \end{bmatrix} \begin{bmatrix} 1.5 & 2 \end{bmatrix} = \begin{bmatrix} 2.25 & 3 \\ 3 & 4 \end{bmatrix}$$

$$m_6 = (x_6 - \mu)(x_6 - \mu)^t = \begin{bmatrix} 2.5 \\ 3 \end{bmatrix} \begin{bmatrix} 2.5 & 3 \end{bmatrix} = \begin{bmatrix} 6.25 & 7.5 \\ 7.5 & 9 \end{bmatrix}$$

Now,
Covariance matrix = $(m_1 + m_2 + m_3 + m_4 + m_5 + m_6) / 6$

On adding the m1~m6 and dividing by 6, we get:

$$\text{Covariance Matrix} = \frac{1}{6} \begin{bmatrix} 17.5 & 22 \\ 22 & 34 \end{bmatrix}$$

$$\text{Covariance Matrix} = \begin{bmatrix} 2.92 & 3.67 \\ 3.67 & 5.67 \end{bmatrix}$$

PCA

Step-05:

Calculate the eigen values and eigen vectors of the covariance matrix.

λ is an eigen value for a matrix M if it is a solution of the characteristic equation $|M - \lambda I| = 0$.

So, we have-

$$\begin{vmatrix} 2.92 & 3.67 \\ 3.67 & 5.67 \end{vmatrix} - \begin{vmatrix} \lambda & 0 \\ 0 & \lambda \end{vmatrix} = 0$$

$$\begin{vmatrix} 2.92 - \lambda & 3.67 \\ 3.67 & 5.67 - \lambda \end{vmatrix} = 0$$

From here,

$(2.92 - \lambda)(5.67 - \lambda) - (3.67 \times 3.67) = 0$

$16.56 - 2.92\lambda - 5.67\lambda + \lambda^2 - 13.47 = 0$

$\lambda^2 - 8.59\lambda + 3.09 = 0$

Solving this quadratic equation, we get $\lambda = 8.22, 0.38$

Thus, two eigen values are $\lambda_1 = 8.22$ and $\lambda_2 = 0.38$.

Clearly, the second eigen value is very small compared to the first eigen value.

So, the second eigen vector can be left out.

Eigen vector corresponding to the greatest eigen value is the principal component for the given data set.

So. we find the eigen vector corresponding to eigen value λ_1.

PCA

We use the following equation to find the eigen vector:

$$MX = \lambda X$$

where

- M = Covariance Matrix
- X = Eigen vector
- λ = Eigen value

Substituting the values in the above equation, we get-

$$\begin{bmatrix} 2.92 & 3.67 \\ 3.67 & 5.67 \end{bmatrix} \begin{bmatrix} X1 \\ X2 \end{bmatrix} = 8.22 \begin{bmatrix} X1 \\ X2 \end{bmatrix}$$

Solving these, we get:

$2.92X_1 + 3.67X_2 = 8.22X_1$

$3.67X_1 + 5.67X_2 = 8.22X_2$

On simplification, we get:

$5.3X_1 = 3.67X_2$ ………(1)

$3.67X_1 = 2.55X_2$ ………(2)

From (1) and (2), $X_1 = 0.69X_2$

From (2), the eigen vector is:

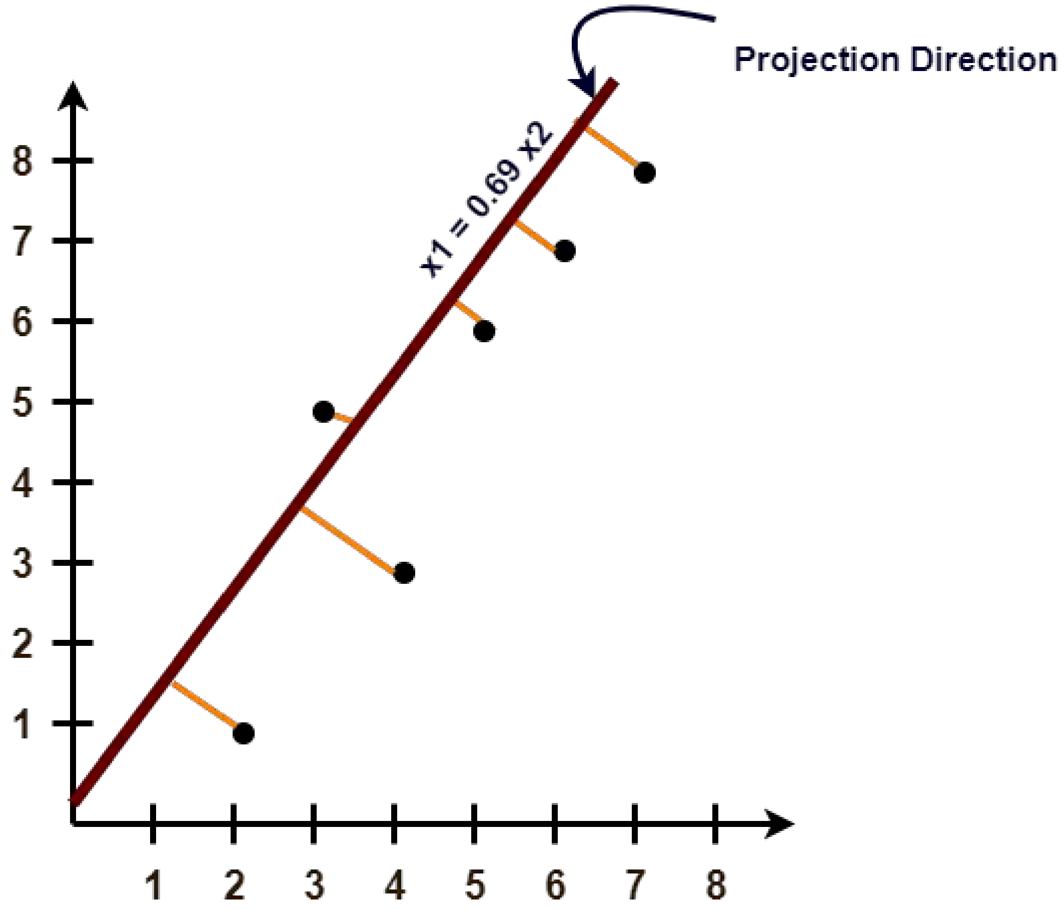
Eigen Vector : $\begin{bmatrix} X1 \\ X2 \end{bmatrix} = \begin{bmatrix} 2.55 \\ 3.67 \end{bmatrix}$

$X_1 = 0.69X_2$

Thus, principal component for the given data set is:

Principal Component : $\begin{bmatrix} X1 \\ X2 \end{bmatrix} = \begin{bmatrix} 2.55 \\ 3.67 \end{bmatrix}$

Lastly, we project the data points onto the new subspace as:



(2, 1) 2D

$$= \begin{bmatrix} 2.55 \\ 3.67 \end{bmatrix}^T \times \left(\begin{bmatrix} 2 \\ 1 \end{bmatrix} - \begin{bmatrix} 4.5 \\ 5 \end{bmatrix} \right)$$

$$= \begin{bmatrix} 2.55 & 3.67 \end{bmatrix} \times \begin{bmatrix} -2.5 \\ -4 \end{bmatrix}$$

$$= -21.055$$

-21.055 1D