Principal Component Analysis

Principal Component Analysis is an unsupervised learning algorithm that is used for the dimensionality reduction in machine learning. It is a statistical process that converts the observations of correlated features into a set of linearly uncorrelated features with the help of orthogonal transformation. These new transformed features are called the **Principal Components**. It is one of the popular tools that is used for exploratory data analysis and predictive modeling. It is a technique to draw strong patterns from the given dataset by reducing the variances.

PCA generally tries to find the lower-dimensional surface to project the high-dimensional data.

PCA works by considering the variance of each attribute because the high attribute shows the good split between the classes, and hence it reduces the dimensionality. Some real-world applications of PCA are ***image processing, movie recommendation system, optimizing the power allocation in various communication channels.*** It is a feature extraction technique, so it contains the important variables and drops the least important variable.

The PCA algorithm is based on some mathematical concepts such as:

Variance and Covariance

o   Eigenvalues and Eigen factors

Some common terms used in PCA algorithm:

o   **Dimensionality:** It is the number of features or variables present in the given dataset. More easily, it is the number of columns present in the dataset.

o   **Correlation:** It signifies that how strongly two variables are related to each other. Such as if one changes, the other variable also gets changed. The correlation value ranges from -1 to +1. Here, -1 occurs if variables are inversely proportional to each other, and +1 indicates that variables are directly proportional to each other.

o   **Orthogonal:** It defines that variables are not correlated to each other, and hence the correlation between the pair of variables is zero.

o   **Eigenvectors:** If there is a square matrix M, and a non-zero vector v is given. Then v will be eigenvector if Av is the scalar multiple of v.

o **Covariance Matrix:** A matrix containing the covariance between the pair of variables is called the Covariance Matrix.

Principal Components in PCA

As described above, the transformed new features or the output of PCA are the Principal Components. The number of these PCs are either equal to or less than the original features present in the dataset. Some properties of these principal components are given below:

o The principal component must be the linear combination of the original features.

o These components are orthogonal, i.e., the correlation between a pair of variables is zero.

o The importance of each component decreases when going to 1 to n, it means the 1 PC has the most importance, and n PC will have the least importance.

Steps for PCA algorithm

1. **Getting the dataset**
   Firstly, we need to take the input dataset and divide it into two subparts X and Y, where X is the training set, and Y is the validation set.

2. **Representing data into a structure**
   Now we will represent our dataset into a structure. Such as we will represent the two-dimensional matrix of independent variable X. Here each row corresponds to the data items, and the column corresponds to the Features. The number of columns is the dimensions of the dataset.

3. **Standardizing the data**
   In this step, we will standardize our dataset. Such as in a particular column, the features with high variance are more important compared to the features with lower variance.
   If the importance of features is independent of the variance of the feature, then we will divide each data item in a column with the standard deviation of the column. Here we will name the matrix as Z.

4. **Calculating the Covariance of Z**
   To calculate the covariance of Z, we will take the matrix Z, and will transpose it. After transpose, we will multiply it by Z. The output matrix will be the Covariance matrix of Z.

5. **Calculating the Eigen Values and Eigen Vectors**
   Now we need to calculate the eigenvalues and eigenvectors for the resultant covariance matrix Z. Eigenvectors or the covariance matrix are the directions of the axes with high information. And the coefficients of these eigenvectors are defined as the eigenvalues.

6. **Sorting the Eigen Vectors**
   In this step, we will take all the eigenvalues and will sort them in decreasing order, which means from largest to smallest. And simultaneously sort the eigenvectors accordingly in matrix P of eigenvalues. The resultant matrix will be named as P*.

7. **Calculating the new features Or Principal Components**
   Here we will calculate the new features. To do this, we will multiply the P* matrix to the Z. In the resultant matrix Z*, each observation is the linear combination of original features. Each column of the Z* matrix is independent of each other.

8. **Remove less or unimportant features from the new dataset.**
   The new feature set has occurred, so we will decide here what to keep and what to remove. It means, we will only keep the relevant or important features in the new dataset, and unimportant features will be removed out.

Applications of Principal Component Analysis

o PCA is mainly used as the dimensionality reduction technique in various AI applications such **as computer vision, image compression, etc.**

o It can also be used for finding hidden patterns if data has high dimensions. Some fields where PCA is used are Finance, data mining, Psychology, etc.

In pattern recognition, Dimension Reduction is defined as-

- It is a process of converting a data set having vast dimensions into a data set with lesser dimensions.
- It ensures that the converted data set conveys similar information concisely.
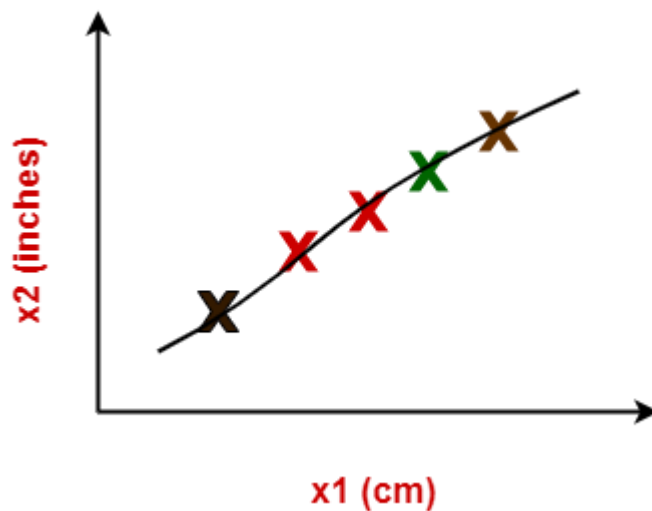
Example-

Consider the following example-

The following graph shows two dimensions x1 and x2.

x1 represents the measurement of several objects in cm.

x2 represents the measurement of several objects in inches.

In machine learning,

- Using both these dimensions convey similar information.
- Also, they introduce a lot of noise in the system.
- So, it is better to use just one dimension.

Using dimension reduction techniques-

- We convert the dimensions of data from 2 dimensions (x1 and x2) to 1 dimension (z1).
- It makes the data relatively easier to explain.


Benefits-

Dimension reduction offers several benefits such as-

- It compresses the data and thus reduces the storage space requirements.
- It reduces the time required for computation since less dimensions require less computation.
- It eliminates the redundant features.
- It improves the model performance.

Dimension Reduction Techniques-

The two popular and well-known dimension reduction techniques are-
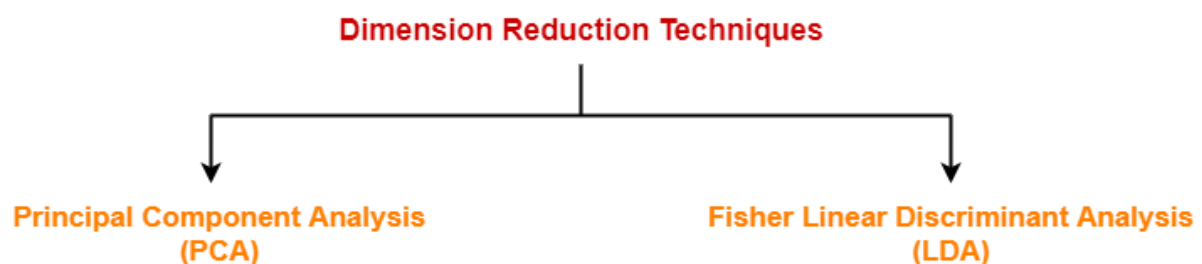
1. Principal Component Analysis (PCA)
2. Fisher Linear Discriminant Analysis (LDA)

In this article, we will discuss about Principal Component Analysis.

Principal Component Analysis-

- Principal Component Analysis is a well-known dimension reduction technique.
- It transforms the variables into a new set of variables called as principal components.
- These principal components are linear combination of original variables and are orthogonal.
- The first principal component accounts for most of the possible variation of original data.
- The second principal component does its best to capture the variance in the data.
- There can be only two principal components for a two-dimensional data set.

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.

PRACTICE PROBLEMS BASED ON PRINCIPAL COMPONENT ANALYSIS-

Problem-01:

Given data = { 2, 3, 4, 5, 6, 7 ; 1, 5, 3, 6, 7, 8 }.

Compute the principal component using PCA Algorithm.

OR

Consider the two dimensional patterns (2, 1), (3, 5), (4, 3), (5, 6), (6, 7), (7, 8).

Compute the principal component using PCA Algorithm.

OR

Compute the principal component of following data-

CLASS 1

$$X = 2 , 3 , 4$$

$$Y = 1, 5, 3$$

CLASS 2

$$X = 5, 6, 7$$

$$Y = 6, 7, 8$$

Solution-

We use the above discussed PCA Algorithm-

Step-01:

Get data.

The given feature vectors are-

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

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

Step-02:

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,

$$\text{Mean vector } (\mu) = \begin{bmatrix} 4.5 \\ 5 \end{bmatrix}$$

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-

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

Step-04:

Calculate the covariance matrix.

Covariance matrix is given by-

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

Now,

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

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

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

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

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

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

Now,

Covariance matrix

$= (m_1 + m_2 + m_3 + m_4 + m_5 + m_6) / 6$

On adding the above matrices and dividing by 6, we get-

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

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

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.

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), **X₁ = 0.69X₂**

From (2), the eigen vector is-

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

Thus, principal component for the given data set is-

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

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