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05-03-2021

LECTURE-59

HIERARCHICAL CLUSTERING:

Also called as Hierarchical cluster analysis, is an algorithm that groups similar objects into groups called clusters.

→ The endpoint is a set of clusters, where each cluster is distinct from each other cluster.

→ The objects with in each cluster are broadly similar to each other.

TYPES OF HIERARCHICAL CLUSTERING:

1. AGGLOMERATIVE CLUSTERING:

   - Also known as AGNES (Agglomerative Nesting).
   - It works in a bottom-up-manner.

2. DIVISIVE HIERARCHICAL CLUSTERING:

- Also known as DIANA (Divise Analysis)
- It works in a top-down manner.

NOTE:

- In Hierarchical clustering, one can stop at any number of clusters.
- One can find appropriate by interpreting the dendrogram.
- One can use median or mean as a cluster centre to represent each cluster.

∴ Hierarchical clusters (or) the hierarchy of clusters is represented as a dendrogram or tree structure.

* On top of the output obtained, we try to implement the K-Means IN INDUSTRY.

This algorithm works by grouping the data one by one on the basis of the nearest distance measured of all the pairwise distance between the data point

→ Again the distance between the data point is recalculated but which distance to consider when the groups has been performed.

To perform this, there are many methods available. They are

1. SINGLE - NEAREST DISTANCE (OR) SINGLE LINKAGE:

It is the shortest distance between the closest points of the clusteres.

2. COMPLETE - FARTHEST DISTANCE (OR) COMPLETE LINKAGE:

It is the farthest distance between the two points of the different clusteres.

* Complete linkage is one of the popular linkage methods as it forms tighter clusters than single-linkage.

3. AVERAGE - AVERAGE DISTANCE (OR) AVERAGE LINKAGE:

It is the distance between each pair of observations in each cluster are added up & divided by the number of pairs to get an average inter-cluster distance.

* Average linkage clus & complete linkage are the two most popular distance metrices in hierarchical clustering.

* Average linkage returns the value of the Arithematic mean.

4. CENTROID LINKAGE:

It is the distance between the centroids of two clusters.

* As the centroids move with new observation it is possible that the smaller clusters are more similar to the new larger cluster than to their individual clusters causing an inversion in the dendogram.

5. WAR'S LINKAGE METHOD:

It is to specify the distance between two clusters computed as the increase in the "Error Sum of Squares (ESS)" after fusing two clusters into a single cluster.

The purpose of them (linkages) is to find the distance.

→ So, these are called as Inter-cluster distance computation.

↳ this is the way we go on grouping the data until one cluster is formed.

* Now on the basis of dendogram graph we can calculate how many number of clusters should be actually present.

STEPS TO BE FOLLOWED TO PERFORM HIERARCHICAL CLUSTERING:

· Let $X = \{x_1, x_2, \ldots, x_n\}$ be the set of data points.

1. Begin with the disjoint clustering having level $L(0) = 0$ & sequence number $m = 0$.

2. Find the least distance pair of clusters

In the current clustering, say pair(r), (s) according to the d[(r),(s)] = min d[(i),(j)] where the minimum is over all pairs of clusters in current clustering

3. Increment the sequence number i.e.,

$m = m + 1$.

Merge clusters (r) & (s) into a single cluster to form the next clustering m. Set the level of this clustering to L(m) = d[(r),(s)].

4. Update the distance matrix D, by deleting the rows and columns corresponding to the clusters (r) & (s) & adding a row & column corresponding to the newly formed cluster.

Then, the distance between the new cluster denoted (r,s) and old Cluster(k) is defined

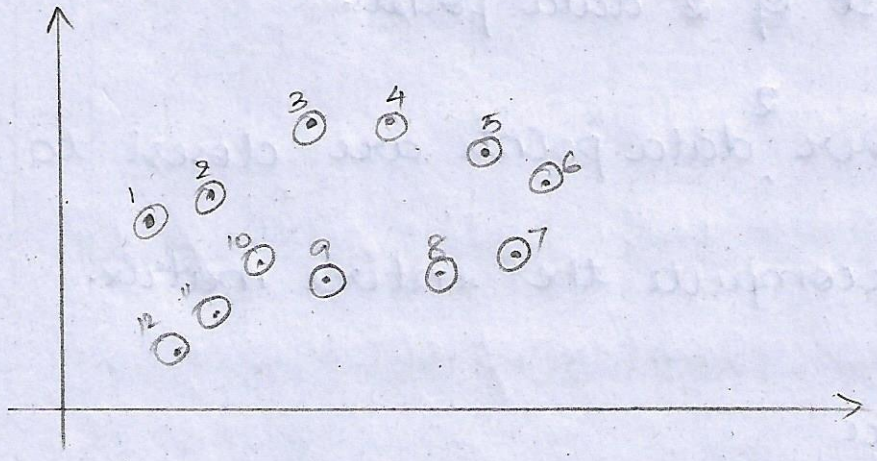
as $d[(k),(r,s)] = \min\left(d[(k),(r)], d[(k),(s)]\right)$.

5. If all the data points are in one cluster then stop else repeat from step 2.

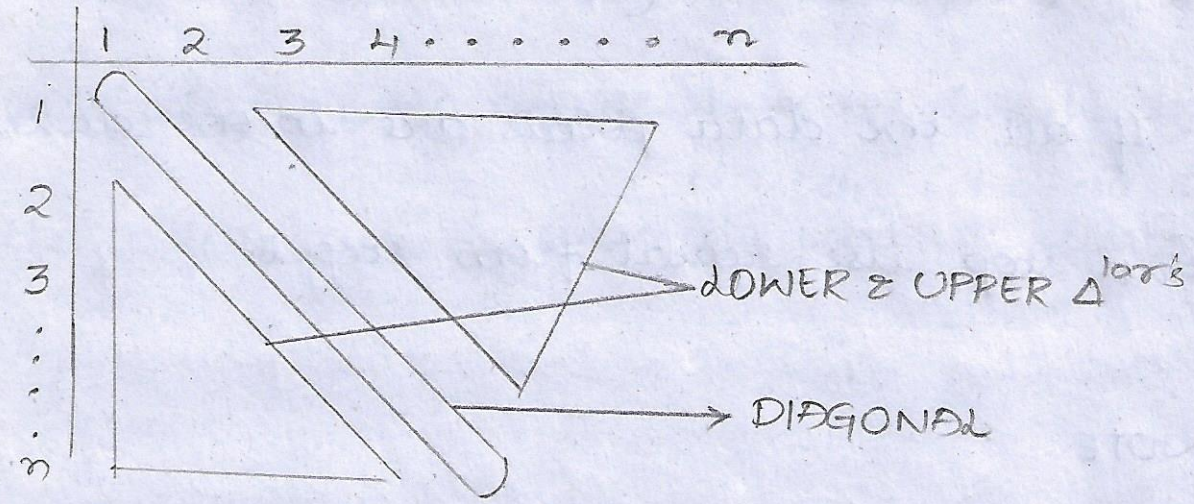
NOTE:

The Divise Hierarchical clustering is just the reverse of Agglomerative Hierarchical clustering.

TASK : TO cluster the data,



→ Now try to create a distance matrix and compute the distance matrix.



NOTE:

We will consider or take values from upper or lower triangular matrices

→ Always try to pick the lower value from the closest of 2 data points.

→ Which ever 2 data points are closest to the cluster, recompute the entire matrix.

SO, overhere

↳ Computing distance matrix is very complex.

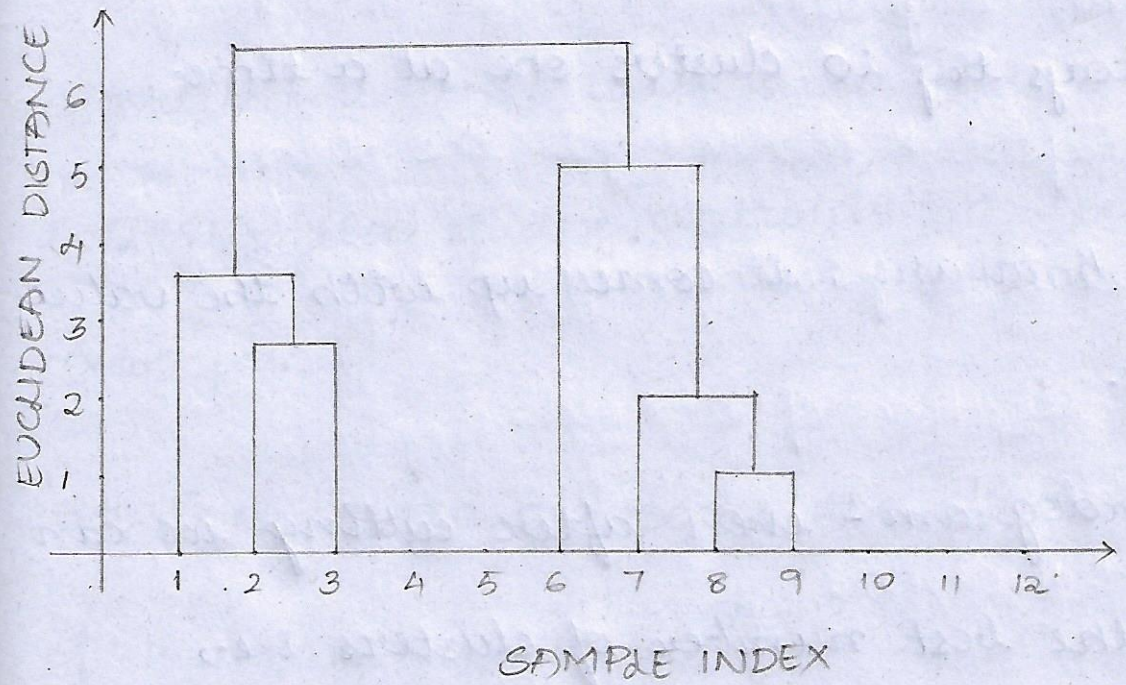
↳ We should be aware of the linkage.

↳ Dendogram is also considered.

DENDOGRAM :

A dendogram is a type of tree diagram showing the hierarchical relationships between different sets of data.

→ So, just by looking at the Dendogram we can tell how the clusters are formed.



NOTE :

→ Distance between the data points represents the dissimilarities.

→ Height of the blocks represents the distance between clusters.

↳ We can cut the dendogram tree with a horizantal line at a height where the line can ~~traverse~~ traverse the maximum distance up & down without intersecting the merging point.

→ Always try to cluster one at a time.

* In K-means ; it comes up with the value of K.

* Dendogram - even after cutting we can see the best number of clusters i.e., allocating the objects to the clusters.

K-MEANS:

The main objective of k-means algorithm is to minimize the sum of distances between the points and their respective cluster centroid.

DRAWBACK:

The only one disadvantage of k-means algorithm is that it is sensitive to the initialization of the centroids (or) the mean points.

So, inorder to overcome the draw back of k-means we use k-means++.

K-MEANS++:

This algorithm ensures a smarter initialization of the centroids and improve the quality of the clustering.

*→ Apart from initialization, the rest of the algorithm is the same as the standard K-means algorithm.

→ Therefore, K-means++ is the standard K-means algorithm coupled with a smarter initialization of centroids.

STEPS INVOLVED:

1. Randomly select the first centroid from the data points.

2. For each data point compute its distance from the nearest, previously choosen

centroid.

3. Select the next centroid from the data points such that the probability of choosing a point as centroid is directly proportional to its distance from the nearest, previously chosen centroid.

i.e.,

the point having maximum distance from the nearest centroid is most likely to be selected next as a centroid.

4. Repeat steps 2 and 3 until 'k' centroids have been sampled.

PRINCIPAL COMPONENT ANALYSIS (PCA):

It is an unsupervised, non-parametric statistical technique primarily used for dimensionality reduction of large data sets, by transforming a large set of variables into a smaller one that still contains most of the information in the large set in machine learning.

→ PCA can also be used to filter noisy data sets, such as image compression.

WHEN IS PCA USED?

PCA forms the basis of multi-variate data analysis based on projection methods.

→ The most important use of PCA is to

represent a multivariate data table as smaller set of variables (summary indices) in order to observe trends, jumps, clusters and outliers.

→ So, by creating new uncorrelated variables that successively maximize the variance.

USES OF PCA :

PCA

VISUALIZATION

↓

- 1D, 2D, 3D

- If it is in 4D, we need to check the pairplot

then ↓ convert From 4D ↔ 2D

↓

Then it is easy

FEATURE SELECTION

↓

- Instead of using "RFE", we can use PCA feature selection

↓

- Then these will be transformed to the features.

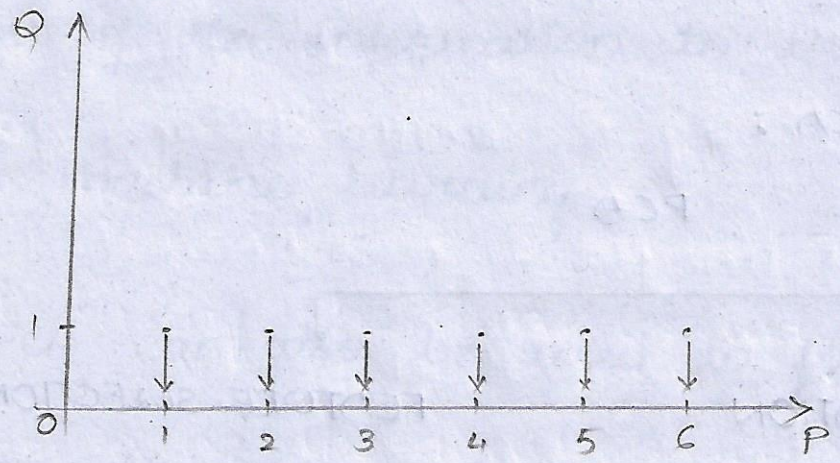
Example:

P	1	2	3	4	5.3	.....
Q	1	1	1	1	1	 1

In the above data,

P → CONTINUOUS , Q → DISCRETE

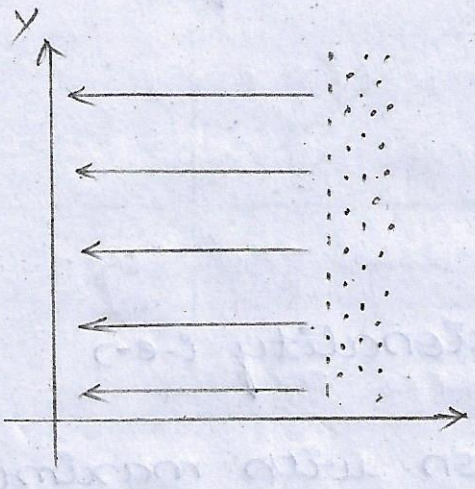
If we try to plot the data, then



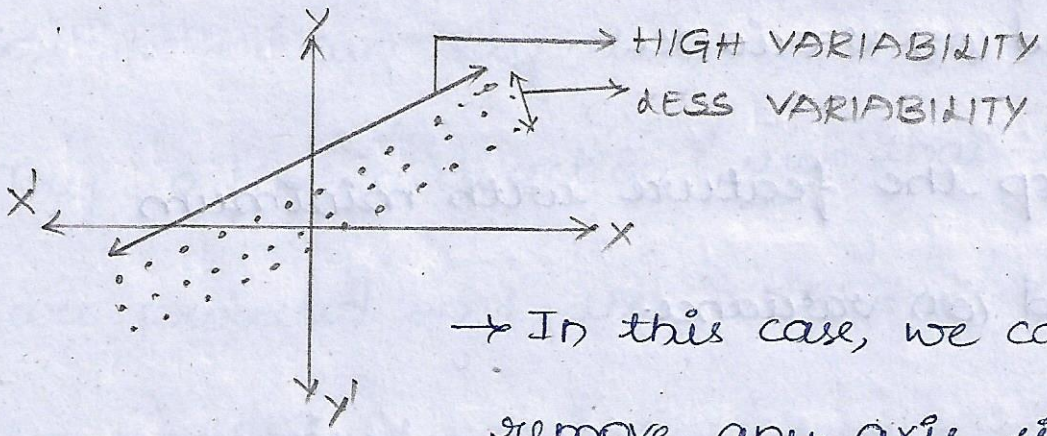
So, As there is no information in Q column, we can drop the column since it is constant. i.e., no variance (zero spread) in the data.

→ As we are dropping down the data i.e., 9 column, now it is reduced & the dimension is 1D after reducing.

→ So, from the above graph we can say that the data is projected only towards the x-axis.

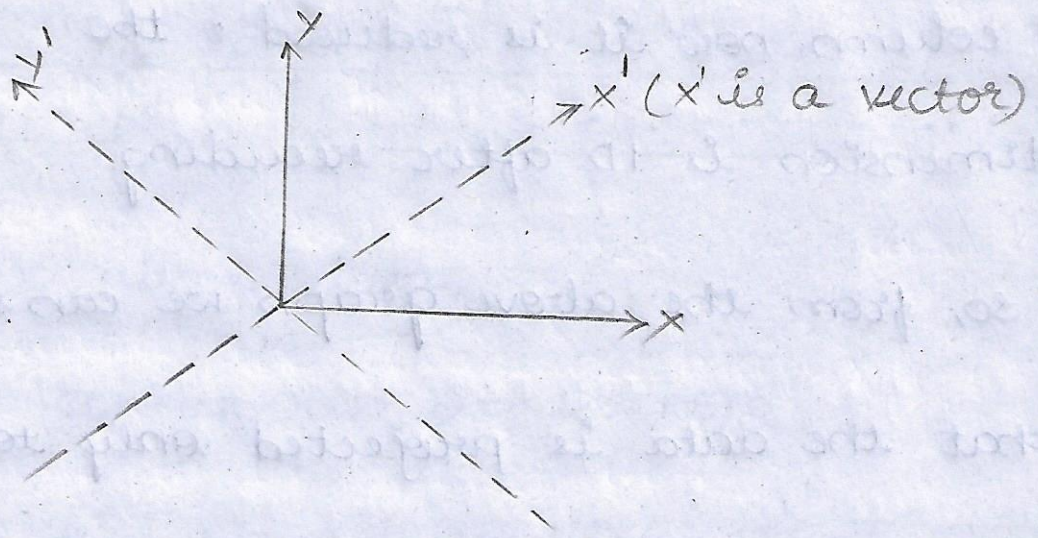


→ In this case, we have variability in x-axis, but its less. Most of the variance is explained by y-axis.



→ In this case, we can't remove any axis since there is an equal spread.

In such cases, try to rotate the axis, then



Now simply drop the Y-axis after the transformation.

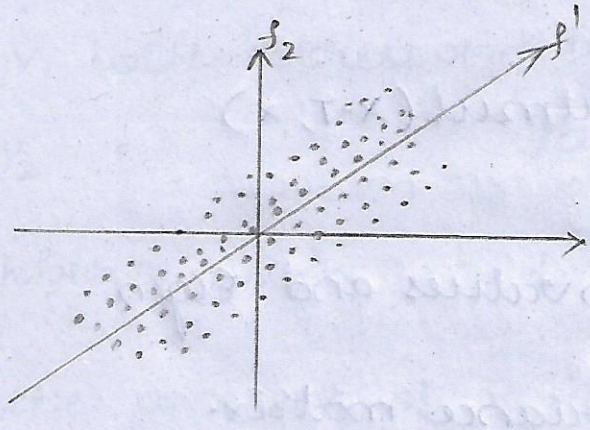
So, In PCA;

→ Reducing the dimensionality i.e.,
Preserving the direction with maximum spread (or) variance

→ Drop the feature with minimum spread (or) variance.

HOW DO PCA SELECT FEATURES?

The basic idea when using PCA as a tool for feature selection is "to select variables according to the magnitude i.e., & from largest to smallest in absolute values of their coefficients.



→ TASK: Try to find that direction where the variance is maximized and simply drop the least variance.

So, now we can say that,

Try to find a direction f' such that if x_i's are projected on f', the variance should be maximized.

⇒ x'_i = Project x_i's on f' i.e., we get new data points

$\Rightarrow$ Try to max.{variance($proj_f x_i$)}

STEPS INVOLVED IN PCA:

1. Standardize (or) Normalize the data.

2. Calculate the covariance matrix for the features in the dataset i.e.,

$$X^T \cdot X = S_{d \times d}$$

In Numpy - np.matmul(X.T, X)

3. Calculate the Eigen values and Eigen vectors for the covariance matrix.

so, if we have dxd covariance matrix then,

Eigen vectors — $V_1, V_2, \ldots\ldots, V_d$

Eigen values — $\lambda_1, \lambda_2, \ldots\ldots, \lambda_d$

4. Sort the eigen values and their corresponding eigen vectors.

$\Rightarrow \lambda_1 \geq \lambda_2 \geq \cdots\cdots\cdots \geq \lambda_d$

So, whenever we have a matrix, we get the vectors, i.e., it gives all the vectors which are orthogonal ($\perp$ or).

→ If we keep eigen values sorted then,

V_1 will correspond to the max. variance.

V_2 " " to the 2nd " "

where $\lambda_1, \lambda_2 \cdots \lambda_d$ are basically give the amount of variance explained by $V_1, V_2, \cdots, V_d$.

∴ We can say that, In real world application, Eigen values & Eigen vectors tells the maximum variance in the data.

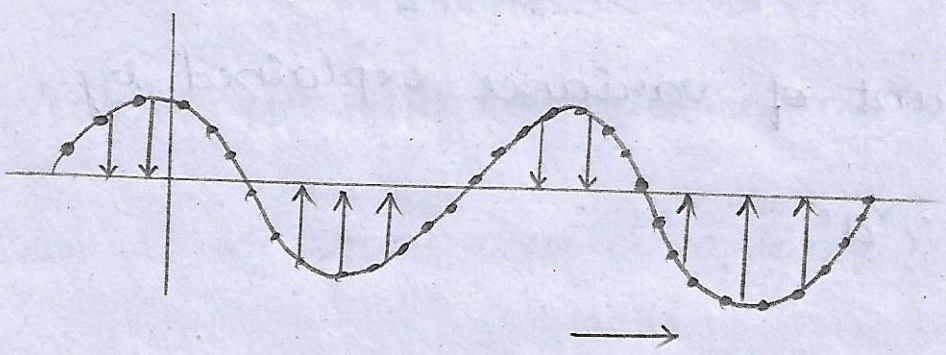
So, 90% of the variance is to preserved; then we try to summate i.e.,

We reduce d to 4d

$$\Rightarrow X_{n \times d} \xrightarrow{PCA} X'_{n \times d'} \text{ where } d' = = d.$$

5. Pick 'K' eigen values and form a matrix of eigen vectors.

6. Transform the original matrix.



In the above case,

If we try to implement PCA,

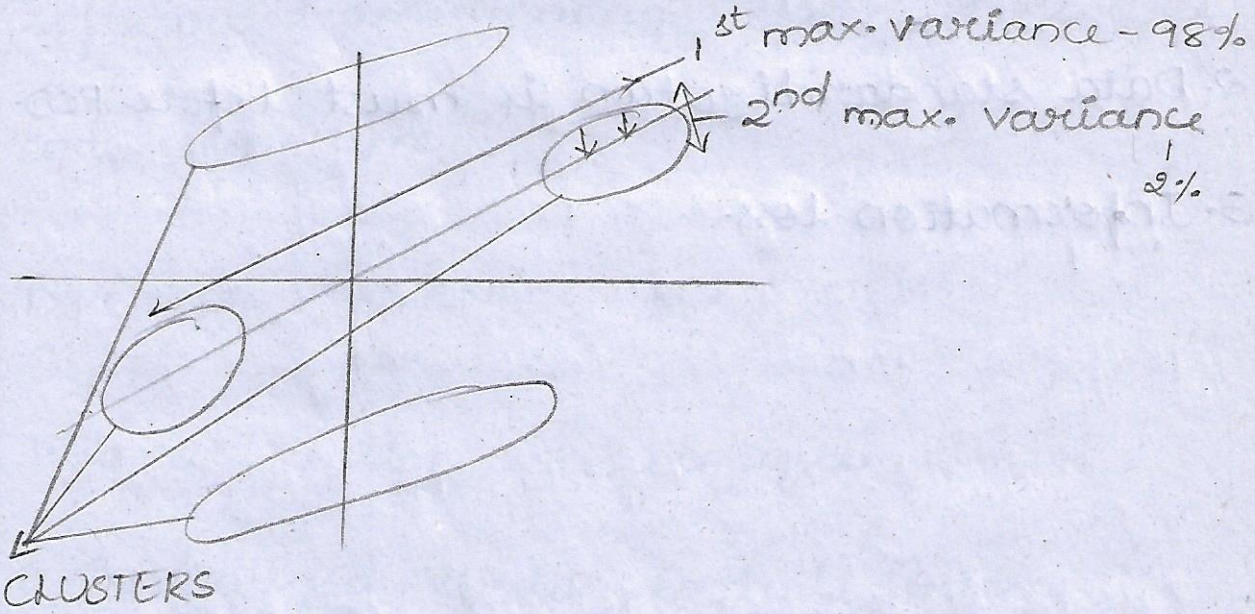
* 1st variance is on x-axis & 2nd variance on y-axis.

So, we project on X-axis and remove Y-axis.

→ then the output is

⇒ X-axis has 98% variance and Y-axis has 2% variance.

We lost the pattern by doing PCA; we removed some information.



In the above case, here we mixed 2 clusters i.e., we missed the cluster information if we perform PCA.

ADVANTAGES OF PCA :

1. Removes correlated features.
2. Improves Algorithm performance.
3. Reduces Overfitting
4. Improves visualization.

DISADVANTAGES OF PCA :

1. Independent variables become less interpretable.
2. Data standardization is must before PCA.
3. Information loss.