An Introduction to Machine Learning with Python Programming
11 Sep 2023 - 20 Oct 2023

Conducted by:
iHUB Divya Sampark, IIT Roorkee
and
Ritvij Bharat Private Limited (RBPL)

Choosing a K Value

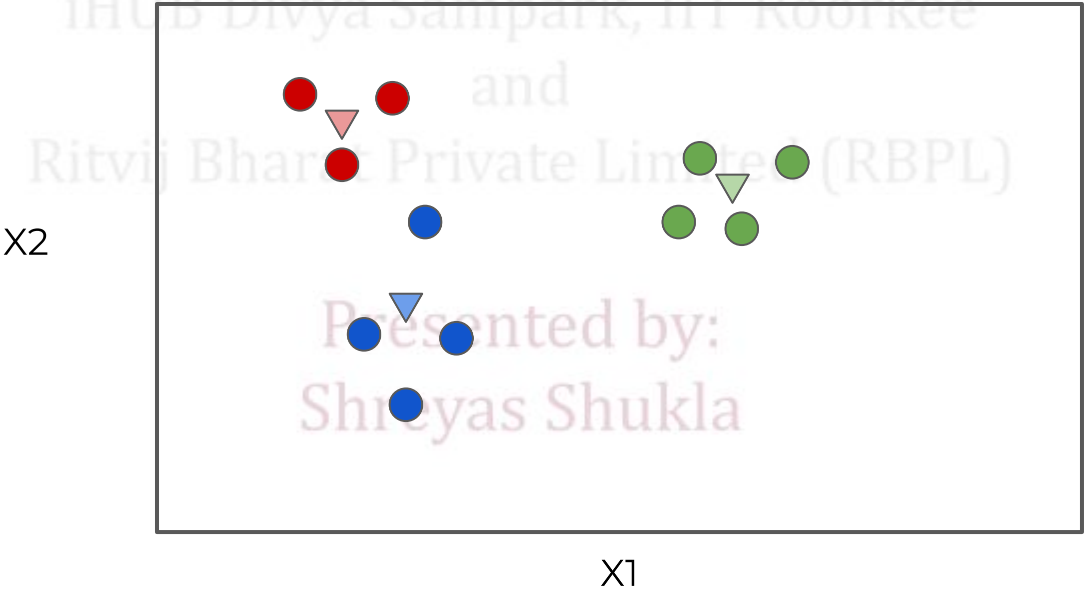
Presented by:
Shreyas Shukla

fig ref: pierian data

Recall our previous considerations:

- How do we choose a reasonable K value?
- Is there any way we can evaluate how good our current K value is at determining clusters?

3 clusters here, how to measure “goodness of fit”? We could measure the sum of the distances from points to cluster centers.



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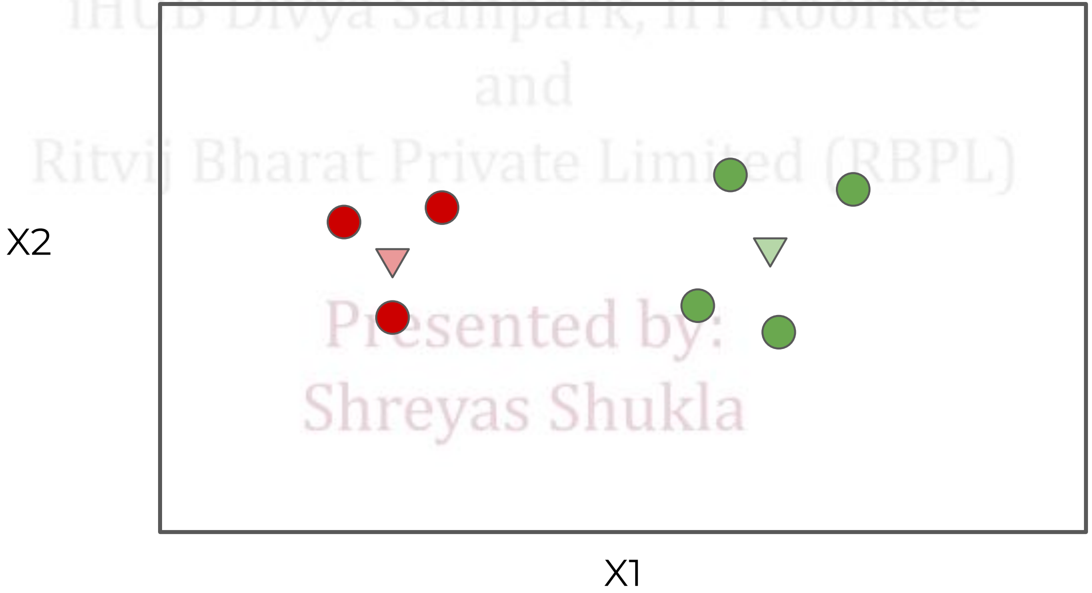
Imagine a simple example starting with K=2.
We measure the sum of the squared distances from points to the cluster center
Then we fit an entirely new KMeans model with K+1



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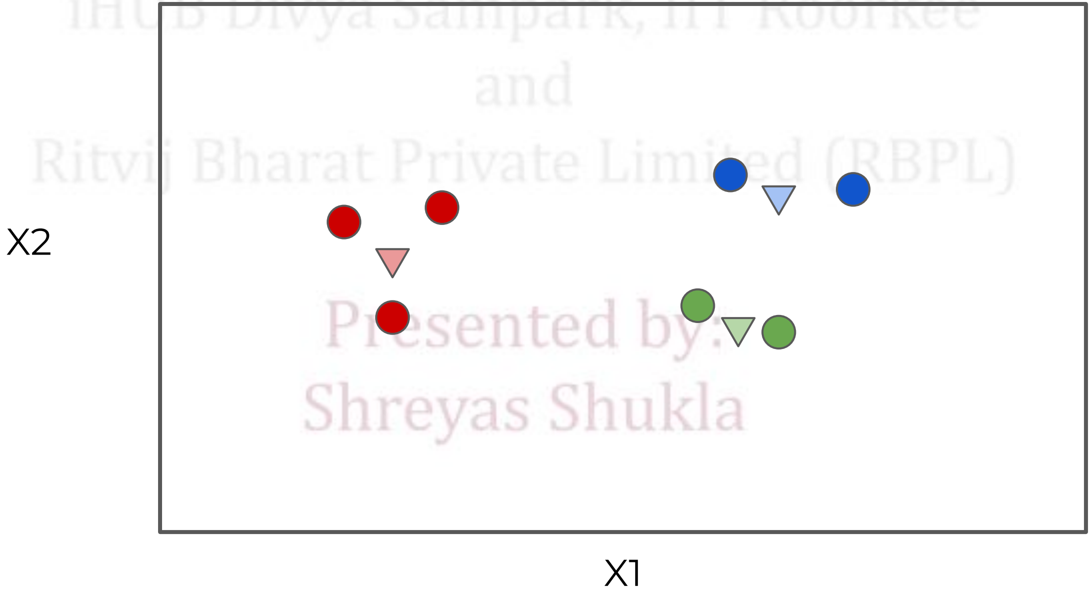
- Then we fit an entirely new KMeans model with K+1
- Then measure again the sum of the squared distance (SSD) to center.
- In theory this SSD would go to zero once K is equal to the number of points.



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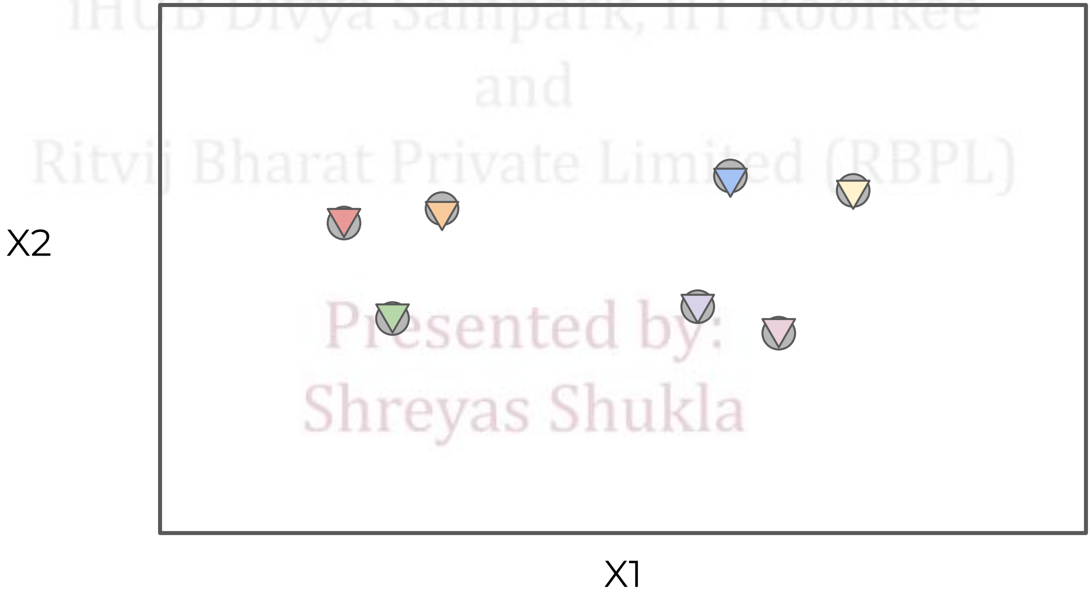
You would have a cluster for each point! SSD would be perfect at 0!



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- Keep track of this SSD value for a range of different K values.
- Then, look for a K value where **rate of reduction in SSD** begins to decline.
- This signifies that adding an extra cluster is **not** obtaining enough clarity of cluster separation to justify increasing K.
- This is known as the “elbow” method since we will track where decrease in SSD begins to flatten out compared to increasing K values.

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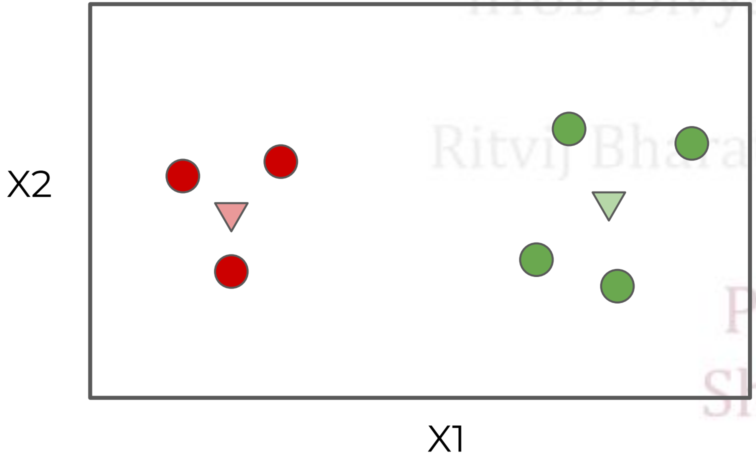
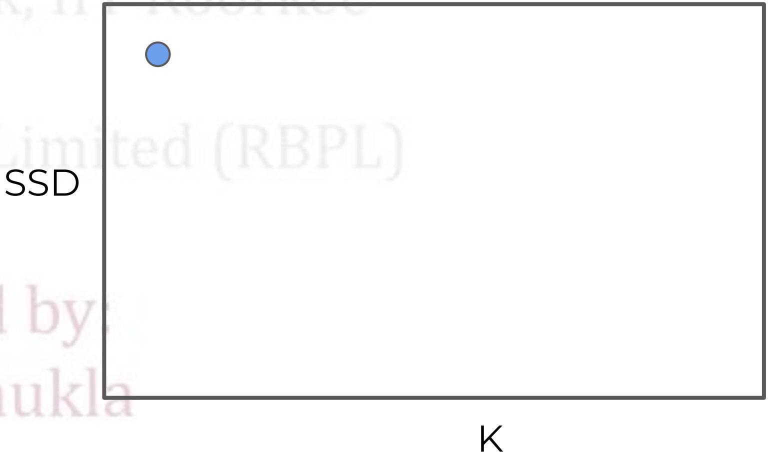
Start with K=2:





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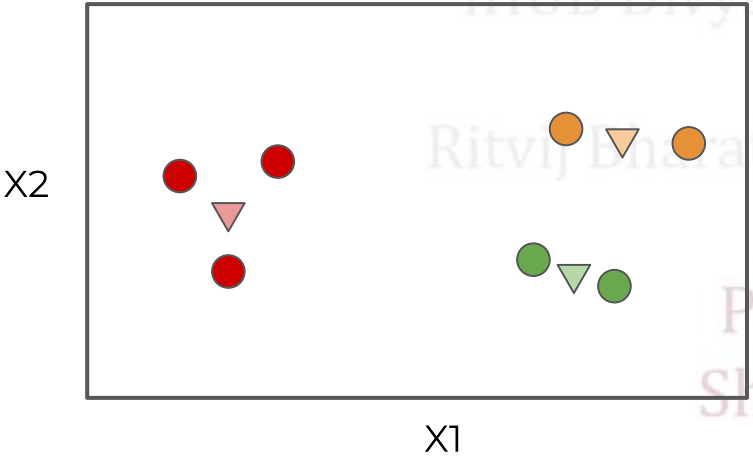
Increase K and measure SSD:



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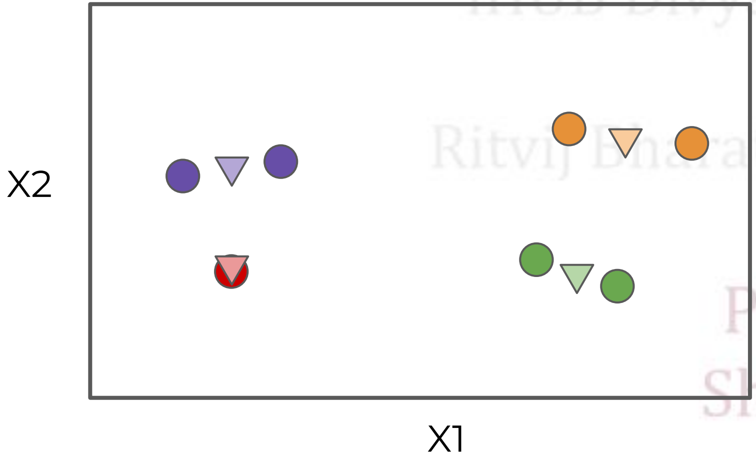
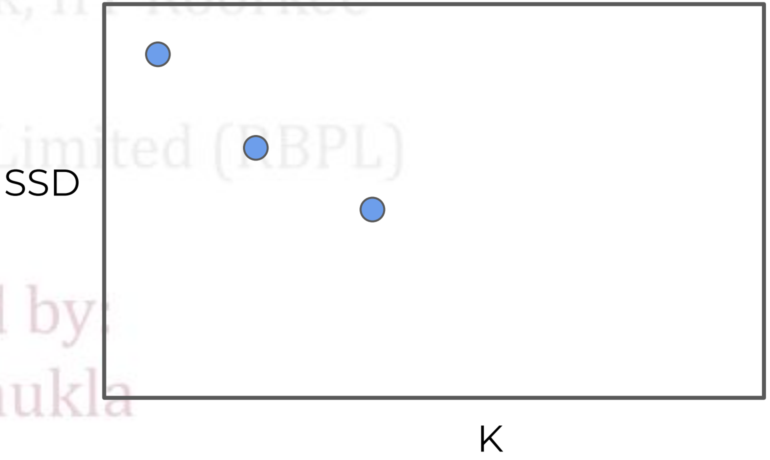
Increase K and measure SSD:





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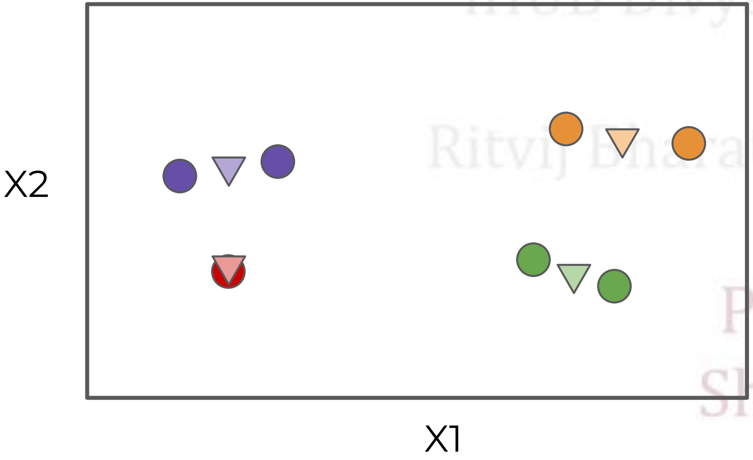
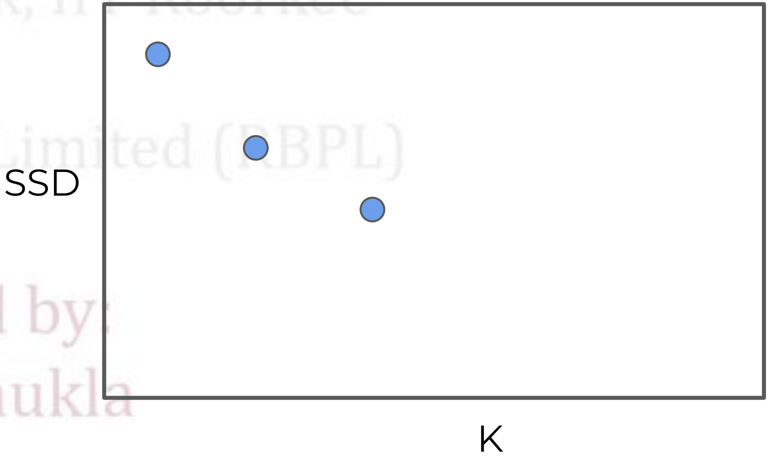
Repeat for some set number of K values:





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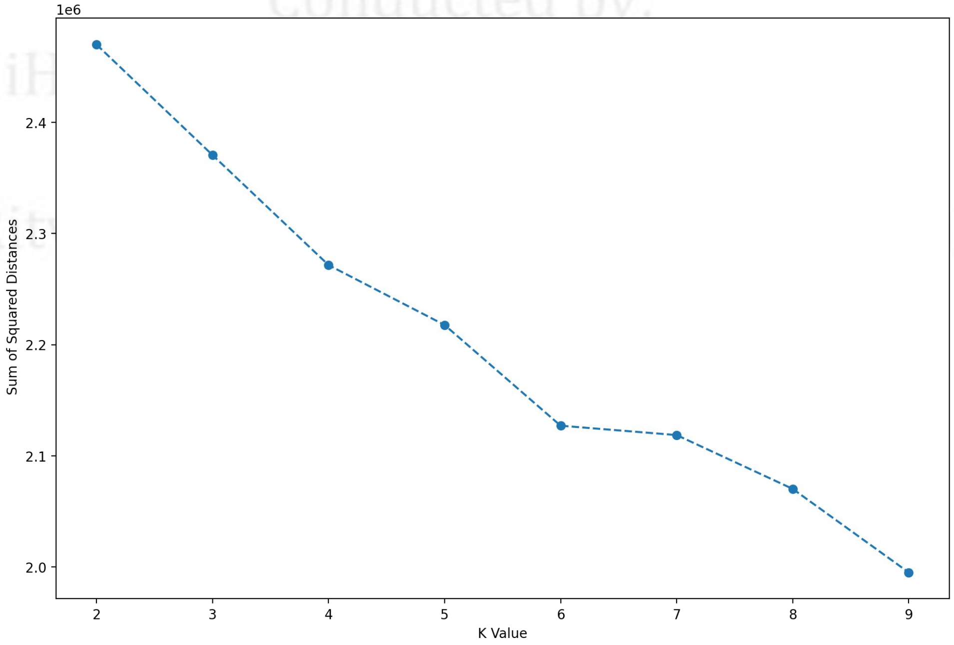
Notice continuous decline.



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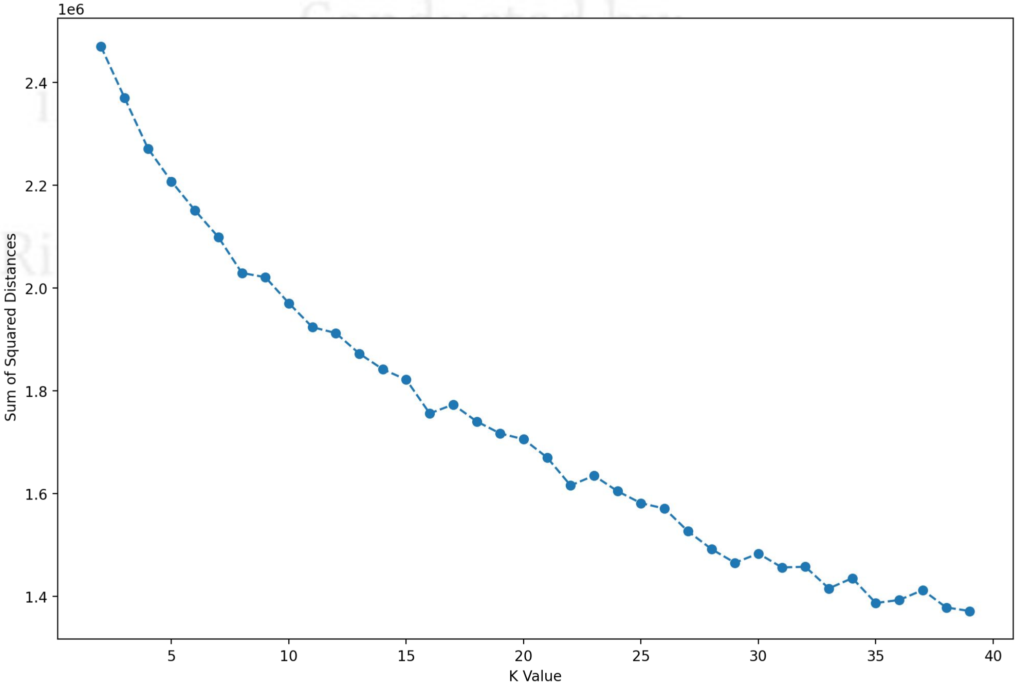
Eventually you will see “elbow” points:



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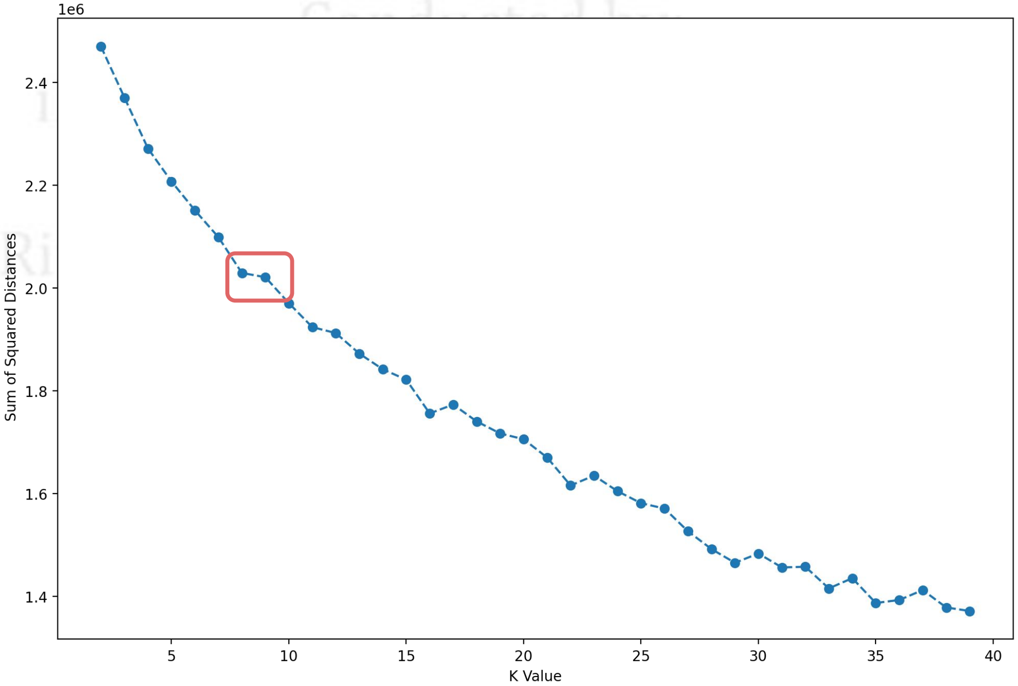

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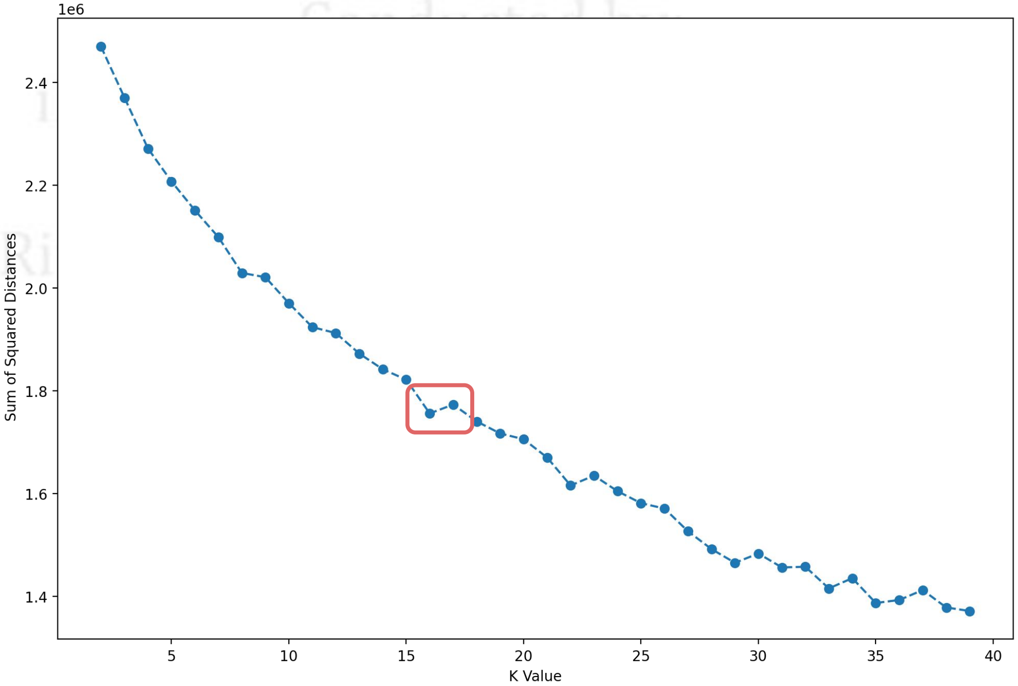

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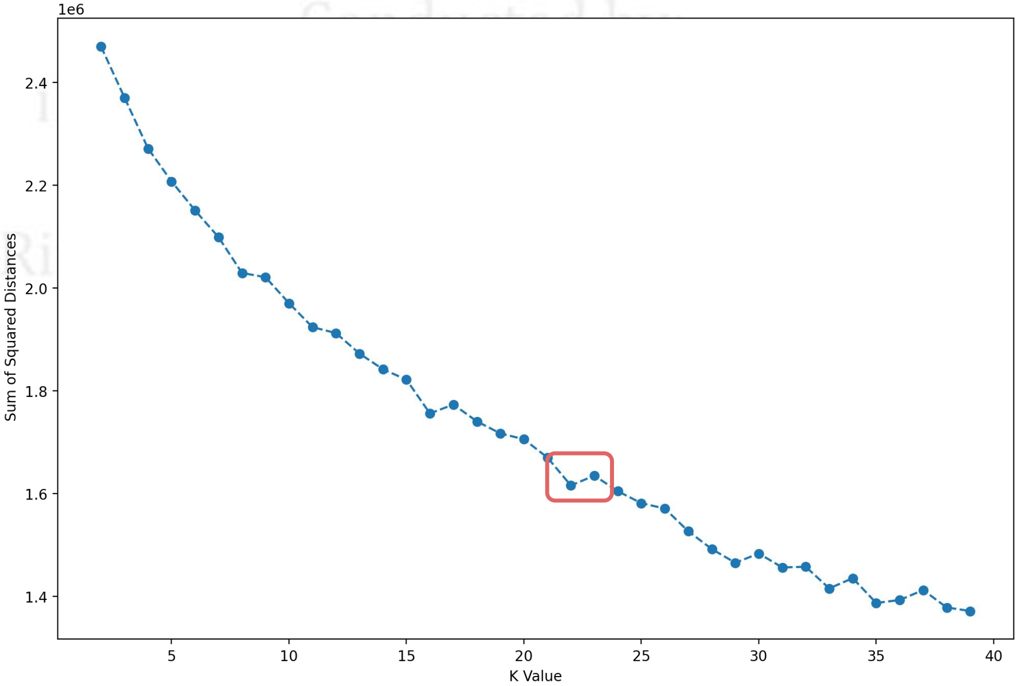

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These points are strong indicators that increasing K further is no longer justified as it is not revealing more “signal”.

Let’s explore this further with code

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Hierarchical Clustering

Conducted by:

and

Presented by:
Shreyas Shukla

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Hierarchical clustering is very common in biology and lends itself nicely to visualizing clusters.

It can also help the user decide on an appropriate number of clusters.

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Overview

1. *Theory and Intuition*
2. *Coding*

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Theory and Intuition

Presented by:
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Like most clustering algorithms, Hierarchical Clustering simply relies on measuring which data points are most “similar” to other data points.

“Similarity” is defined by choosing a distance metric.

Benefits of Hierarchical Clustering

- Easy to understand and visualize.
- Helps users decide how many clusters to choose.
- Not necessary to choose cluster amount **before** running the algorithm.

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So why use Hierarchical Clustering?

- Divides points into ***potential*** clusters:

fig ref: pierian data

So why use Hierarchical Clustering?

- Divides points into ***potential*** clusters:
  - Agglomerative Approach:
    - Each point begins as its own cluster, then clusters are joined.
  - Divisive Approach:
    - All points begin in the same cluster, then clusters are split.

fig ref: pierian data

Agglomerative:

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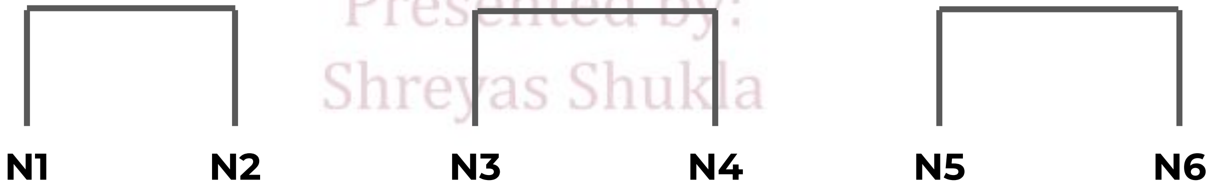
Agglomerative:



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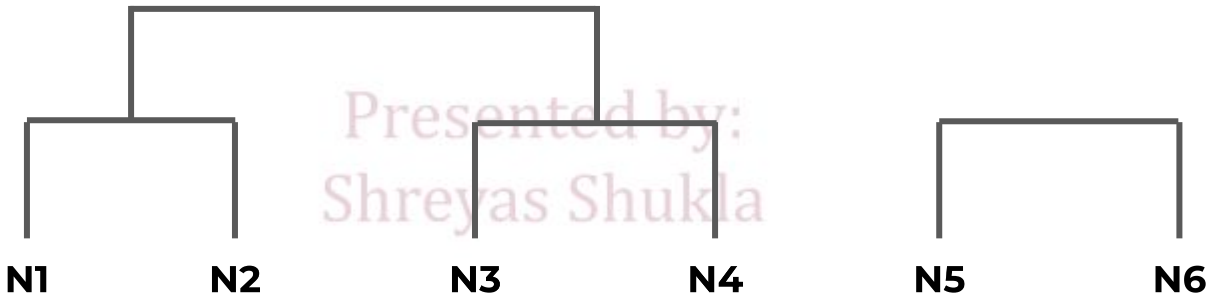
Agglomerative:



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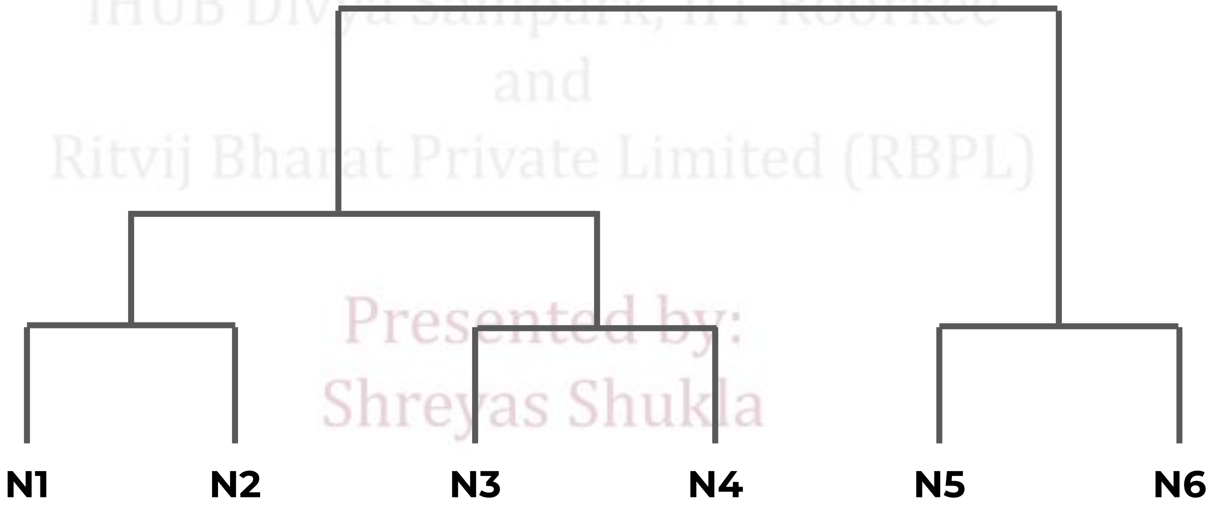
Agglomerative:



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Opposite of the Agglomerative approach is a **Divisive** approach, which starts with all points belonging to the same cluster, and the begins divisions to separate out clusters.

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Hierarchical Clustering Process

- Compare data points to find most similar data points to each other.
- Merge these to create a cluster.
- Compare clusters to find most similar clusters and merge again.
- Repeat until all points in a single cluster.

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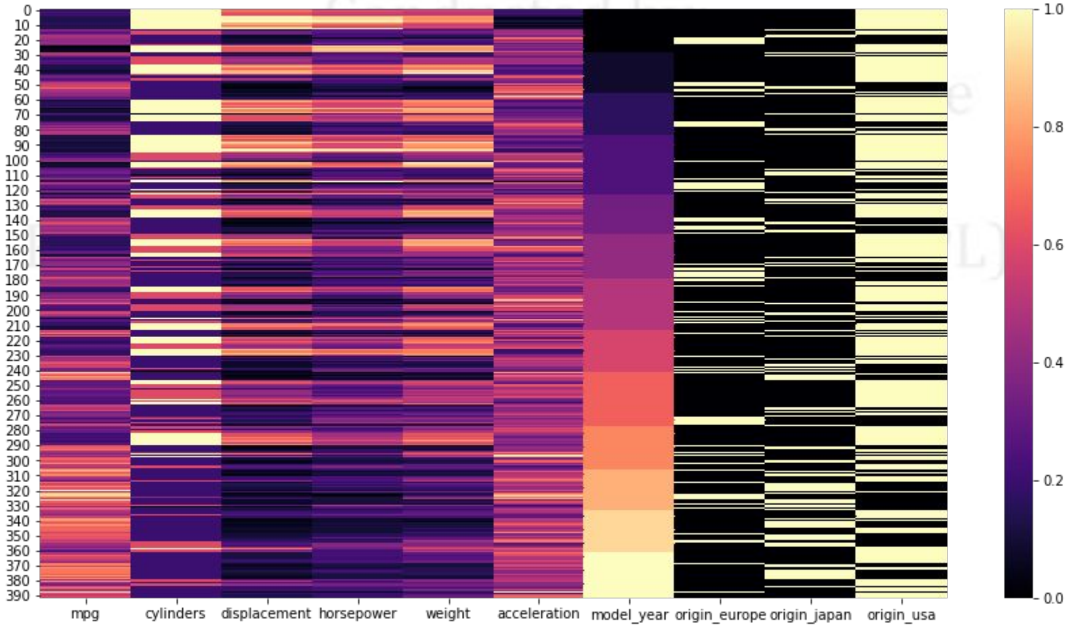
Hierarchical Clustering Process



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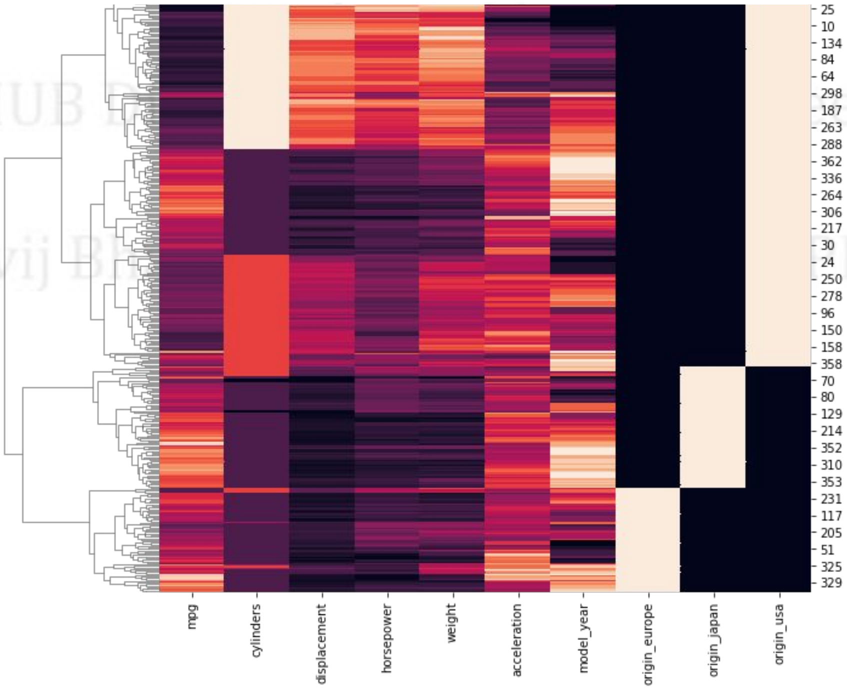
Hierarchical Clustering Process



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Topics which we still need to understand for Hierarchical Clustering:

- Similarity Metric
- Dendrogram
- Linkage Matrix

fig ref: pierian data

Similarity Metric

Measures distance between two points.

Many types:

- Euclidean Distance
- Manhattan
- Cosine
- and many more...

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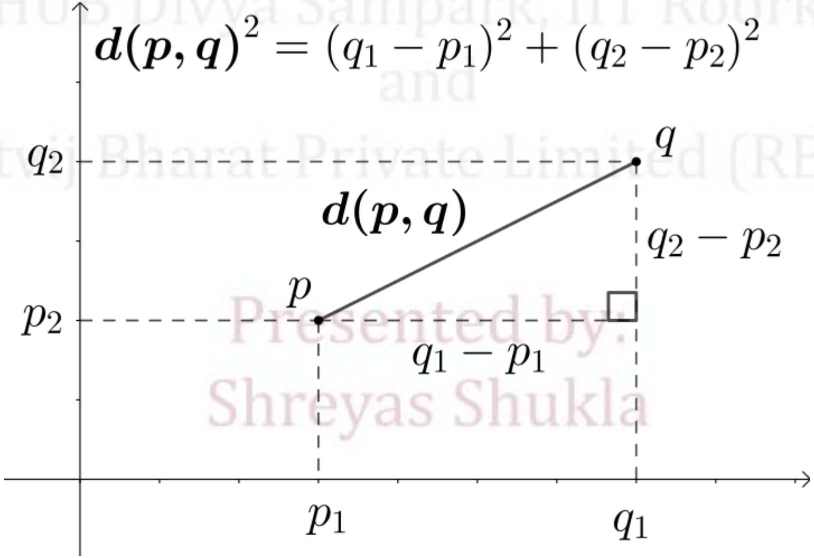
Similarity Metric

Default choice is Euclidean



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Similarity Metric

- Each dimension would be a feature
- For **n** data points and **p** features:
  - $D^2 = (x_{11} - x_{12})^2 + \ldots + (x_{n-1p-1} - x_{np})^2$

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Similarity Metric

- Each dimension would be a feature
- For **n** data points and **p** features:
  - $D^2 = (x_{11} - x_{12})^2 + \dots + (x_{n-1p-1} - x_{np})^2$
- Using MinMaxScaler we can scale all features to be between 0 and 1.
- This allows for maximum distance between a feature to be 1.

fig ref: pierian data

Dendrogram:

- Plot displaying all potential clusters.
- Very computationally expensive to compute and display for larger data sets.
- Very useful for deciding on number of clusters.

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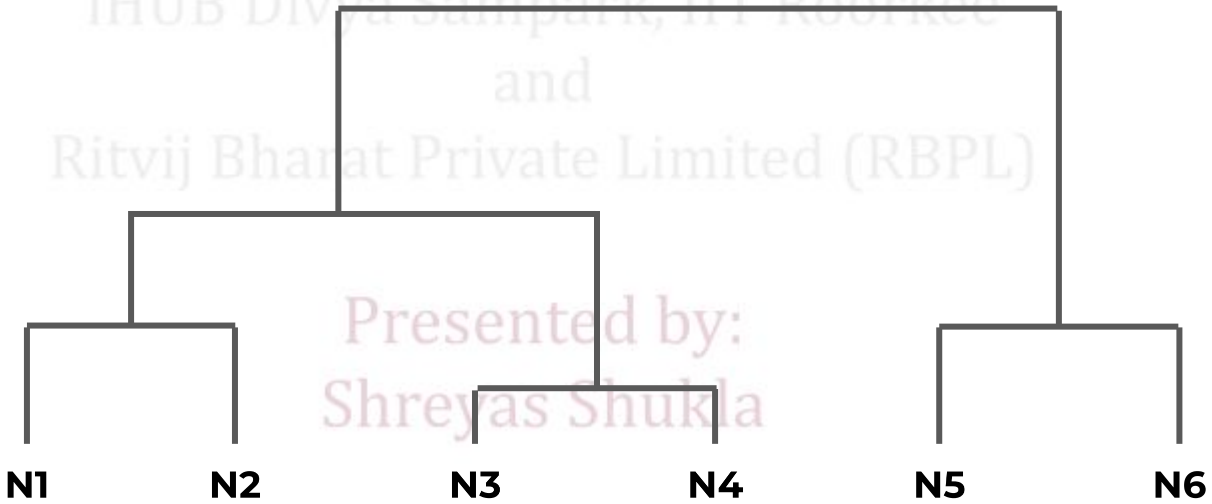
Dendrogram:



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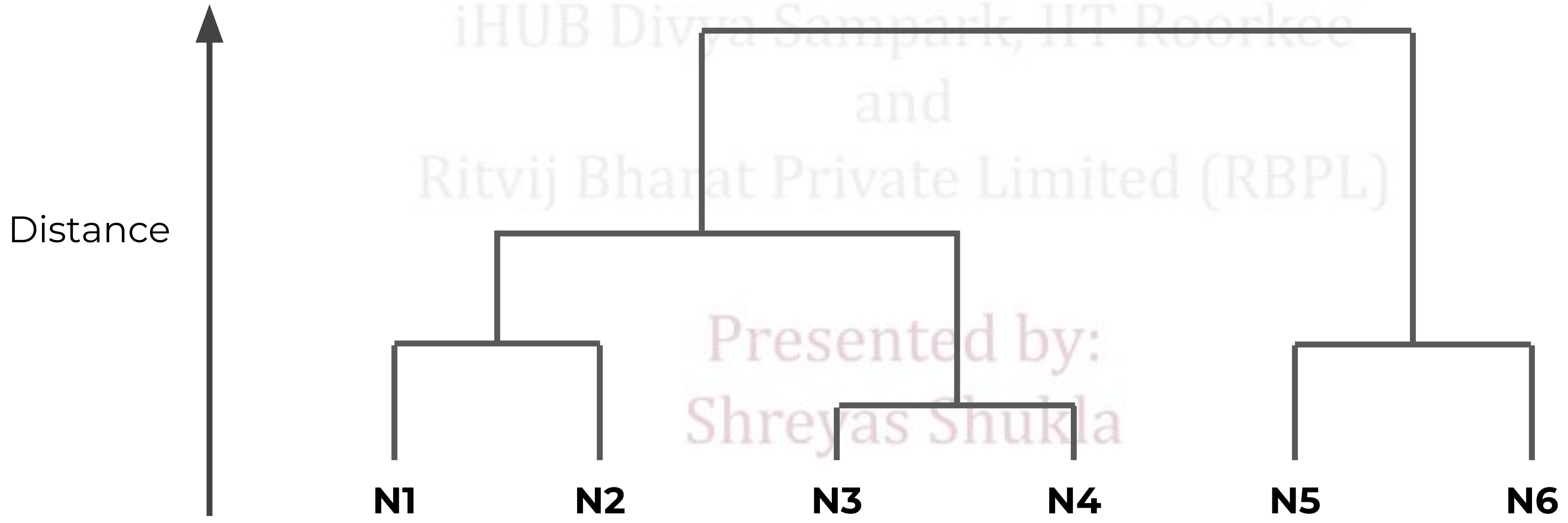
Dendrogram:



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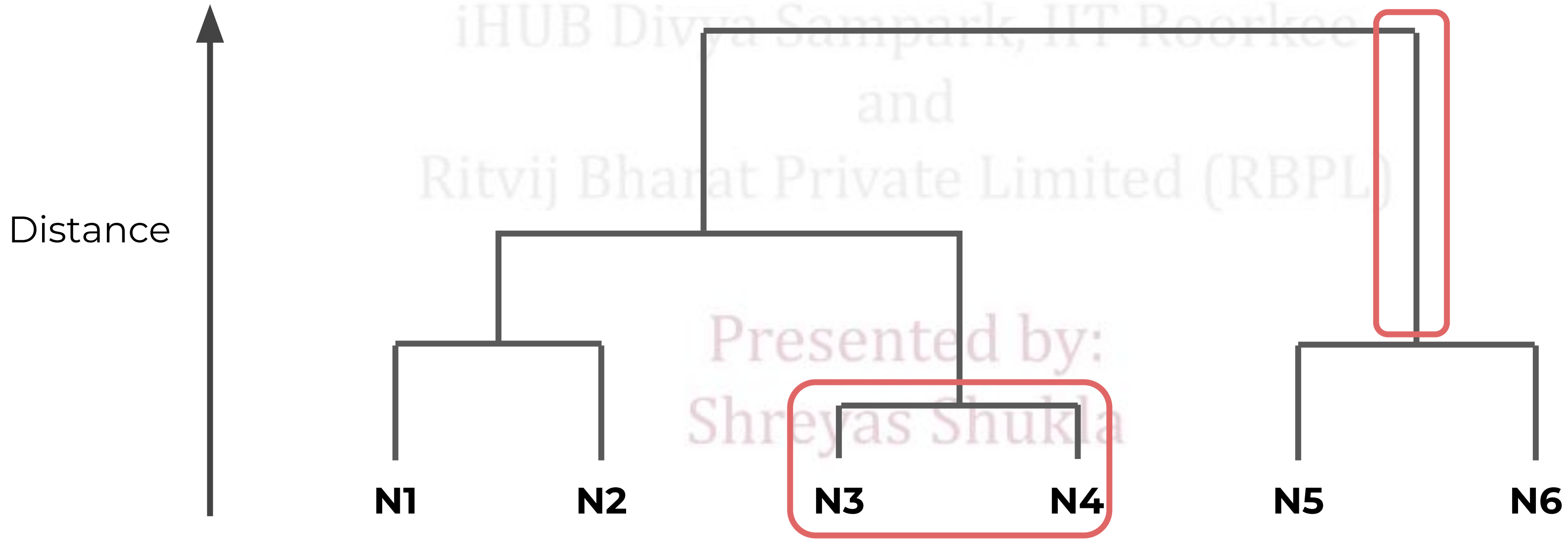
Dendrogram:



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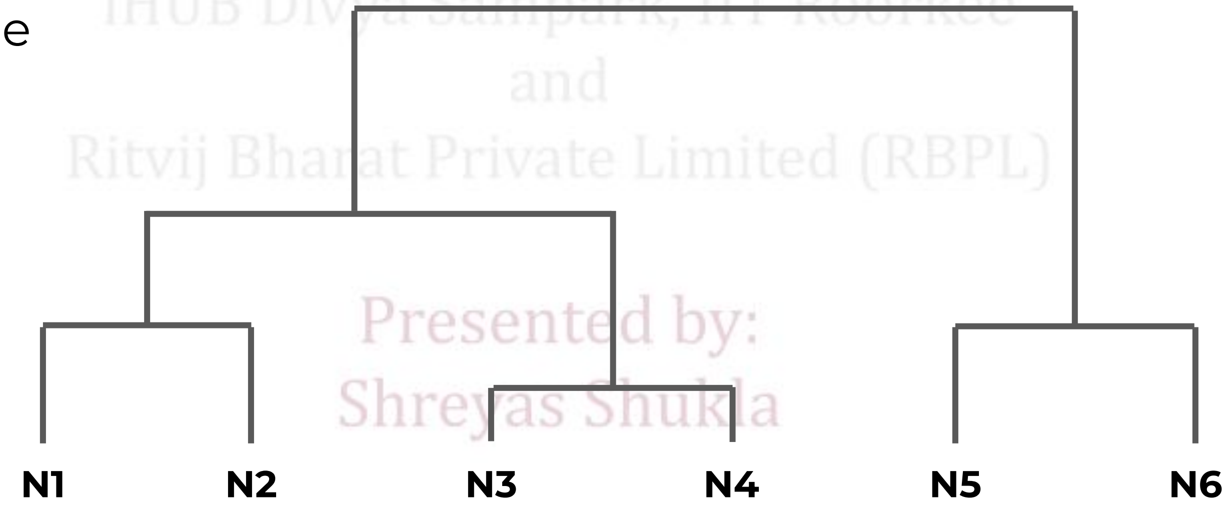
Dendrogram:

“Slice” to decide cluster count



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Dendrogram:

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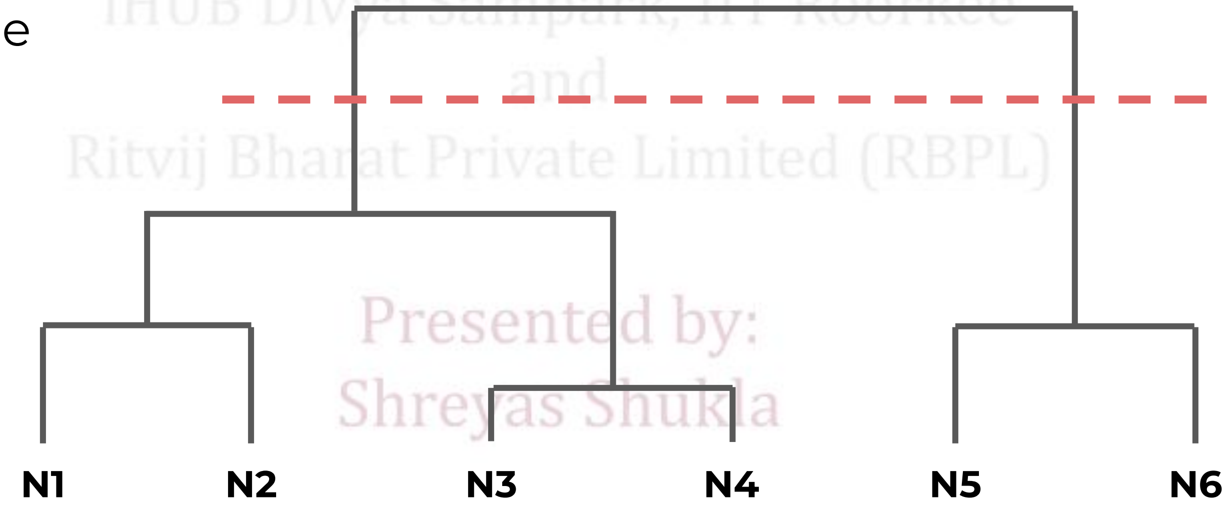

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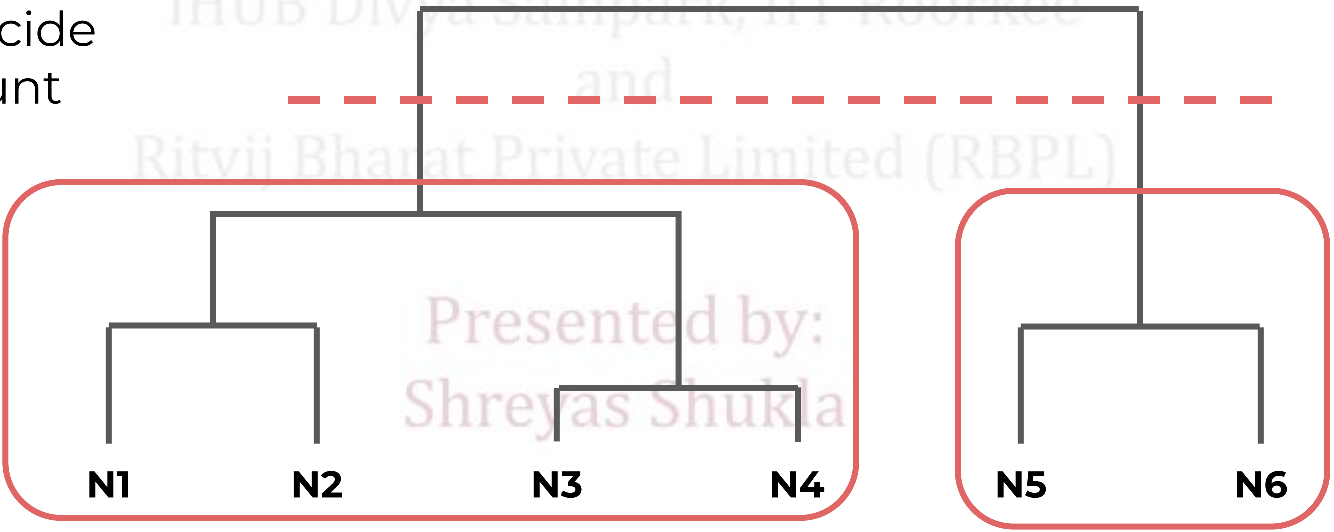

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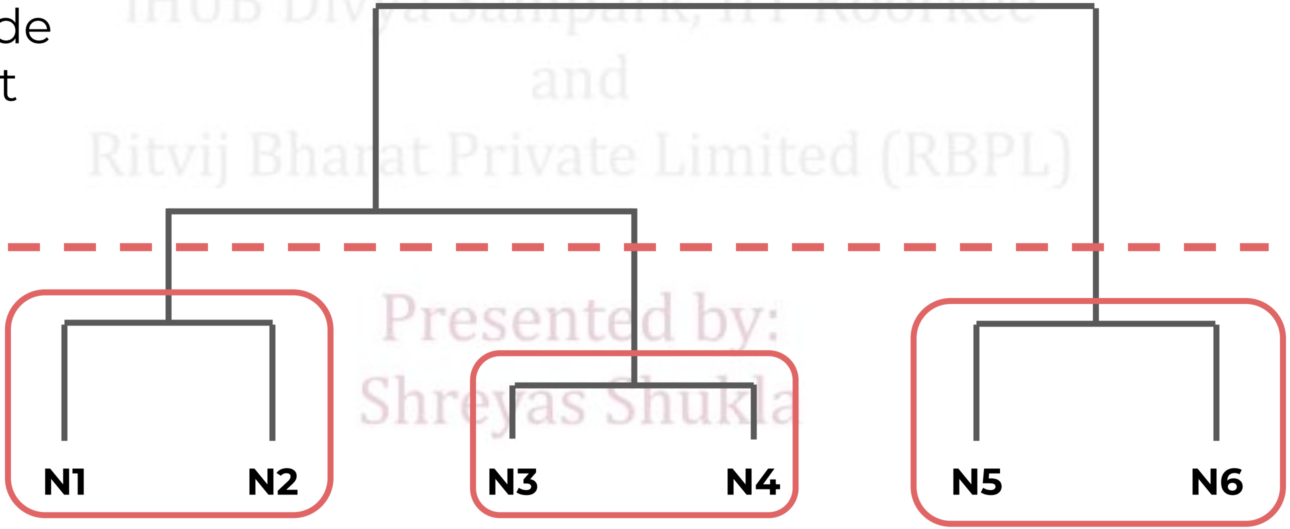

Linkage

- How do we measure distance from a point to an entire cluster?
- How do we measure distance from a cluster to another cluster?

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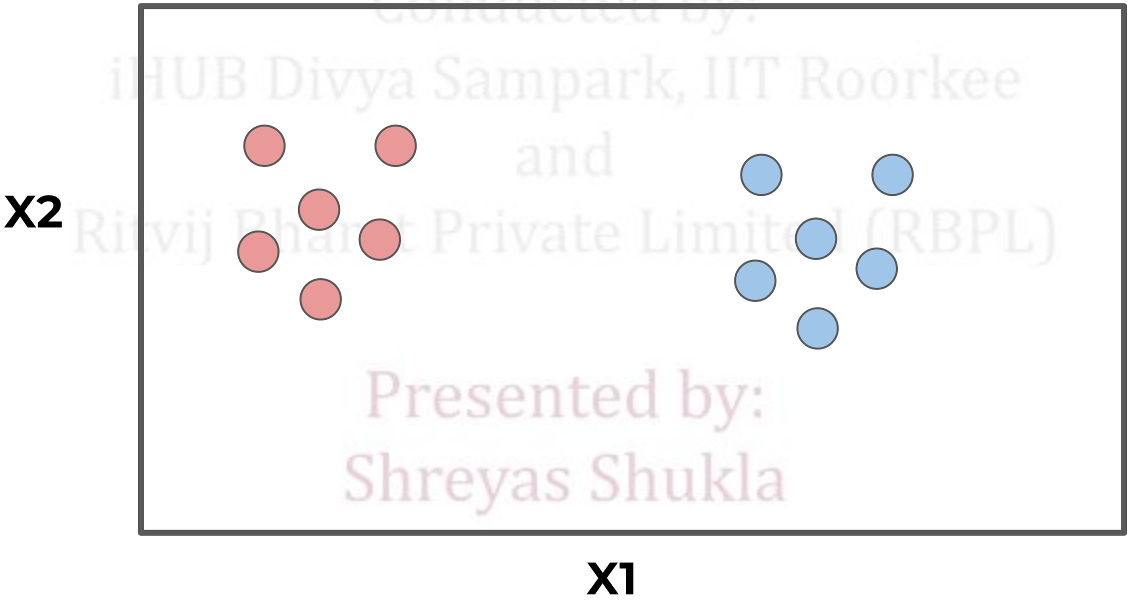
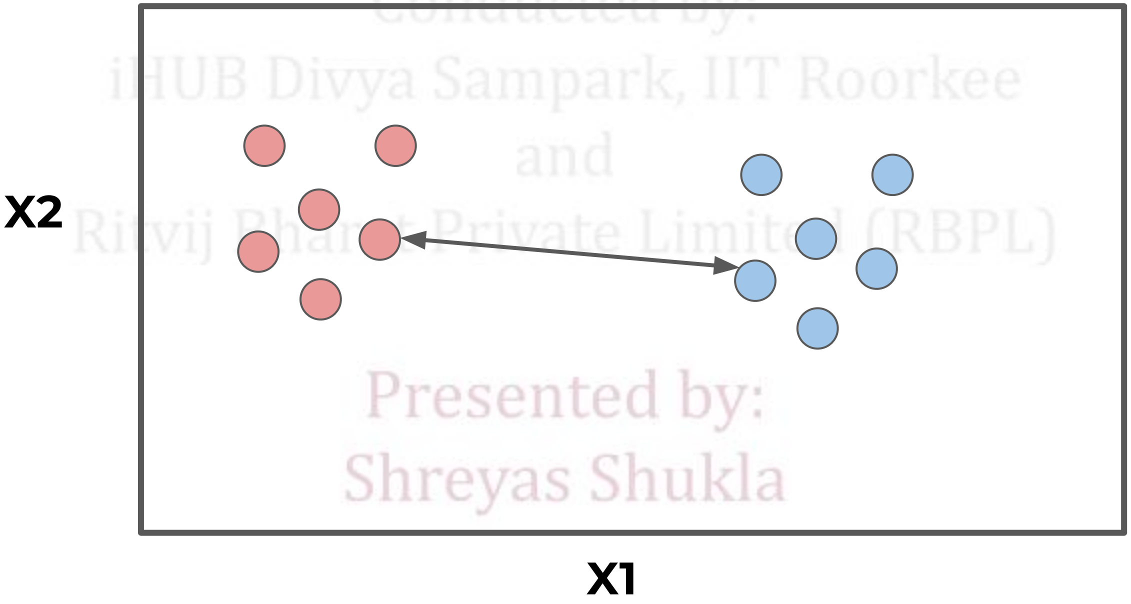
Linkage

Once two or more points are together and we want to continue agglomerative clustering to join clusters, we need to decide on a **linkage** parameter.


X2
X1



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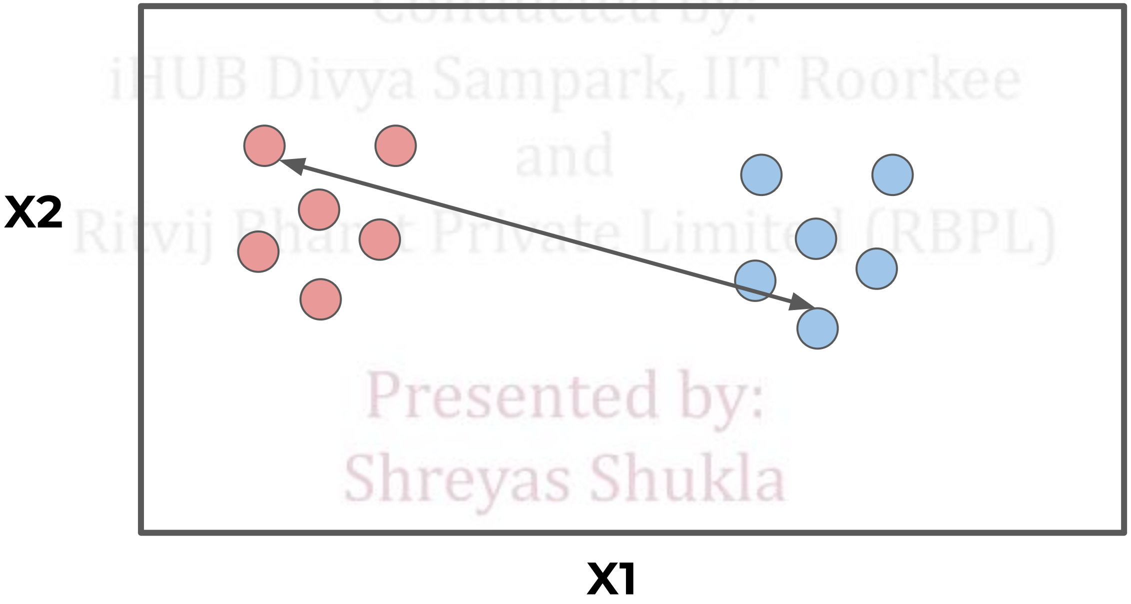

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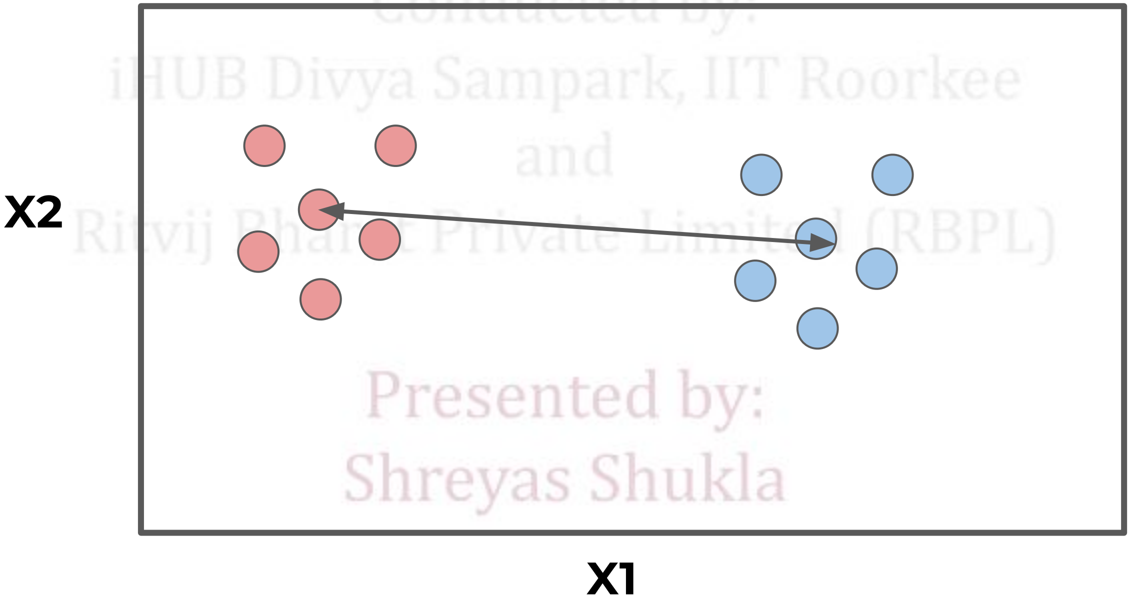

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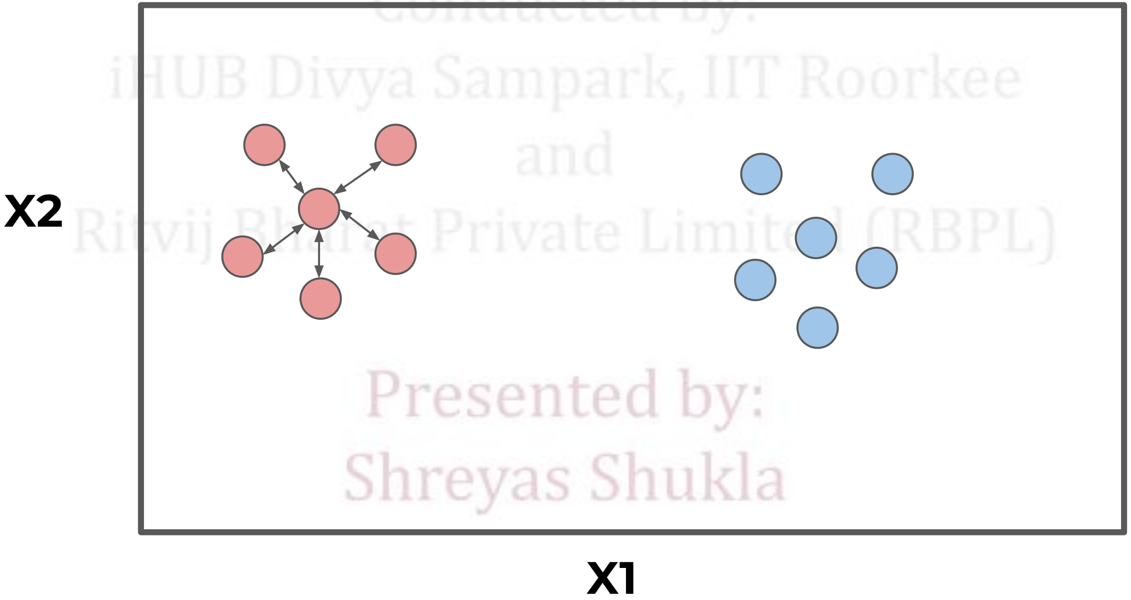

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Linkage

- Criterion determining which distance to use between sets of observation.
- Algorithm will merge pairs of clusters that minimizes the criterion.

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Linkage:

- **Ward:** minimizes variance of clusters being merged.
- **Average:** uses average distances between two sets.
- **Minimum** or **Maximum** distances between all observations of the two sets.

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