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

Unsupervised Learning

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Let’s learn about Unsupervised Learning!

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Supervised Learning

Using historical **labeled** data, predict a label on new data (regression or classification).

Unsupervised Learning

Using **unlabeled** data, discover patterns, clusters, or significant components.

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Unsupervised Learning:

- Clustering:
  - Using features, group together data rows into distinct clusters.
- Dimensionality Reduction:
  - Using features, discover how to combine and reduce into fewer components.

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Supervised performance metrics will not apply for unsupervised learning!

Then How can we compare to a correct label answer, if there was no label?

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We will need to figure out other ways of assessing unsupervised model performance or reasonableness.

Infact, our understanding of what “performance” actually means will need to change with unsupervised learning!

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Machine Learning Pathway for Unsupervised Learning

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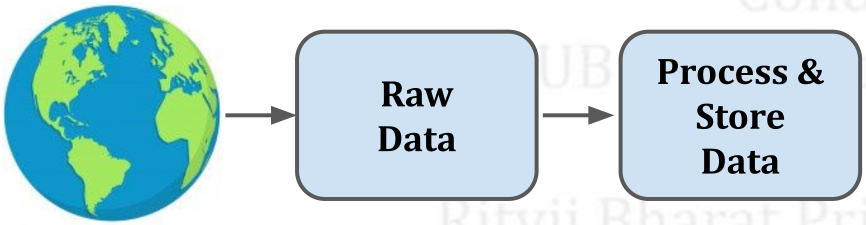

Real
World

SQL Database, CSV
files, Excel, Cloud
Storage

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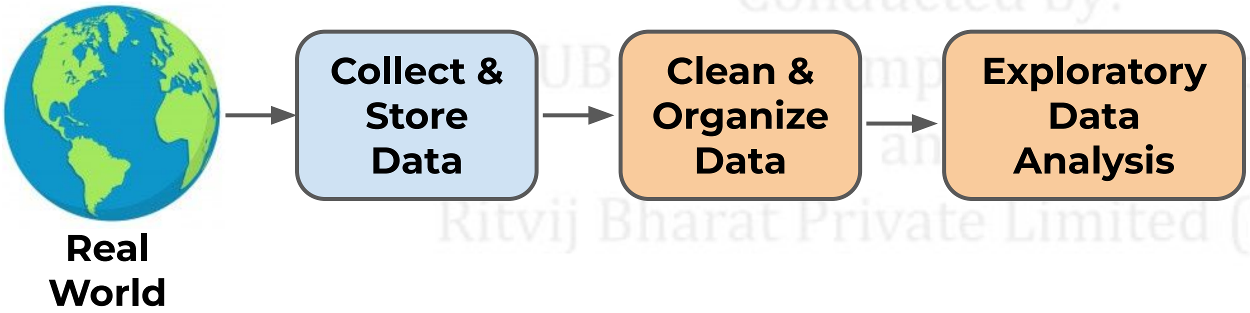

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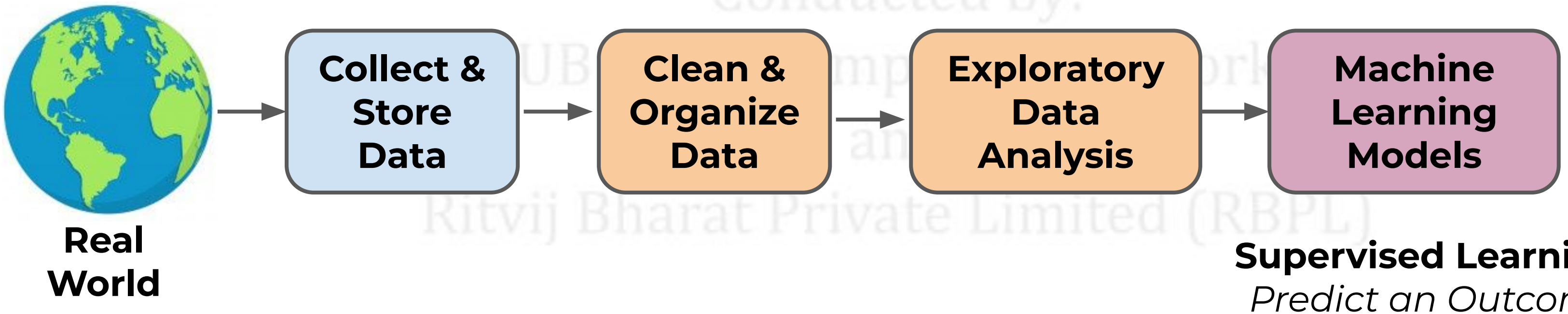

Supervised Learning:
Predict an Outcome
Unsupervised Learning:
Discover Patterns in Data

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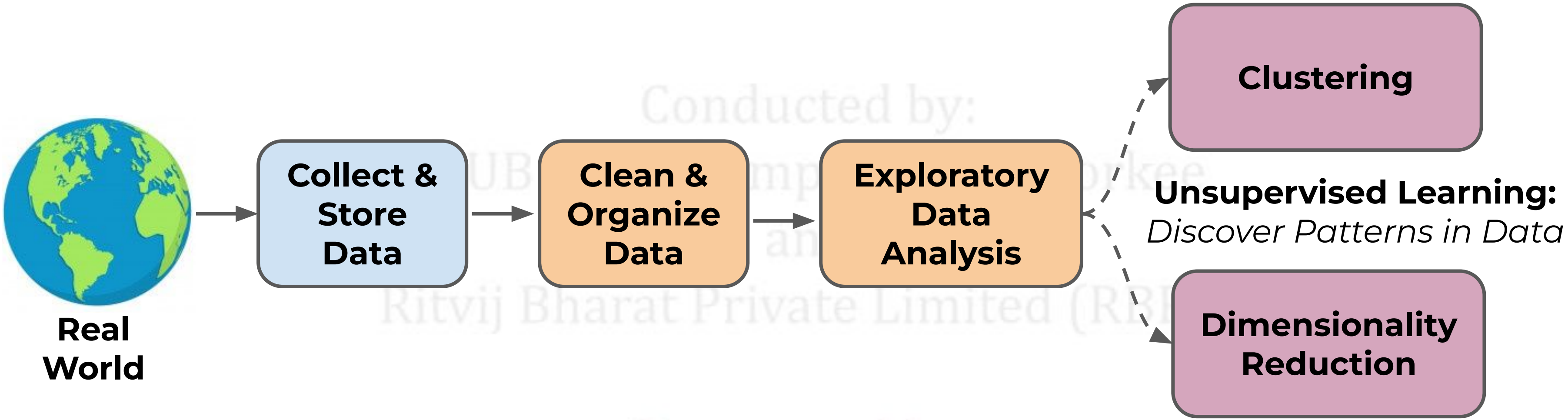

Real World

Collect & Store Data

Clean & Organize Data

Exploratory Data Analysis

Clustering

Unsupervised Learning:
Discover Patterns in Data

Dimensionality Reduction

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Clustering: If we have unlabeled data, can we attempt to cluster or group similar data points together to "discover" possible labels for clusters?

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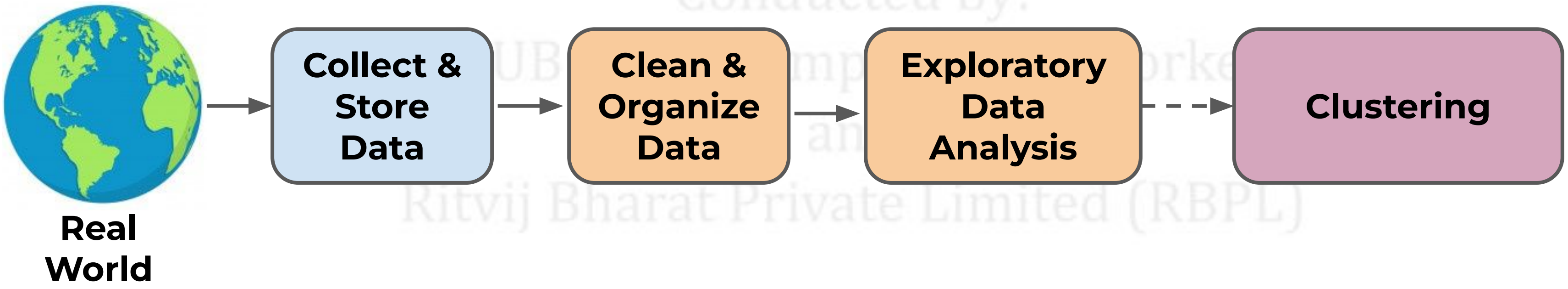

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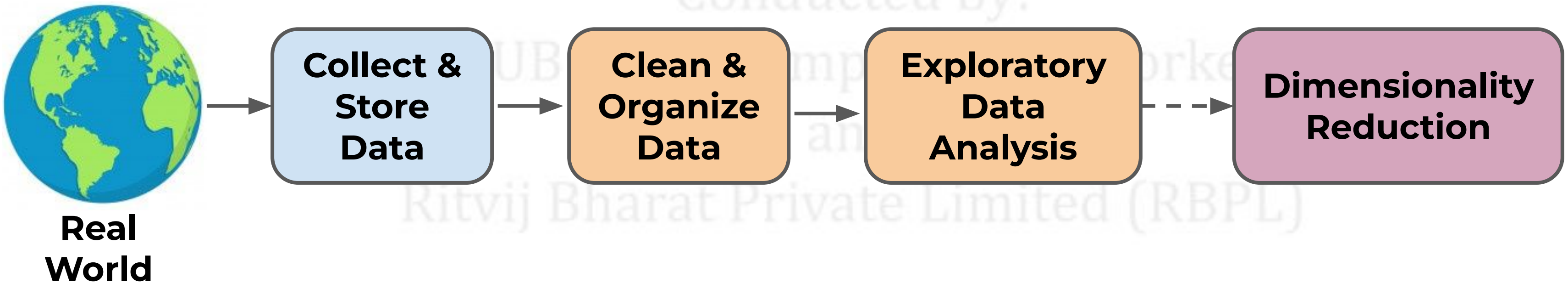
Dimensionality Reduction: If we have unlabeled data, can we attempt to reduce the number of features by combining them into new components? Do these new components give us further insight for the data?



Real World

Collect & Store Data

Clean & Organize Data

Exploratory Data Analysis

Dimensionality Reduction

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1. K-Means
2. Hierarchical clustering
3. Dimensionality reduction.

Methods for interpreting the model results

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Things keep in mind:

○ *What does it really mean to “discover” labels through clustering?*

○ *Without known labels how do we measure performance?*

○ *Do combinations of features hold important insights?*

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Let’s get started!

and

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K-Means Clustering

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○ Understanding Clustering

○ Intuition of K-Means

○ Mathematical Theory of K-Means

○ Example of K-Means

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Do not confuse K-Means with KNN!

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General Concepts

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Clustering uses **unlabeled data**
It looks for similarities between groups (clusters) in order to attempt to segment the data into separate clusters.

Keep in mind that we don’t actually know the true correct label for this data!

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Imagine an example data set:

X1	X2
2	4
6	3
...	...
1	2

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How could we cluster this data together?

X1	X2
2	4
6	3
...	...
1	2

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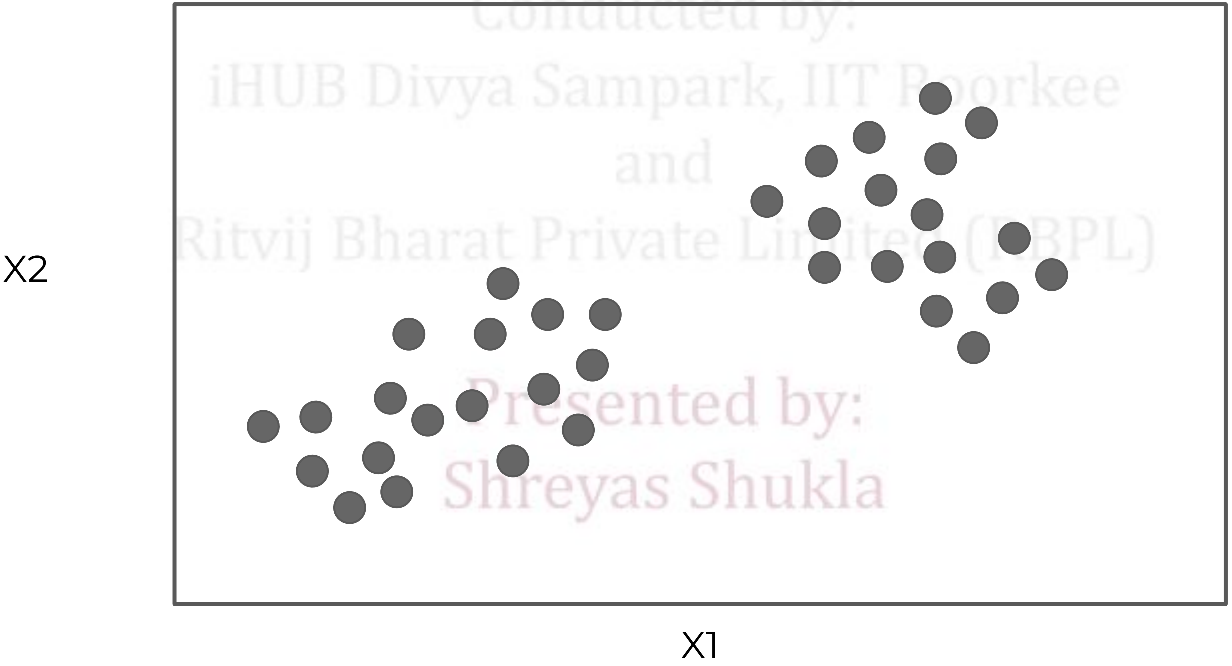
Intuitively, we see 2 groupings:



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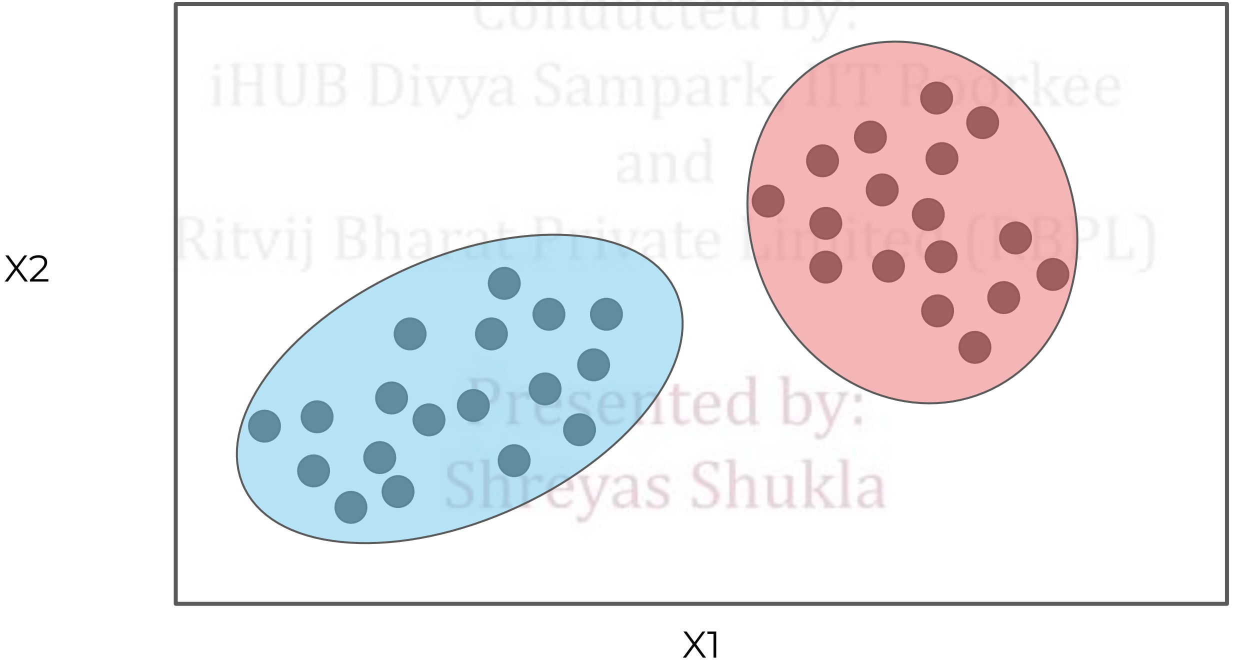
Note how distance is the intuitive metric:



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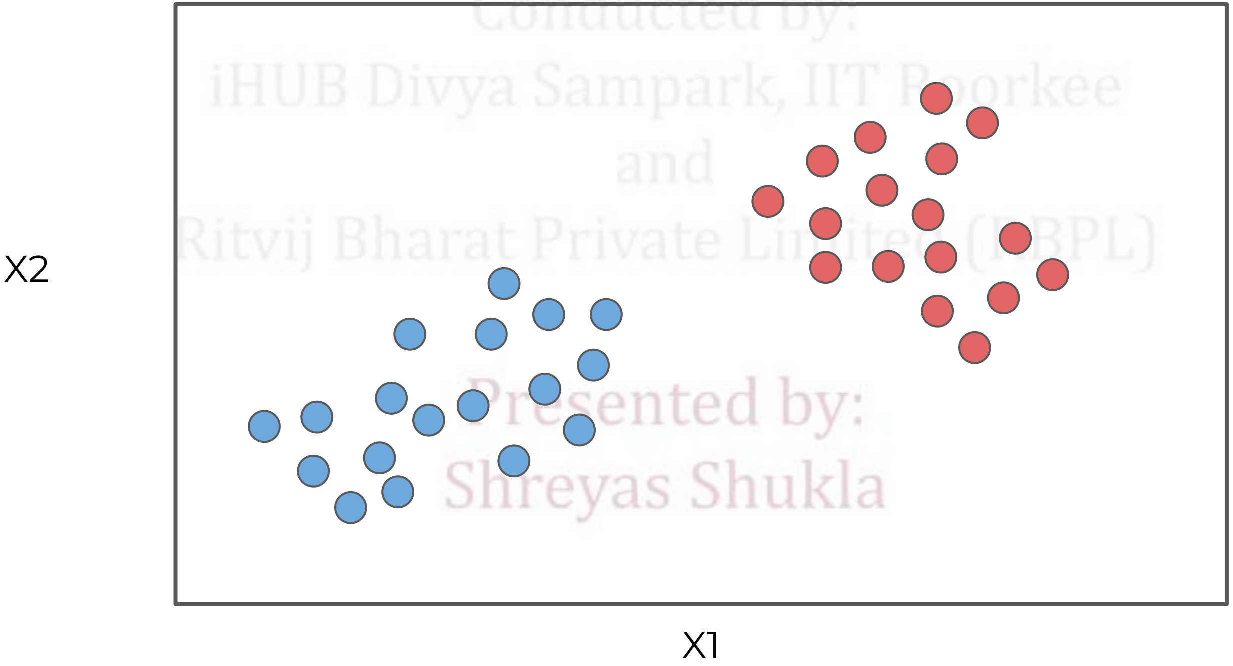
Assign clusters:



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We don’t actually know for sure if this is a correct way of grouping together these data points, there was no correct label to begin with!

Also what about situations that are not so obvious or multi-dimensional?

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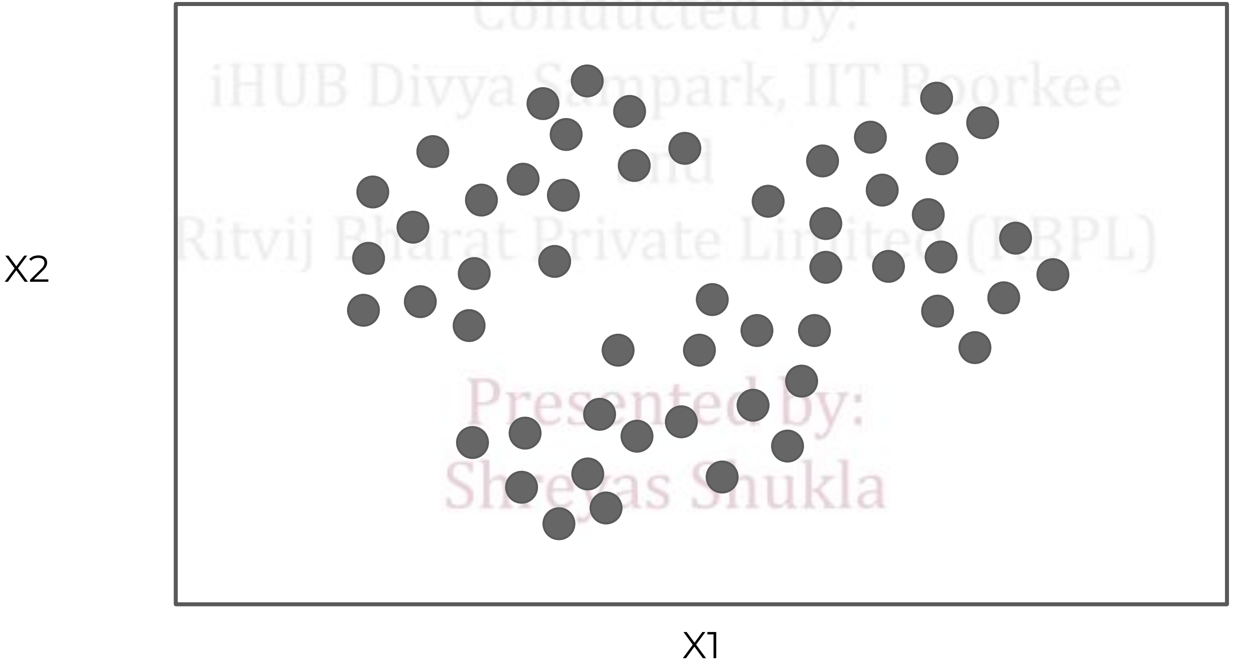
2 or 3 clusters could both be reasonable:



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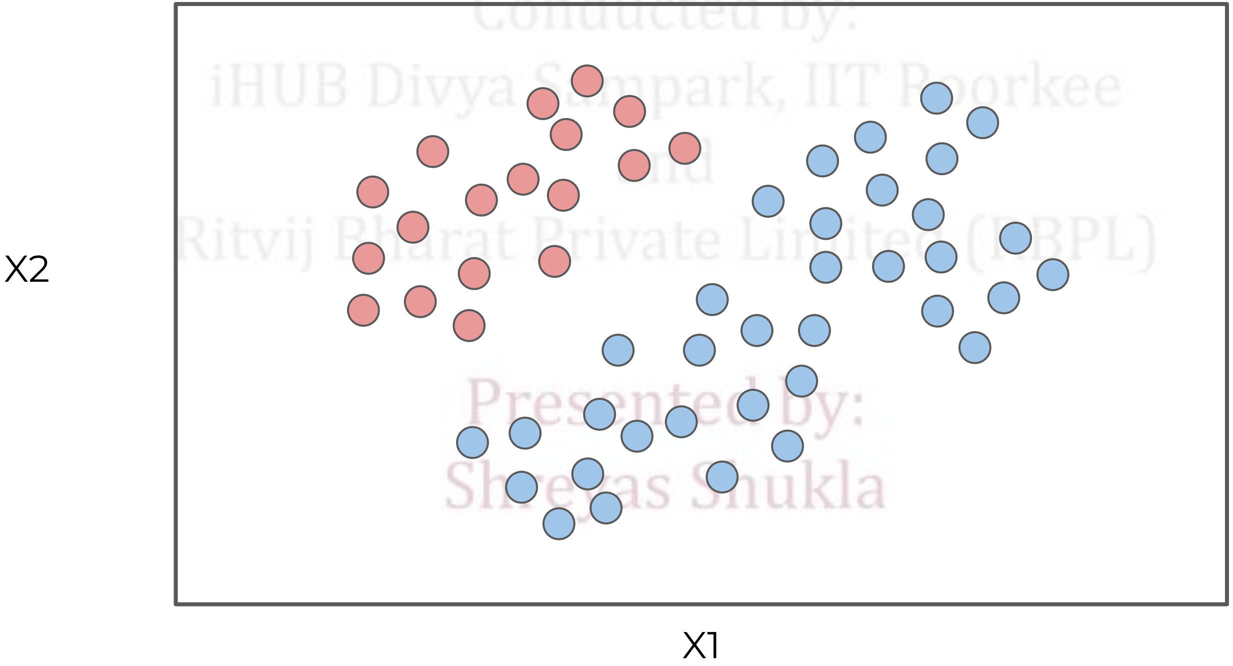

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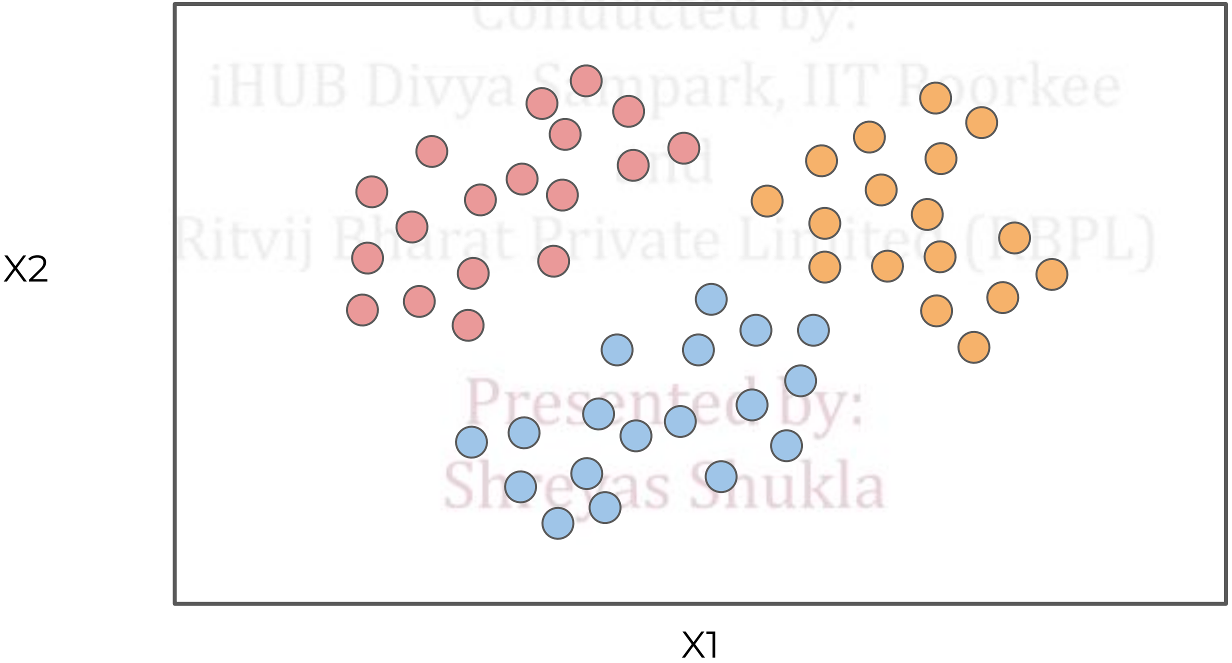

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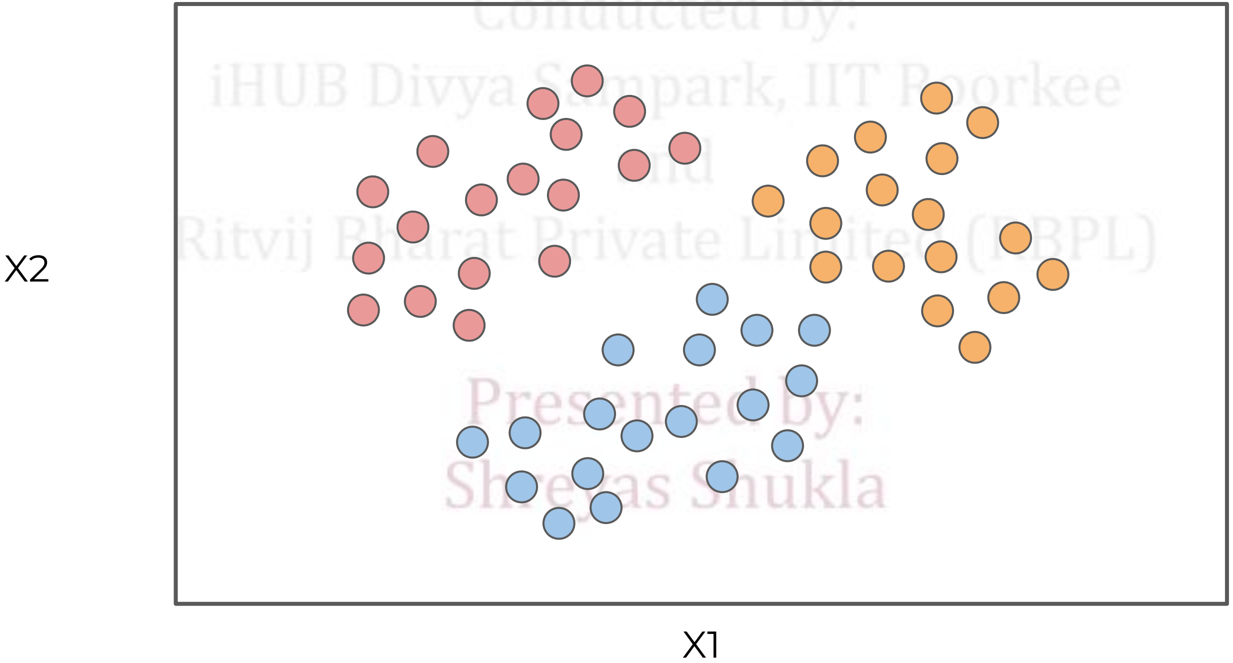
Different methods can be used to decide!



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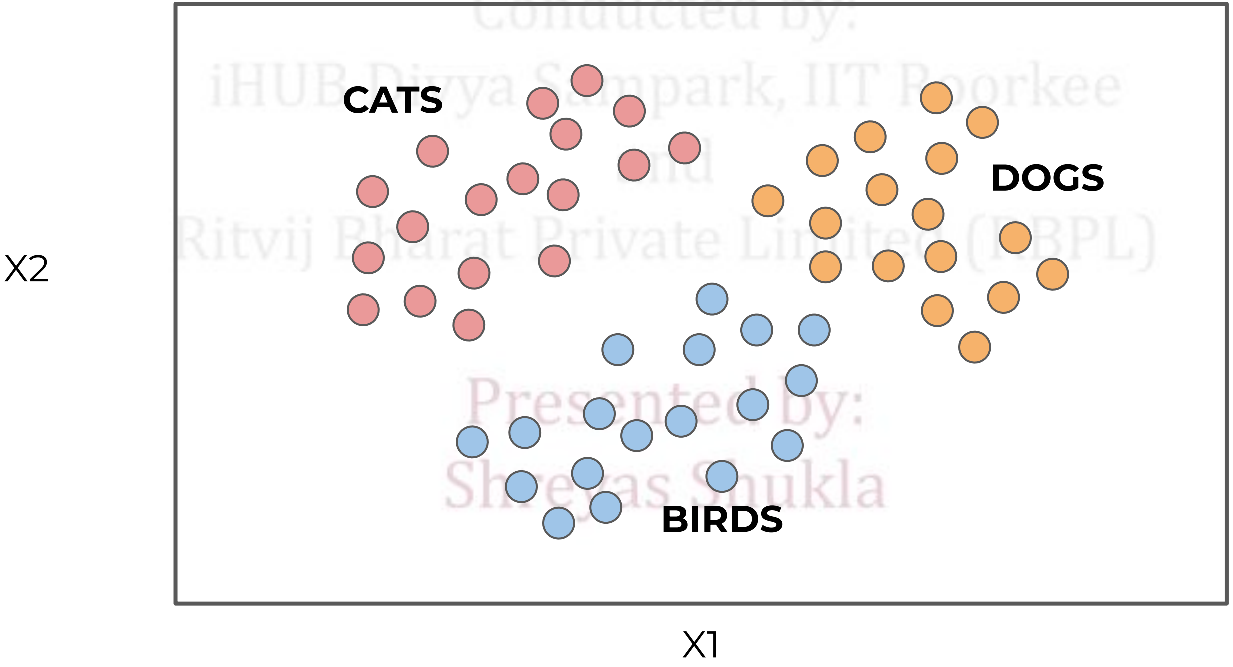
Clustering doesn’t “label” these for you!



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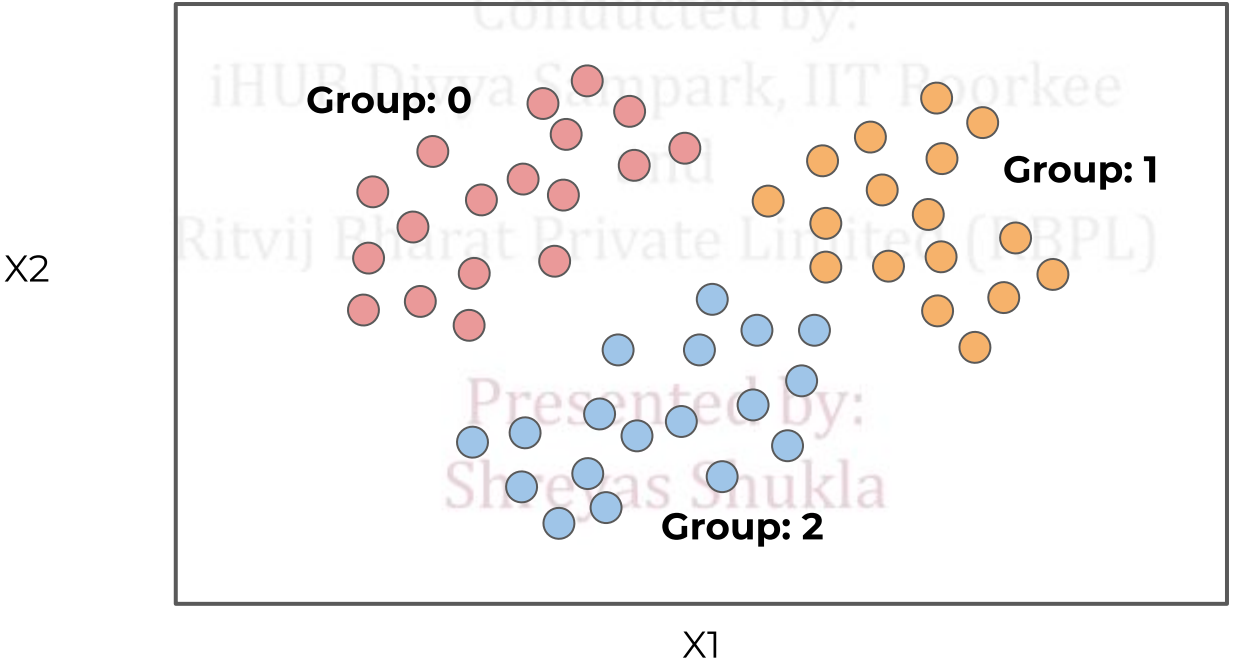

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Main Clustering Ideas:

1. Use features to decide which points are most similar to other points.
2. There is no final correct **y** label to compare cluster results to.
3. Clustering is an unsupervised learning process that “discovers” potential labels.

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- *What about a new unlabeled data point?*
- *How do we assign it to a cluster?*
- *Was it the correct cluster for assignment?*

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- *How do we assign a new data point to a cluster?*
  - Different approaches depending on the unsupervised learning algorithm used.
  - Use features to assign most appropriate cluster.

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- ○ *If we've discovered these new cluster labels, could we use that as a **y** for supervised training?*
  - ■ Yes! We can use unsupervised learning to discover possible labels, then apply supervised learning on new data points.

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- *If we’ve discovered these new cluster labels, could we use that as a **y** for supervised training?*
  - What’s the trade-off?

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If we’ve discovered these new cluster labels, could we use that as a ***y*** *for supervised training?*

- Clustering doesn’t tell you what these new cluster labels represent, no real way of knowing if these clusters are truly significant.

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- How do we decide which number of clusters is best?
- Do we decide or let the algorithm decide?
- How can we measure “goodness of fit” for clustering without a **y** label for comparison?

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Machine Learning as an art

What is ground truth?

What trade-offs are we making by using unsupervised learning as a substitute for ground truth of the y label that was not given?

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It is much harder to compare unsupervised algorithms against each other due to the lack of ground truth based performance metrics like accuracy or RMSE.

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K-Means Clustering

Intuition and Theory

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Working of K-Means clustering

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First, a set of properties each point we must satisfy:

- ○ Each point must belong to a cluster.
- ○ Each point can only belong to one cluster (no single point can belong to multiple clusters).

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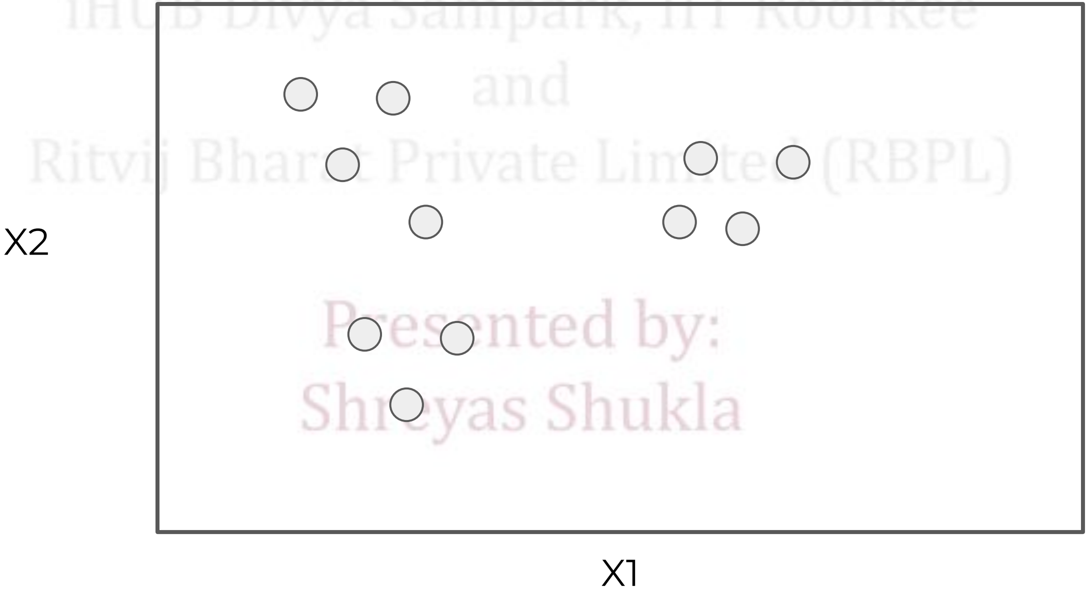
We’ll work with a simple dataset with only 2 features. The process shown here easily extends to **N** feature dimensions.

- Step 0: Start with unlabeled data (only features).



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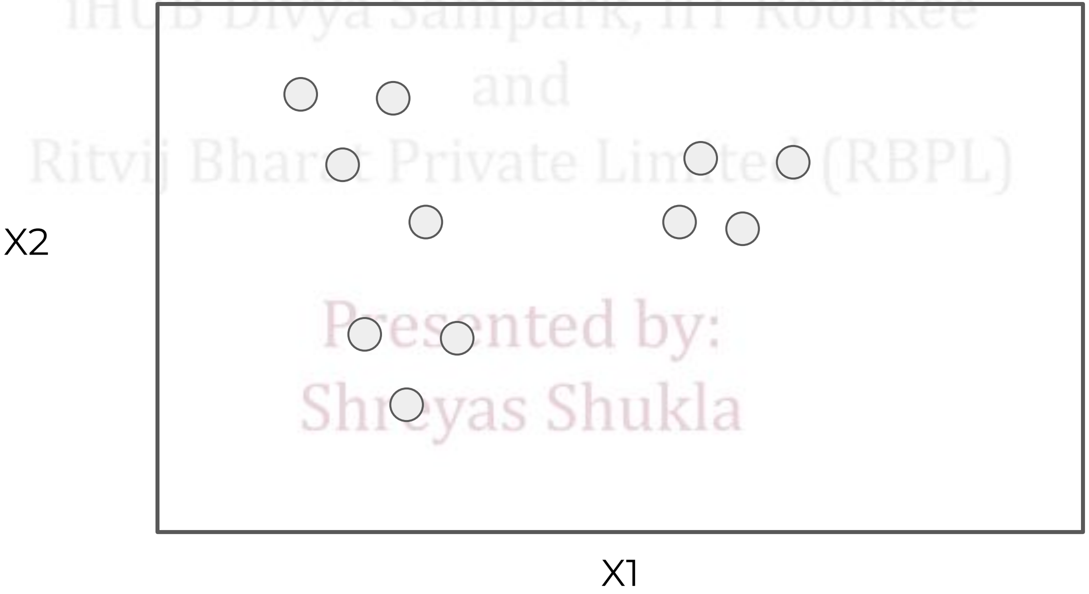
Note: *If we had the group labels, it wouldn't make sense to cluster!*



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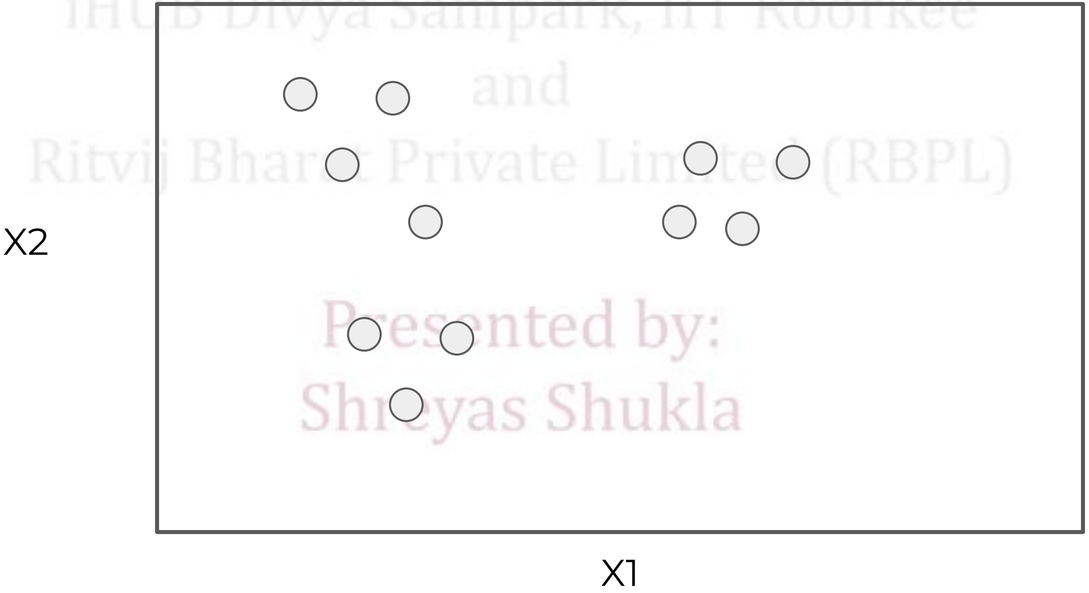
Step 1: Choose the number of clusters to create (this is the K value).



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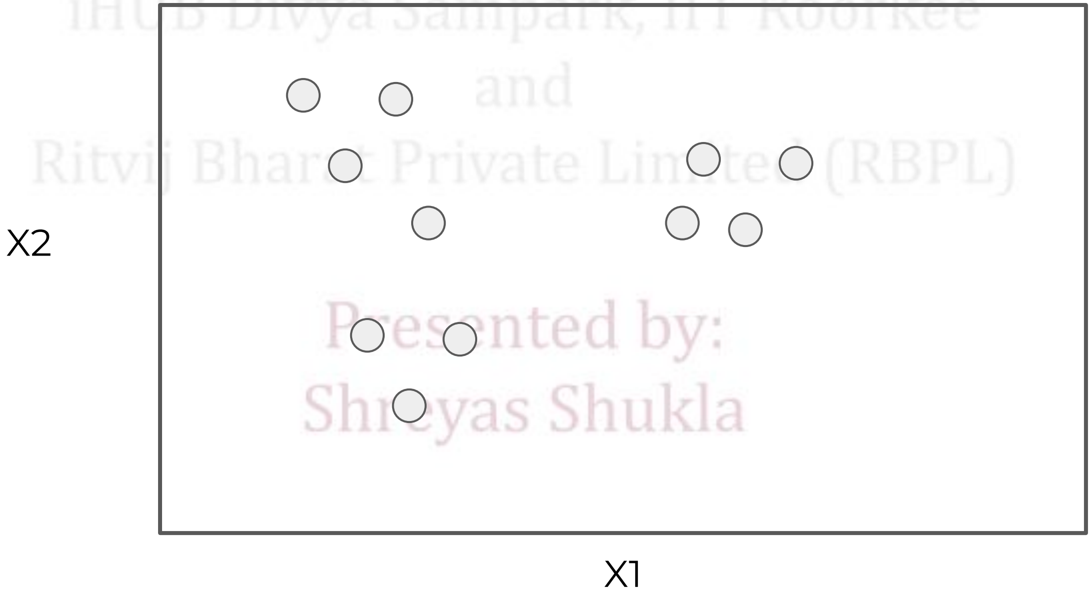
Step 1: We’ll choose K=3. Note in most situations you won’t visualize the data!



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Step 2: Randomly select K distinct data points.

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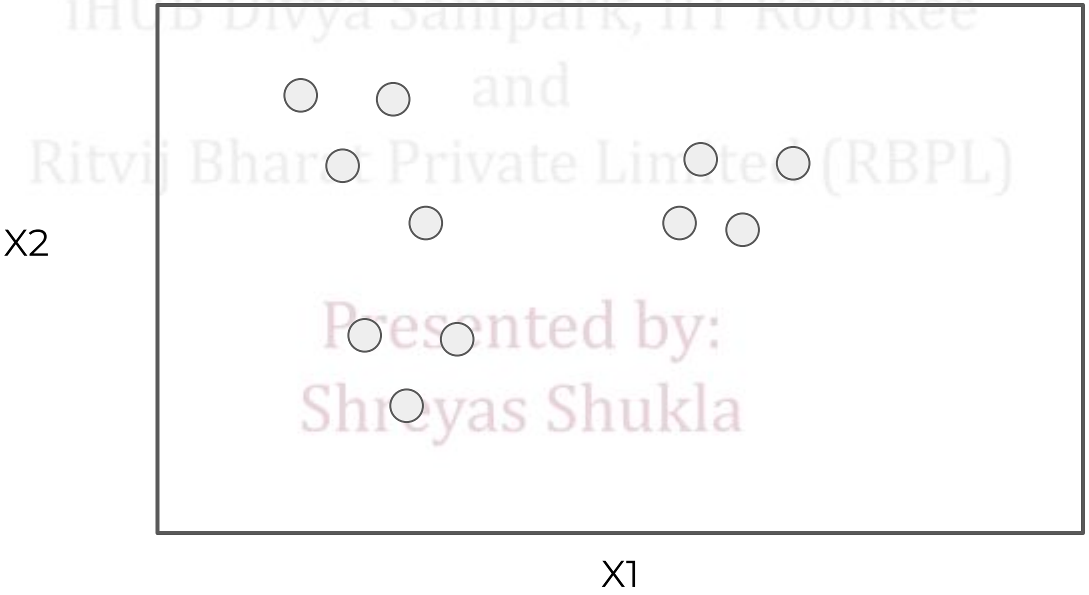

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Step 2: Randomly select K distinct data points. Our K=3. We’ll treat these new K points as our cluster points.

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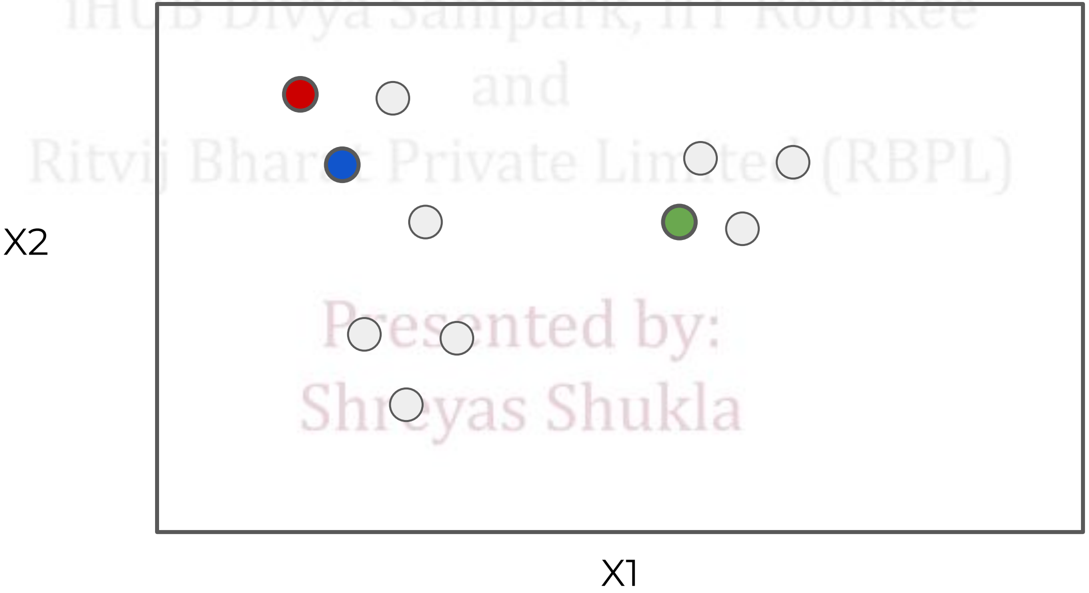

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Step 3: Assign each remaining point to the nearest “cluster” point.

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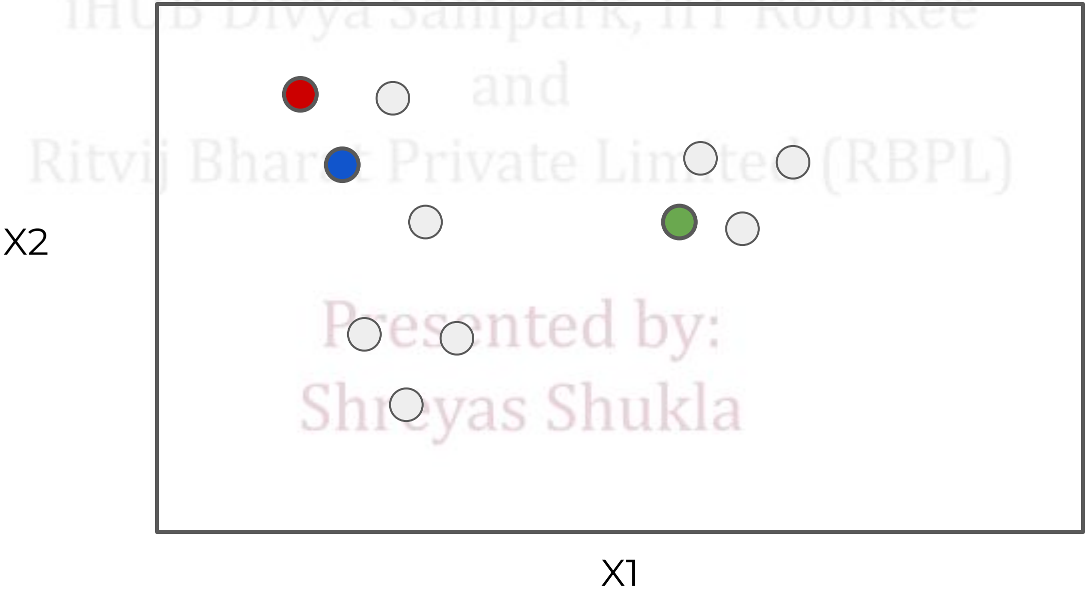

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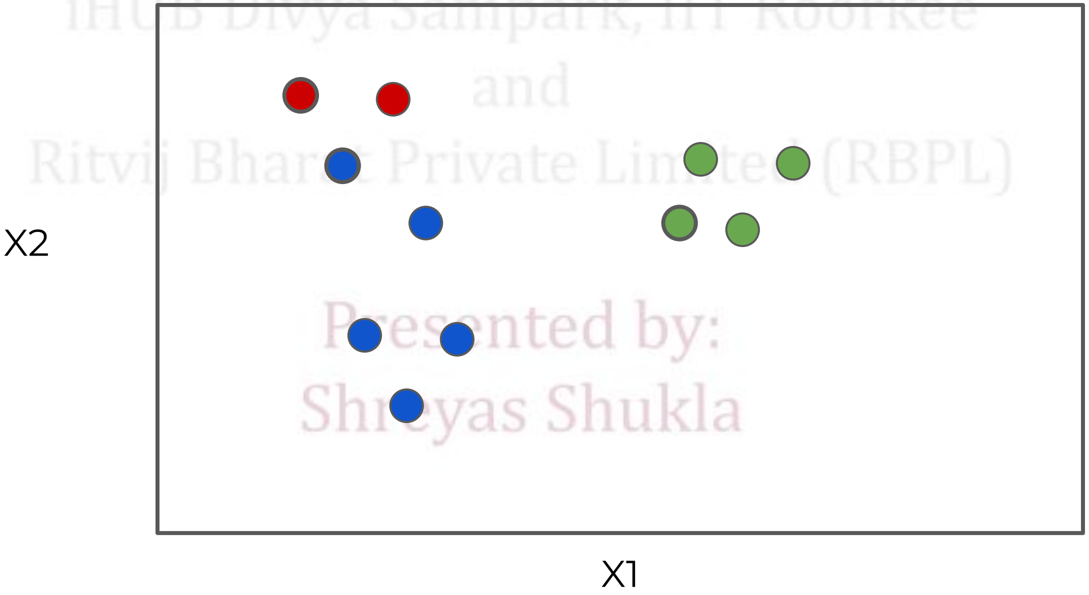
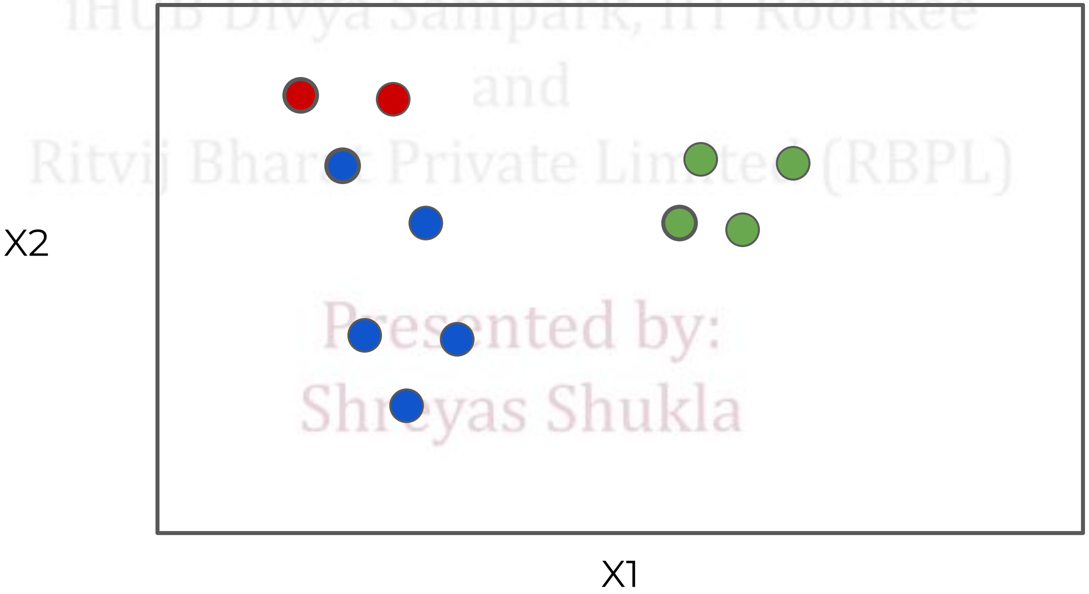


fig ref: pierian data

Step 3: Note how this is using a distance metric to judge the nearest point.



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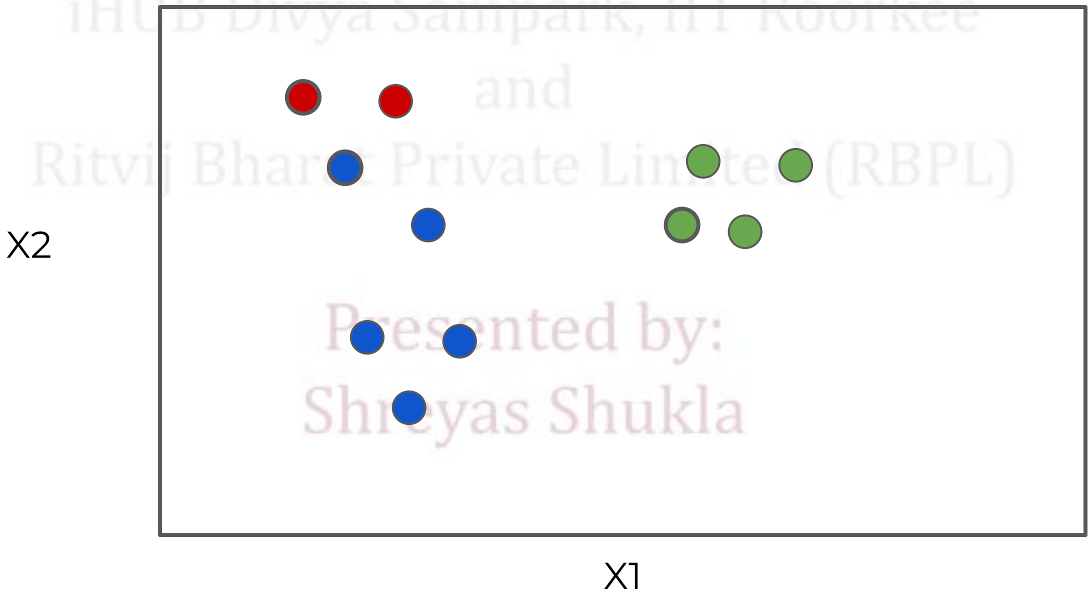
Step 4: Calculate the center of the cluster points (mean value of each point vector).



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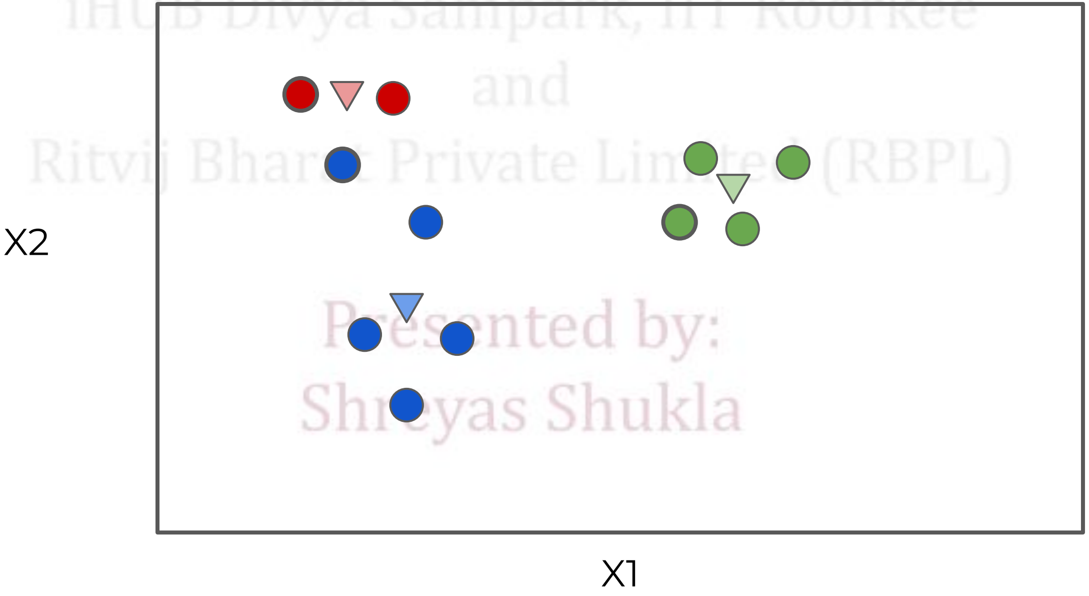

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Step 5: Now assign each point to the nearest cluster center.

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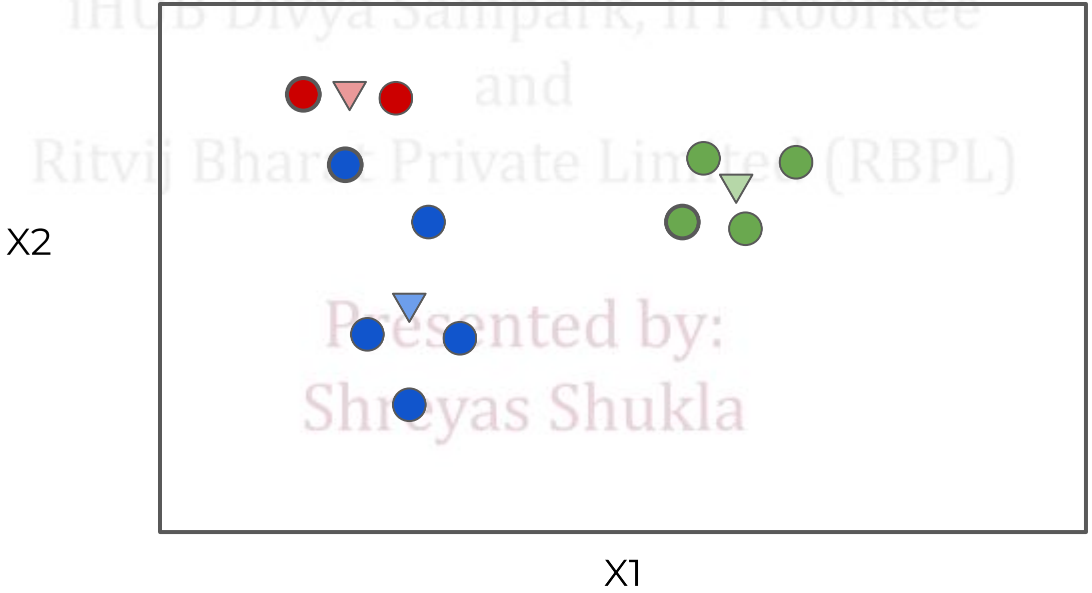

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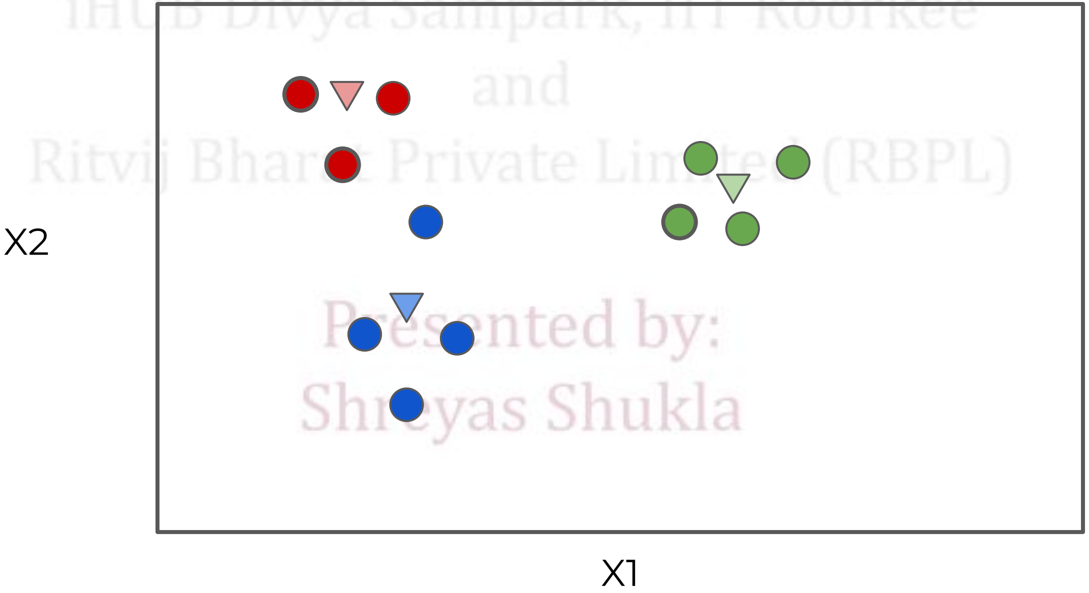

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We repeat steps 4 and 5 until there are no more cluster reassignments.

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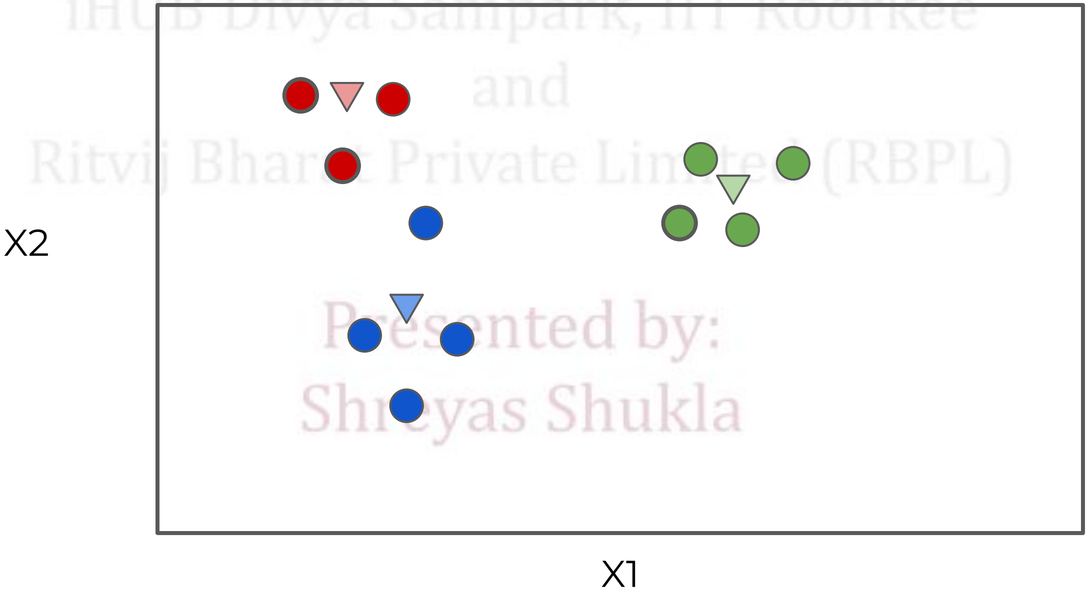

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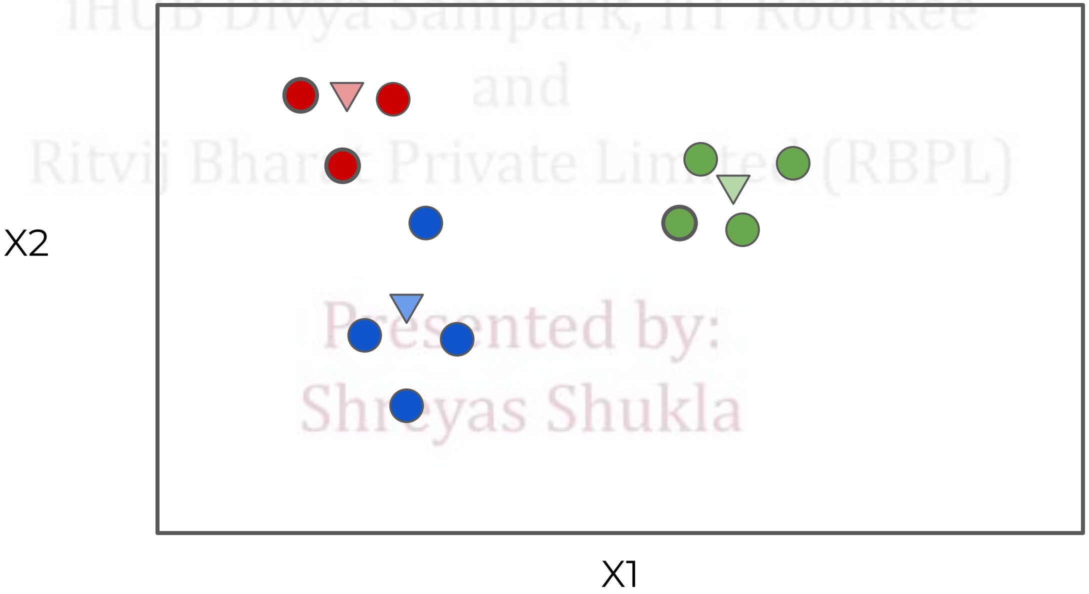
Step 4b: Recalculate new cluster centers:



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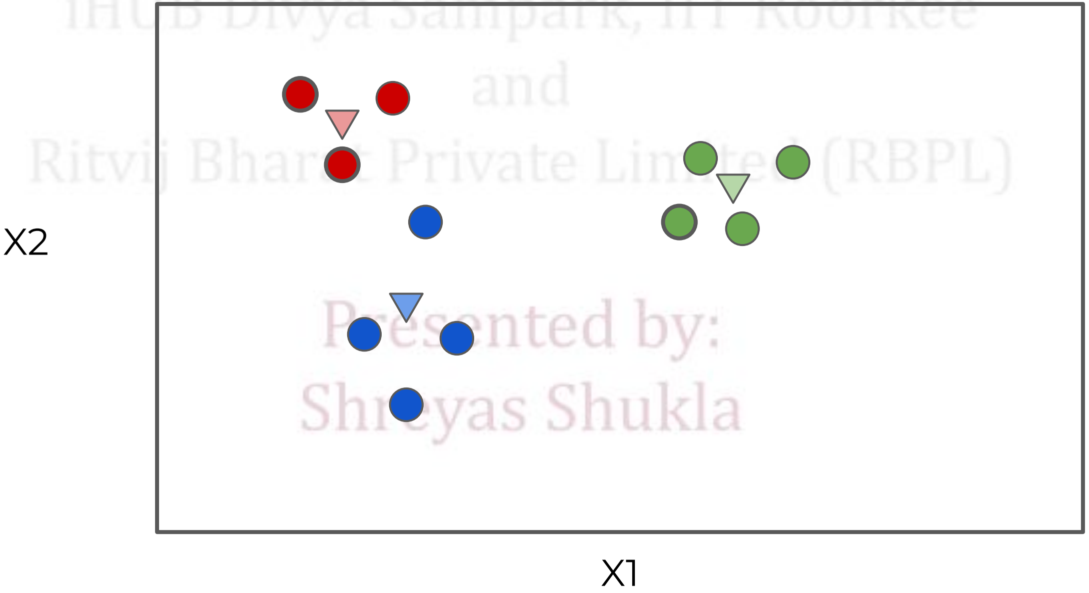

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Step 5b: Assign points to nearest cluster center.

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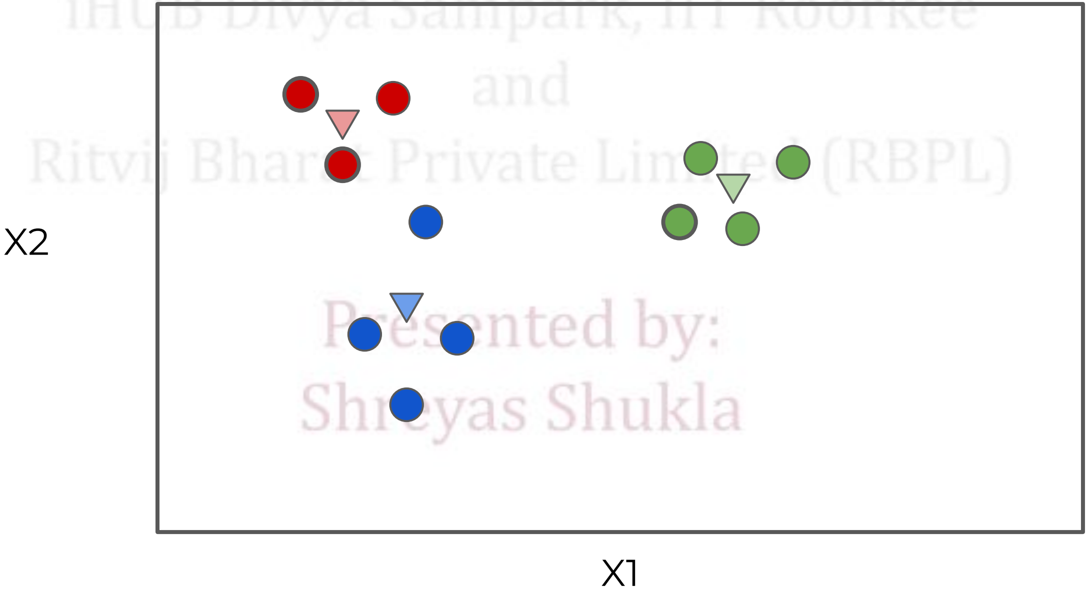
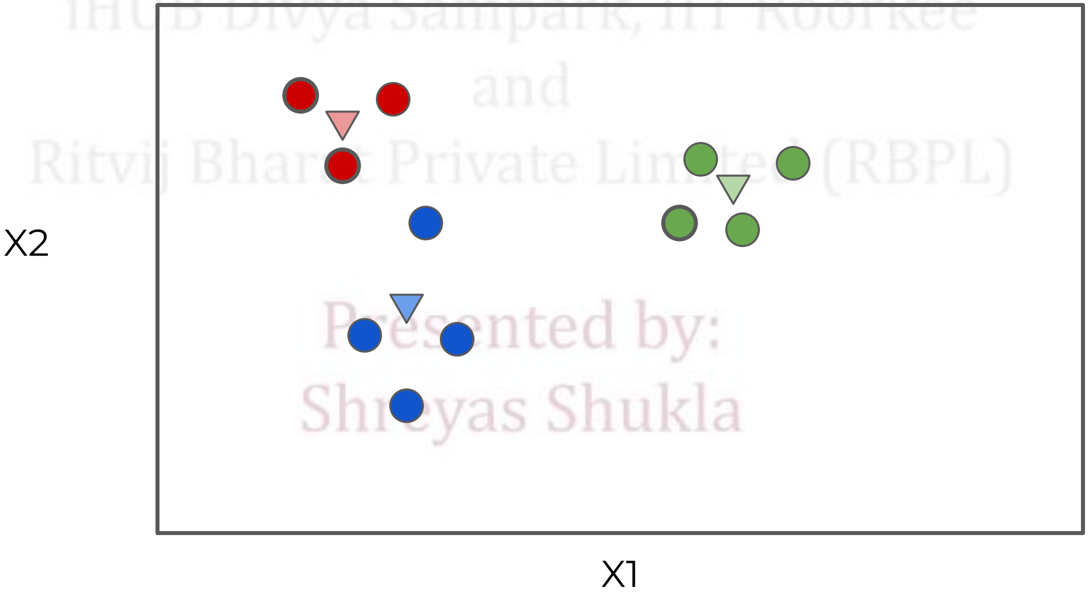


fig ref: pierian data

If there are no more reassignments, we're done! The clusters have been found.



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Upcoming considerations:

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

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Let’s code out an example of K-Means clustering,

then we’ll revisit these considerations when they naturally appear after we find the first set of clusters for a given K.

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Let’s Code !!

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