Intro to Unsupervised Learning

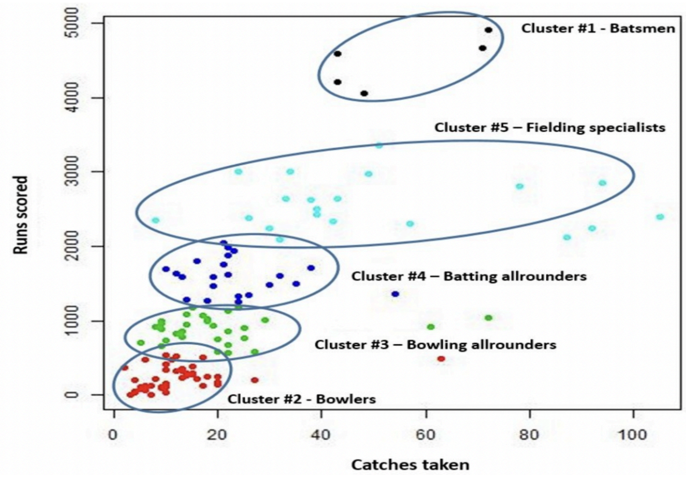
- In the case of supervised, we are trying to find a function that is used to predict y_i when x_i s are given as the input. (the models are trained with a target variable.)
- Unsupervised learning deals with data that is unlabelled or hasn't a target variable.

Clustering

- The process of grouping any kind of data based on the similarity in their features, automatically, without human expertise, is called **clustering**. It is a type of **unsupervised learning**.

- Intuitively, clustering is dividing a population into groups such that the points in one group are similar to each other. Each group is called a **cluster**.
    - The points in the same cluster are closer and similar to each other.
    - The points in different clusters are more distant and distinct from each other.

- So, the task in clustering is grouping the points of a similar kind based on our definition of similarity. For example,
    - In the image below, we can see clusters of different kinds of players based on runs scored and catches taken.

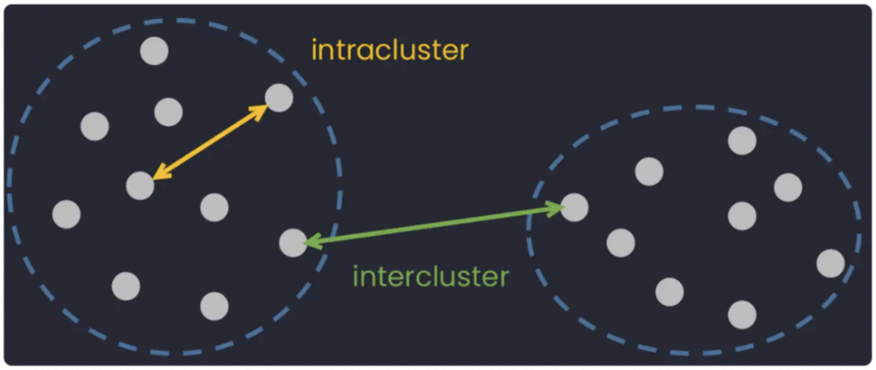


- **Similarity** can be measured using different distance metrics like Euclidean distance, manhattan distance, and Hamming distance.

Distances used while clustering:

- **Inter-cluste**r distance represents the distance between two clusters
  - Distance between average values of the clusters.
  - Distance between closest points from the clusters (min distance)
  - Distance between farthest points from the clusters (max distance)

- **Intra-cluster** distance represents the distance within a certain cluster.
  - Average distance between the points of a cluster.
  - Distance between farthest points of a cluster



- Having only one inter or intra-cluster distance won't tell us how good or bad our clusters are, therefore we need a metric to evaluate our clusters.

Dunn Index

- It is calculated as a ratio of the **smallest** inter-cluster distance to the **largest** intra-cluster distance.

i.e. $D = \dfrac{minimum \;\; inter-cluster \;\; distance}{maximum \;\; intra-cluster \;\; distance}$

- The objective of the Dunn index is to identify clusters that are:
  - compact with a small variance between members of the cluster
  - and well separated

- A **higher Dunn Index** means **better clustering** since observations in each cluster are closer together, while clusters themselves are further away from each other.

- The Dunn Index is **unbound**, so it can only be interpreted in a relative sense.

Introduction to K-Means

- The value 'K' in the K-means algorithm denotes the number of clusters.
- In k-means, data is divided into k clusters where each cluster has a centroid which is the average of all the points in the cluster.
- The centroid (C_i) of the cluster (S_i) can be defined as

$$C_i = \frac{1}{|S_i|} \sum_{x_j \epsilon S_i} x_j$$

  where $|S_i|$ represents the number of points belonging to the i^{th} cluster.
- K-Means assign only one cluster to each point.
- Steps in In K-Means:
  - Every point is assigned to the cluster centroid closest to it.
  - Update the centroid.
  - Repeat the above two steps until convergence.

Improving centroids

- If after each iteration, the value of the Dunn Index **increases**, it is a sign that the clusters have become better after each iteration.
- The **objective** for the optimization of clusters can be represented as

$$L : \max_{c} \; dunn(x, argmin(c, x))$$

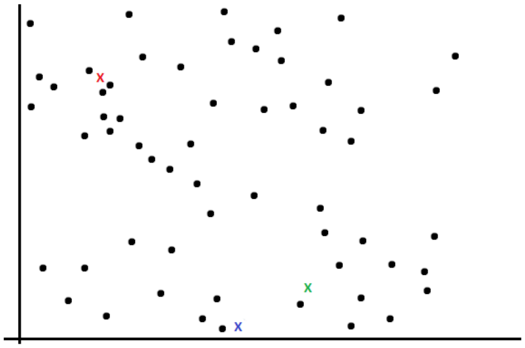
- The above equation can be read as
  - ➔ Take a point **x** and calculate its distance from all the **centroids,**
  - ➔ Choose the center having minimum distance from the point, that would be the cluster to which the point **x** would be assigned,
  - ➔ Using the cluster and the data point, calculate the Dunn index and maximize that over the centers.

- **Problems** while performing the above optimization steps:
  1. The objective function is not differentiable.
  2. Assigning a point **x** to a group is a discrete problem, and there is no good way to convert the expression into a function that is continuous and differentiable.
- We cannot use calculus or gradient descent for optimization. Gradient descent can lead to fractional assignments.

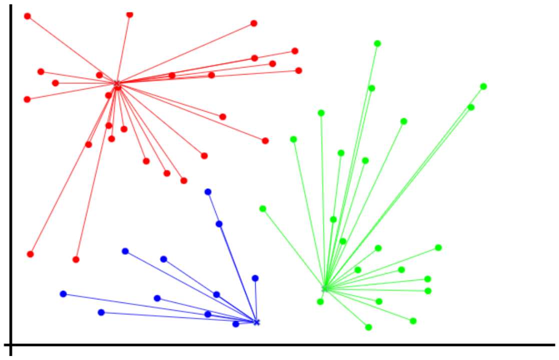
Lloyd's algorithm (K-means algorithm)

- This algorithm is used to cope with the problem of updating the centers.
- It has 4 basic steps:

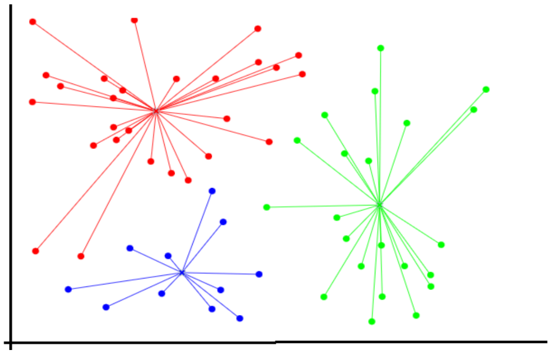
  ➔ **Initialization**: Randomly initialize **k** centers from the dataset.



  ➔ **Assignment**: For each point, we find the distance of existing centroids from it and assign the point to that cluster whose centroid has the minimum distance.



- ➔ **Update** the centroids of the clusters by taking the average of points from each cluster.



- ➔ Repeat the previous two steps until convergence (the center of new cluster centroids stops changing their positions).

ANIMATION LINK: http://tech.nitoyon.com/en/blog/2013/11/07/k-means/

Within-cluster sum of squares (WCSS)

- Measure of the variability of the data points within each cluster.

$$wcss = \sum_{i=1}^{k} \sum_{j=1}^{m_i} (x_{ij} - c_i)^2$$

where $\mathbf{x_{ij}}$ is the $\mathbf{j}^{\text{th}}$ point belonging to the $\mathbf{i}^{\text{th}}$ cluster and $\mathbf{m_i}$ is the number of points in the $\mathbf{i}^{\text{th}}$ cluster.

- A **variation** of the above formula:

$$wcss = \sum_{i=1}^{k} \sum_{j=1}^{m_i} d(x_{ij}, c_i)$$

where, $\mathbf{d(x_{ij}, c_i)}$ represents a distance metric (any of Euclidean, manhattan, etc.) that calculates the distance between the point $\mathbf{x_{ij}}$ and the centroid $\mathbf{c_i}$ of the cluster.

Silhouette score

- Measure how similar an object is to its cluster (cohesion) compared to other clusters (separation).

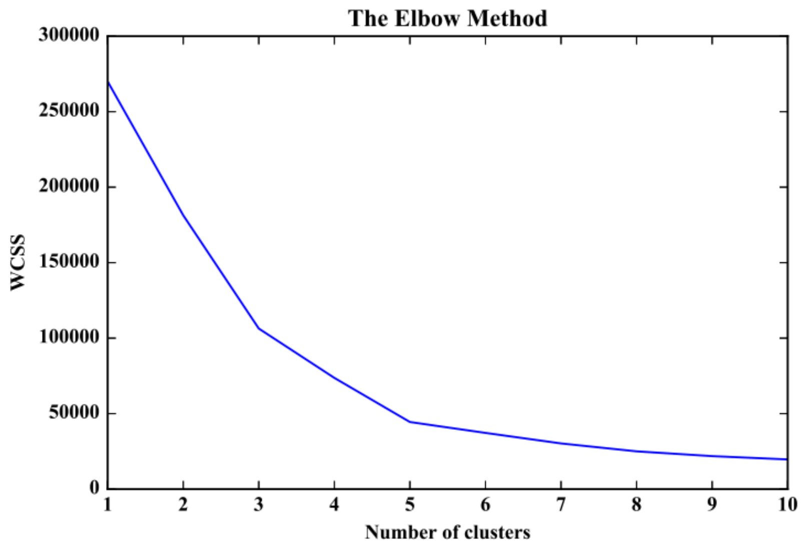
$$S(x_i) = \frac{b - a}{max(b, a)}$$

where **a** = average distance of point $\mathbf{x_i}$ from points in its own cluster and,
b = average distance of point $\mathbf{x_i}$ from all the points of the nearest cluster.

- The range of the Silhouette score is **[-1, 1]**.
  - ➔ A Silhouette score near +1 indicates that the sample is far away from its neighboring cluster.
  - ➔ A value near 0 represents overlapping clusters with samples very close to the decision boundary of the neighboring clusters.
  - ➔ A Silhouette score of -1 indicates that the samples have been assigned to the wrong clusters.

Elbow method

- It is a method to determine the optimal number of clusters (**k**) for k-means clustering.
- We perform the k-means clustering for a range of values of **k** and for each iteration, we calculate the value of the WCSS metric.
- When the value of WCSS is plotted against a range of **k** values, we get a plot that looks like an elbow.



- We can see that the WCSS value decreases as the number of clusters (k) increases.

- At some point on the graph, there is a sharp change in the slope (k = 5) after which the change in slope is very small. The k value corresponding to this point is the optimal K value or an **optimal** number of clusters.

- If we do not get a sharp change in the slope of the elbow plot while using the WCSS metric on the y-axis, we can try using the **Silhouette score** to get significant results or to get confidence in our decision.