

COMP 3010J Tutorial

Clustering

Q1(a)

The dataset contains 10 examples represented by 4 numeric features.

These examples have been randomly assigned to two clusters in order to initialise the k-Means algorithm.

The assignments are as follows:

$$C1 = \{ x1, x3, x7, x8 \}$$

$$C2 = \{ x2, x4, x5, x6, x9, x10 \}$$

| | f1 | f2 | f3 | f4 |
|-----|-----|-----|-----|-----|
| x1 | 5.1 | 3.8 | 1.6 | 0.2 |
| x2 | 4.6 | 3.2 | 1.4 | 0.2 |
| x3 | 5.3 | 3.7 | 1.5 | 0.2 |
| x4 | 5 | 3.3 | 1.4 | 0.2 |
| x5 | 7 | 3.2 | 4.7 | 1.4 |
| x6 | 6.4 | 3.2 | 4.5 | 1.5 |
| x7 | 6.9 | 3.1 | 4.9 | 1.5 |
| x8 | 5.5 | 2.3 | 4 | 1.3 |
| x9 | 6.5 | 2.8 | 4.6 | 1.5 |
| x10 | 5.7 | 2.8 | 4.5 | 1.3 |

Based on the data and cluster assignments, calculate the centroid vector for each cluster.

Q1(a)

- Recall - k -Means objective:

Centroid = mean of examples in cluster

$$SSE(C) = \sum_{c=1}^k \sum_{x_i \in C_c} D(x_i, \mu_c)^2 \quad \text{where} \quad \mu_c = \frac{\sum_{x_i \in C_c} x_i}{|C_c|}$$

| | f1 | f2 | f3 | f4 |
|-----|-----|-----|-----|-----|
| x1 | 5.1 | 3.8 | 1.6 | 0.2 |
| x2 | 4.6 | 3.2 | 1.4 | 0.2 |
| x3 | 5.3 | 3.7 | 1.5 | 0.2 |
| x4 | 5 | 3.3 | 1.4 | 0.2 |
| x5 | 7 | 3.2 | 4.7 | 1.4 |
| x6 | 6.4 | 3.2 | 4.5 | 1.5 |
| x7 | 6.9 | 3.1 | 4.9 | 1.5 |
| x8 | 5.5 | 2.3 | 4 | 1.3 |
| x9 | 6.5 | 2.8 | 4.6 | 1.5 |
| x10 | 5.7 | 2.8 | 4.5 | 1.3 |

$$C1 = \{ x1, x3, x7, x8 \}$$

$$C2 = \{ x2, x4, x5, x6, x9, x10 \}$$

| Cluster 1 | f1 | f2 | f3 | f4 |
|------------|------|------|------|------|
| x1 | 5.1 | 3.8 | 1.6 | 0.2 |
| x3 | 5.3 | 3.7 | 1.5 | 0.2 |
| x7 | 6.9 | 3.1 | 4.9 | 1.5 |
| x8 | 5.5 | 2.3 | 4 | 1.3 |
| Centroid 1 | 5.70 | 3.23 | 3.00 | 0.80 |

| Cluster 2 | f1 | f2 | f3 | f4 |
|------------|------|------|------|------|
| x2 | 4.6 | 3.2 | 1.4 | 0.2 |
| x4 | 5 | 3.3 | 1.4 | 0.2 |
| x5 | 7 | 3.2 | 4.7 | 1.4 |
| x6 | 6.4 | 3.2 | 4.5 | 1.5 |
| x9 | 6.5 | 2.8 | 4.6 | 1.5 |
| x10 | 5.7 | 2.8 | 4.5 | 1.3 |
| Centroid 2 | 5.87 | 3.08 | 3.52 | 1.02 |

(rounded to 2 decimal places)

Q1(b)

- Based on the centroids calculated above, which clusters will the examples $x1$ and $x10$ next be assigned to? Calculate distances using the Euclidean distance measure.

| | f1 | f2 | f3 | f4 |
|-------------------|------|------|------|------|
| x1 | 5.10 | 3.80 | 1.60 | 0.20 |
| Centroid 1 | 5.70 | 3.23 | 3.00 | 0.80 |
| Centroid 2 | 5.87 | 3.08 | 3.52 | 1.02 |

$$D(x, \mu) = \sqrt{\sum_{l=1}^m (x_l - \mu_l)^2}$$

$$D(x1, C1) = \sqrt{(5.10 - 5.70)^2 + (3.80 - 3.22)^2 + (1.60 - 3.00)^2 + (0.20 - 0.80)^2} = 1.74$$

$$D(x1, C2) = \sqrt{(5.10 - 5.87)^2 + (3.80 - 3.08)^2 + (1.60 - 3.52)^2 + (0.20 - 1.02)^2} = 2.33$$

$$D(x1, C1) = 1.74 \quad D(x1, C2) = 2.33 \quad \Rightarrow \quad \text{Assign to C1}$$

Q1(b)

- Based on the centroids calculated above, which clusters will the examples $x1$ and $x10$ next be assigned to? Calculate distances using the Euclidean distance measure.

| | f1 | f2 | f3 | f4 |
|-------------------|------|------|------|------|
| x10 | 5.70 | 2.80 | 4.50 | 1.30 |
| Centroid 1 | 5.70 | 3.23 | 3.00 | 0.80 |
| Centroid 2 | 5.87 | 3.08 | 3.52 | 1.02 |

$$D(x, \mu) = \sqrt{\sum_{l=1}^m (x_l - \mu_l)^2}$$

$$D(x10, C1) = \sqrt{(5.70 - 5.70)^2 + (2.80 - 3.22)^2 + (4.50 - 3.00)^2 + (1.30 - 0.80)^2} = 1.64$$

$$D(x10, C2) = \sqrt{(5.70 - 5.87)^2 + (2.80 - 3.08)^2 + (4.50 - 3.52)^2 + (1.30 - 1.02)^2} = 1.07$$

$$D(x10, C1) = 1.64 \quad D(x10, C2) = 1.07 \quad \Rightarrow \quad \text{Assign to C2}$$

Q2

- If the cluster $C1 = \{x1, x3\}$, use the Euclidean distance measure to calculate the distances between the example $x2$ and cluster $C1$ based on *single*, *complete*, and *average linkage*.

| | f1 | f2 |
|----|-----|-----|
| x1 | 1.3 | 1.5 |
| x2 | 0.5 | 2.4 |
| x3 | 0.0 | 3.0 |

Step 1: Calculate Euclidean distances

$$D(x1, x2) = 1.20$$

$$D(x1, x3) = 1.98$$

$$D(x2, x3) = 0.78$$

Step 2: Calculate linkage metrics

$$\text{Single: } D(x2, C1) = \min(1.20, 0.78) = 0.78$$

$$\text{Complete: } D(x2, C1) = \max(1.20, 0.78) = 1.20$$

$$\text{Average: } D(x2, C1) = (1.20 + 0.78) / 2 = 0.99$$

Q3

- The following table depicts a pairwise distance matrix for 5 examples.
- Calculate the dendrogram representing the agglomerative hierarchical clustering of these examples based on the single-linkage method.
- The answer should illustrate the distance matrices originating from each clustering step.

e.g. $D(x_3, x_1) = 6$
and $D(x_1, x_3) = 6$

| | x1 | x2 | x3 | x4 | x5 |
|----|----|----|----|----|----|
| x1 | 0 | | | | |
| x2 | 2 | 0 | | | |
| x3 | 6 | 5 | 0 | | |
| x4 | 10 | 9 | 4 | 0 | |
| x5 | 9 | 8 | 5 | 3 | 0 |

Q3

| | x1 | x2 | x3 | x4 | x5 |
|----|----|----|----|----|----|
| x1 | 0 | | | | |
| x2 | 2 | 0 | | | |
| x3 | 6 | 5 | 0 | | |
| x4 | 10 | 9 | 4 | 0 | |
| x5 | 9 | 8 | 5 | 3 | 0 |

- 1** Start with everything in its own cluster:
Clusters: $\{x1\}, \{x2\}, \{x3\}, \{x4\}, \{x5\}$
Identify nearest pair via single linkage
Min distance $\Rightarrow D(x1, x2) = 2$
Merge: $C1 = \{x1, x2\}$

- 2** Clusters: $C1, \{x3\}, \{x4\}, \{x5\}$
Calculate distance matrix via single linkage
e.g. $D(C1, x3) = \min(6, 5)$
Min distance $\Rightarrow D(x4, x5) = 3$
Merge: $C2 = \{x4, x5\}$

| | C1 | x3 | x4 | x5 |
|----|----|----|----|----|
| C1 | 0 | | | |
| x3 | 5 | 0 | | |
| x4 | 9 | 4 | 0 | |
| x5 | 8 | 5 | 3 | 0 |

- 3** Clusters: $C1, \{x3\}, C2$
Calculate distance matrix via single linkage
e.g. $D(C1, C2) = \min(10, 9, 9, 8) = 8$
Min distance $\Rightarrow D(C2, x3) = 4$
Merge: $C3 = \{x3, x4, x5\}$

| | C1 | x3 | C2 |
|----|----|----|----|
| C1 | 0 | | |
| x3 | 5 | 0 | |
| C2 | 8 | 4 | 0 |

Q3

- 4** Clusters: $C1$, $C3$ where $C1 = \{x1, x2\}$, $C3 = \{x3, x4, x5\}$
Only 2 clusters remain, so merge into root node $C4$

Construct dendrogram based on the merges at each level...

