COMP47460 Tutorial

Clustering

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Tutorial 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.

Tutorial Q1(a)

- Recall - *k*-Means objective:

Centroid = mean of examples in cluster

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

	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)

Tutorial 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   *D(x1,C2) = 2.33*   =>   Assign to C1

Tutorial 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 *D(x10,C2) = 1.07* => Assign to C2

Tutorial 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

Single: D(x2,C1) = min(1.20,0.78) = 0.78

Complete: D(x2,C1) = max(1.20,0.78) = 1.20

Average: D(x2,C1) = (1.20+0.78)/2 = 0.99

Tutorial 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(x3,x1) = 6
and D(x1,x3) = 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

Tutorial 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 ⇒ 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 ⇒ 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 ⇒ D(C2,x3) = 4

Merge: C3 = {x3,x4,x5}

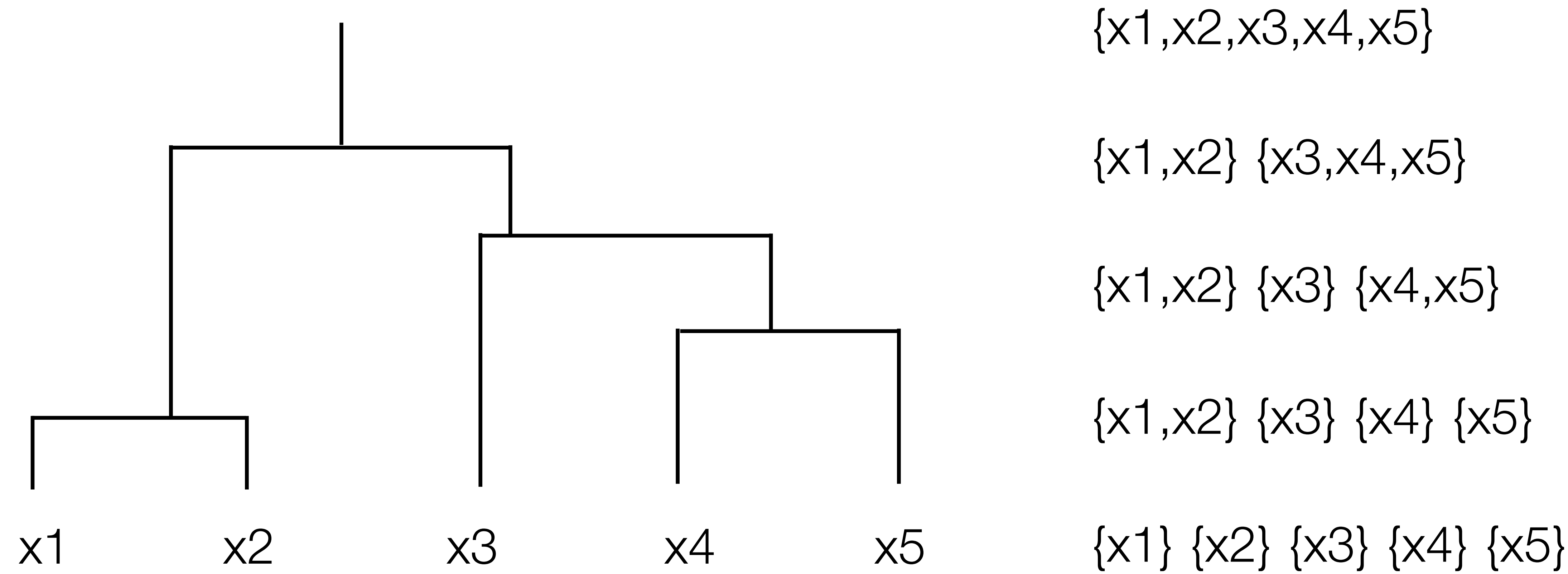
	C1	x3	C2
C1	0		
x3	5	0	
C2	8	4	0

Tutorial 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…

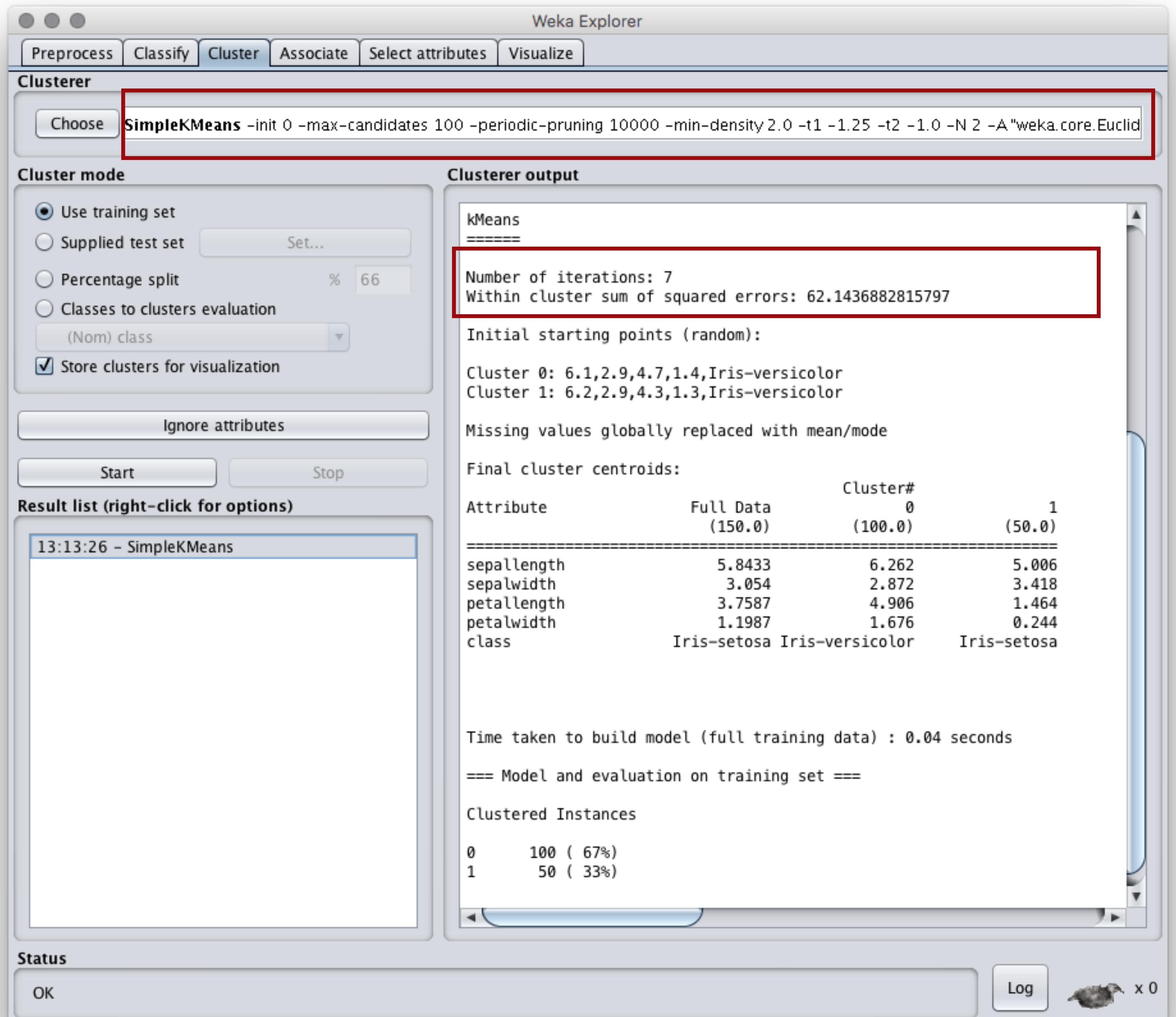


Tutorial Q4

In Weka, apply *k*-Means with Euclidean distance to the Iris ARFF dataset. Report the Within cluster sum of squared errors (SSE) for runs with different numbers of clusters: *k=2, k=3* and *k=4.*

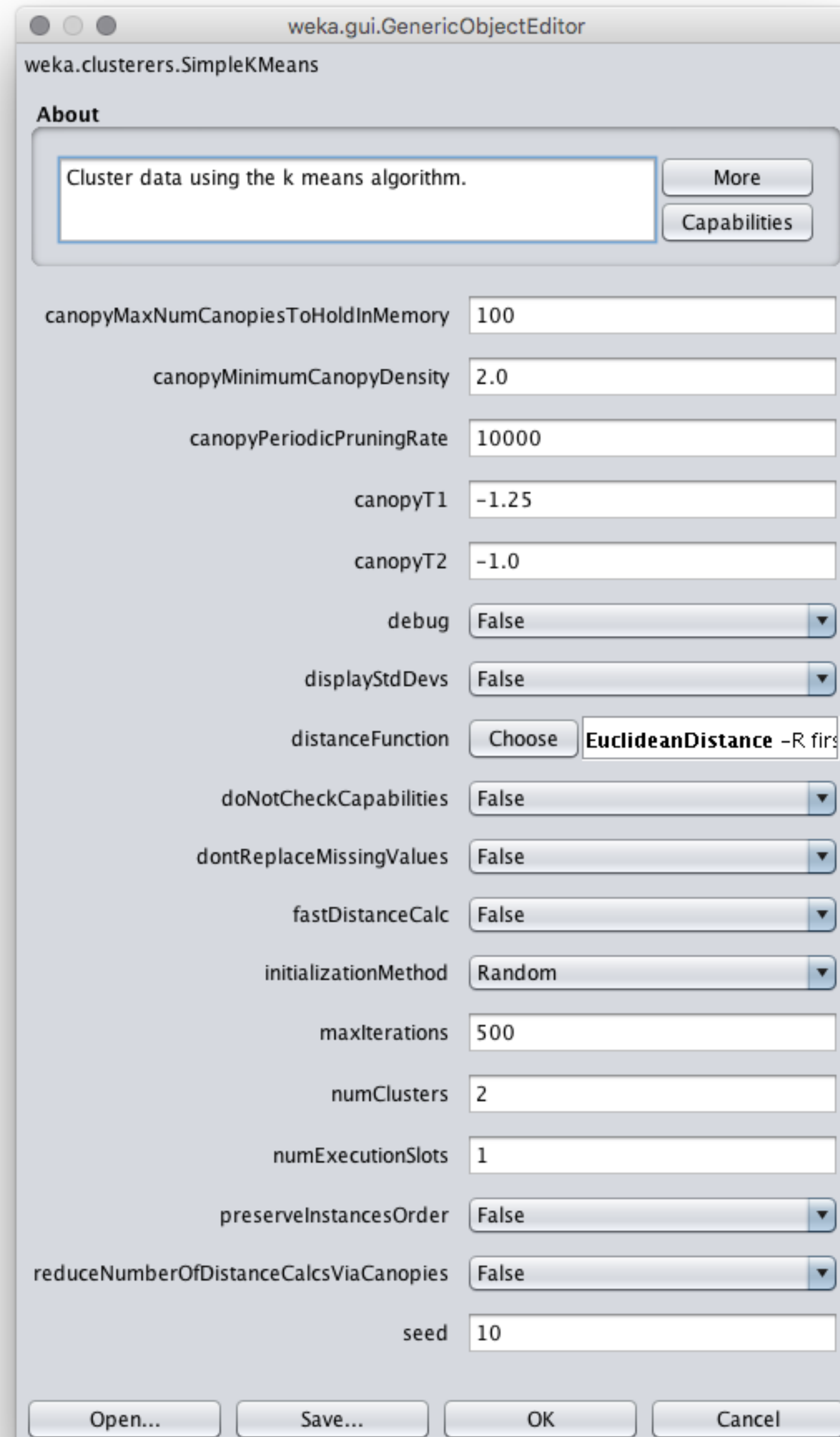
Tutorial Q4

- In *Cluster* tab, choose *SimpleKMeans* as the clusterer. Change options for *numClusters* to 2, 3, 4.



Tutorial Q4

- In the *Cluster* tab, choose *SimpleKMeans* as the clusterer.
- Change options for *numClusters* to 2, 3, 4.
- Use the default random *seed* (10).



Tutorial Q4

- Report the within cluster *sum of squared errors* (SSE) for runs with different numbers of clusters: *k=2, k=3* and *k=4.*
- Use default random seed (*seed=10*)

numClusters=2

Within cluster sum of squared errors: 62.1436882815797

numClusters=3

Within cluster sum of squared errors: 7.817456892309574

numClusters=4

Within cluster sum of squared errors: 6.613823274690356

Tutorial Q4

- Repeat the above process again, but change the random seed parameter for k-Means. Are the SSE scores identical? If not, explain why not.

Set random seed to - e.g seed = 100

Changing random seed affects initial random clusters

numClusters=2

Within cluster sum of squared errors: $\boxed{62.143688281579706}$

numClusters=3

Within cluster sum of squared errors: $\boxed{60.90827498962252}$

numClusters=4

Within cluster sum of squared errors: $\boxed{6.856549502288228}$