COMP30120 Tutorial

Clustering

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Autumn 2015

Tutorial Q1(a)

The data set contains 10 items represented by 4 numeric features.

These items 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 }

Item	Feature1	Feature2	Feature3	Feature4
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 items in cluster

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

Item	Feature1	Feature2	Feature3	Feature4
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	Feature1	Feature2	Feature3	Feature4
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	Feature1	Feature2	Feature3	Feature4
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 items *x1* and *x10* next be assigned to? Calculate distances using the Euclidean distance measure.

	Feature1	Feature2	Feature3	Feature4
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 items *x1* and *x10* next be assigned to? Calculate distances using the Euclidean distance measure.

	Feature1	Feature2	Feature3	Feature4
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(a)

- Describe the difference between the *single-linkage, complete* and *average linkages*, which are used as cluster metrics in Agglomerative Hierarchical Clustering.

- Single linkage: Define cluster distance as the smallest pairwise distance between items from each cluster.

$$d(C_a, C_b) = \min_{x_i \in C_a, x_j \in C_b} D_{ij}$$

- Complete linkage: Define cluster distance as the largest pairwise distance between items from each cluster.

$$d(C_a, C_b) = \max_{x_i \in C_a, x_j \in C_b} D_{ij}$$

- Average linkage: Define cluster distance as the average of all pairwise distances between items from each cluster.

$$d(C_a, C_b) = \frac{\sum_{x_i \in C_a} \sum_{x_j \in C_b} D_{ij}}{|C_a|\,|C_b|}$$

Tutorial Q2(b)

- Calculate the distances between *x2* and *C1* using single, complete and average linkage for the data below, if the cluster *C1 = {x1, x3}*. Assume that distances between items are calculated using Euclidean distance.

Item	Feature1	Feature2
x1	1.3	1.5
x2	0.5	2.4
x3	0.0	3.0

Pairwise Euclidean distances

D(x1,x2) = 1.20

D(x1,x3) = 1.98

D(x2,x3) = 0.78

Linkage scores

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 items.
- Calculate the dendrogram representing the agglomerative hierarchical clustering of these items based on the single-linkage method.
- The answer should illustrate the distance matrices originating from each clustering step.

	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}

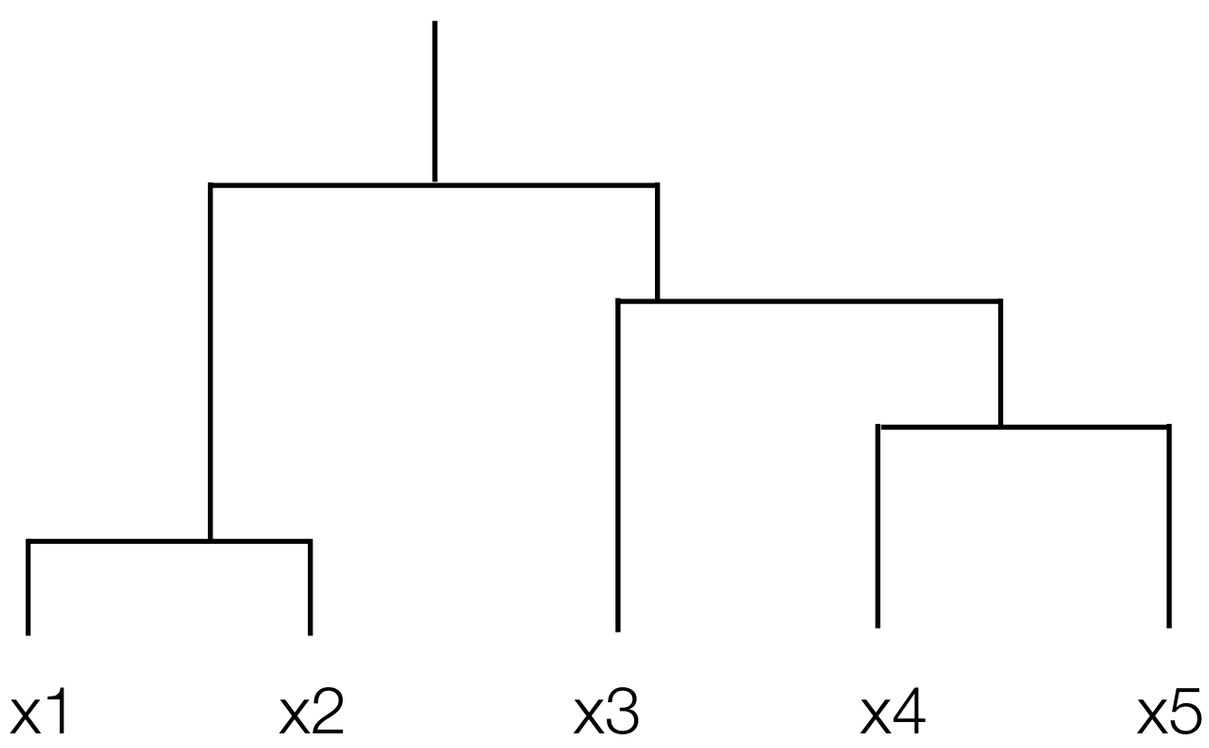
	C1	x3	C2
C1	0		
x3	5	0	
C2	8	4	0

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…



{x1,x2,x3,x4,x5}

{x1,x2} {x3,x4,x5}

{x1,x2} {x3} {x4,x5}

{x1,x2} {x3} {x4} {x5}

{x1} {x2} {x3} {x4} {x5}

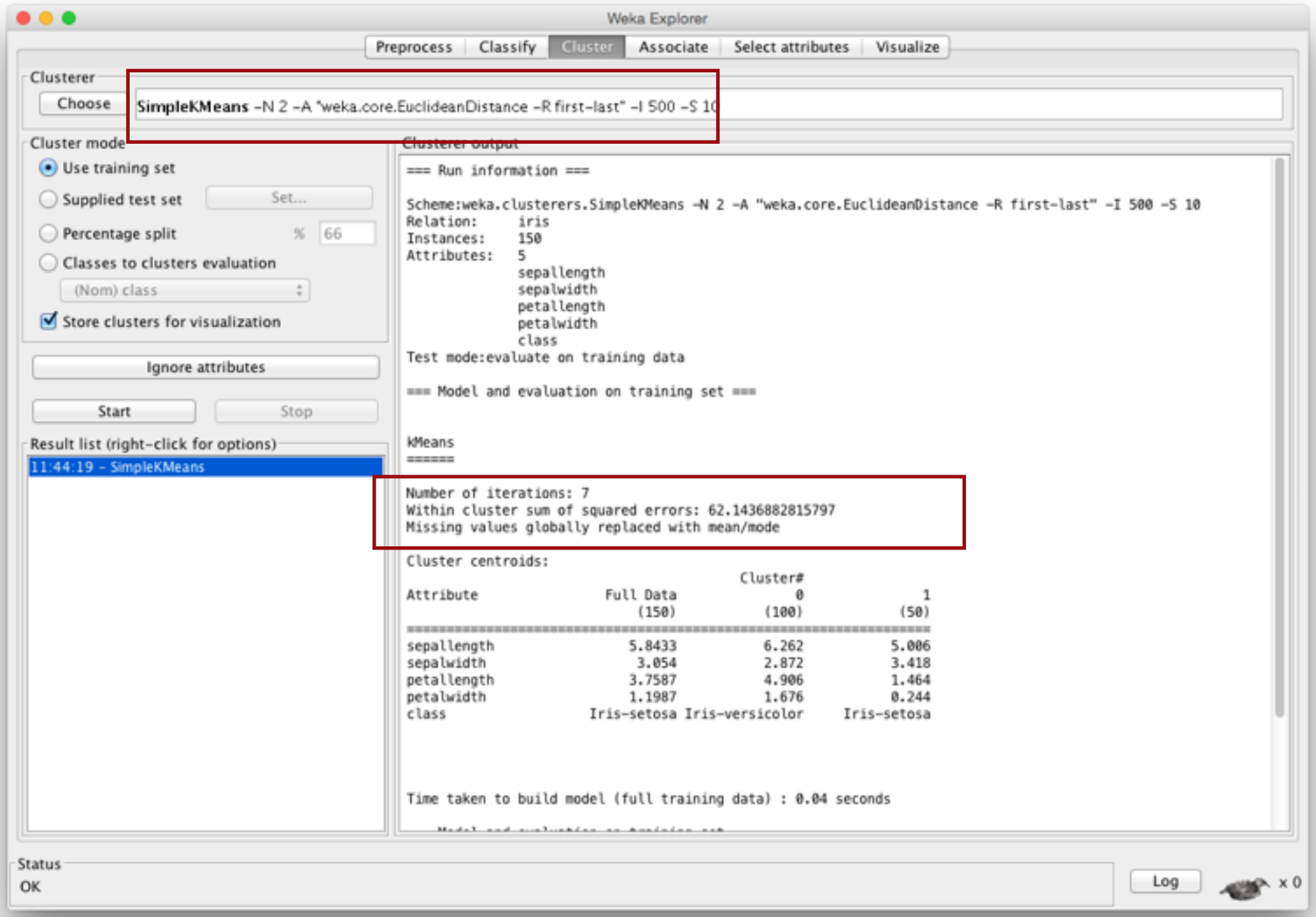
Tutorial Q4

In Weka, apply *k*-Means with Euclidean distance to the Iris ARFF dataset provided on the course Moodle page.

Report the Within cluster sum of squared errors (SSE) for runs with different numbers of clusters: *k=2, k=3* and *k=4.*

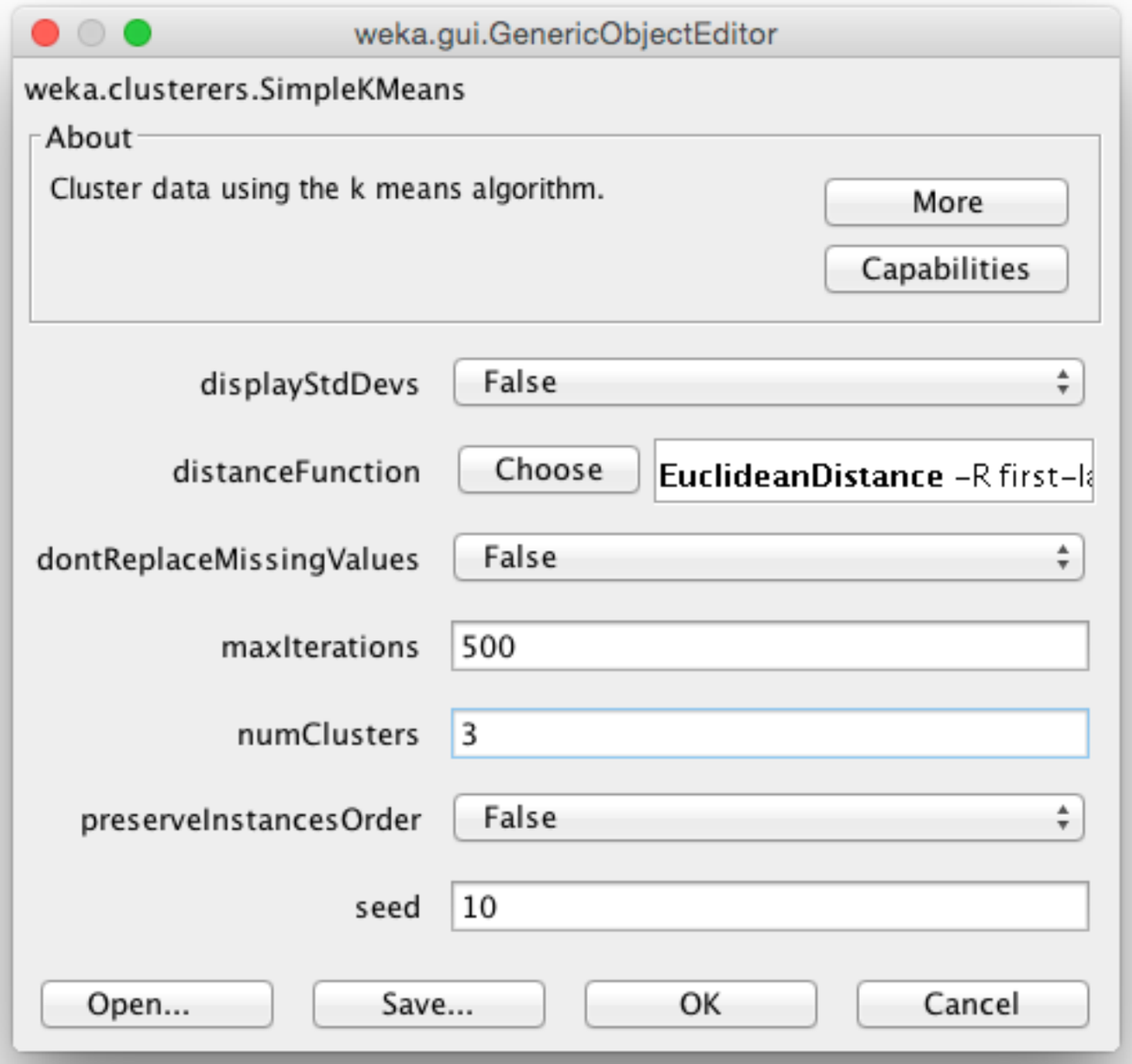
Tutorial Q4

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



Tutorial Q4

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



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.*

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