Workshop Week 6

COMP20008

Consider the 1-dimensional data set with 10 data points {1,2,3,...10}. Show the iterations of the k-means algorithm using Euclidean distance when k = 2, and the random seeds are initialized to {1, 2}.

- Iteration 1 Data points: [1 2 3 4 5 6 7 8 9 10] Assignments: [0, 1, 1, 1, 1, 1, 1, 1, 1, 1] Centroids: [1.0, 6.0]

- Iteration 2 Data points: [1 2 3 4 5 6 7 8 9 10] Assignments: [0, 0, 0, 1, 1, 1, 1, 1, 1, 1] Centroids: [2.0, 7.0]

- Iteration 3 Data points: [1 2 3 4 5 6 7 8 9 10] Assignments: [0, 0, 0, 0, 1, 1, 1, 1, 1, 1] Centroids: [2.5, 7.5]

Consider the 1-dimensional data set with 10 data points {1,2,3,...10}. Show the iterations of the k-means algorithm using Euclidean distance when k = 2, and the random seeds are initialized to {1, 2}.

- Iteration 4 Data points: [1 2 3 4 5 6 7 8 9 10] Assignments: [0, 0, 0, 0, 0, 1, 1, 1, 1, 1] Centroids: [3.0, 8.0]

- Iteration 5 Data points: [1 2 3 4 5 6 7 8 9 10] Assignments: [0, 0, 0, 0, 0, 1, 1, 1, 1, 1] Centroids: [3.0, 8.0]

Repeat Exercise 1 using agglomerative hierarchical clustering and Euclidean distance,
with single linkage (min) criterion.

	1	2	3	4	5	6	7	8	9	10
1	0									
2	1	0								
3	2		0							
4	3			0						
5	4				0					
6	5					0				
7	6						0			
8	7							0		
9	8								0	
10	9									0

Initially, how many clusters do we have?

Dissimilarity Matrix

	1	2	3	4	5	6	7	8	9	10
1	0	1	2	3	4	5	6	7	8	9
2	1	0	1	2	3	4	5	6	7	8
3	2	1	0	1	2	3	4	5	6	7
4	3	2	1	0	1	2	3	4	5	6
5	4	3	2	1	0	1	2	3	4	5
6	5	4	3	2	1	0	1	2	3	4
7	6	5	4	3	2	1	0	1	2	3
8	7	6	5	4	3	2	1	0	1	2
9	8	7	6	5	4	3	2	1	0	1
10	9	8	7	6	5	4	3	2	1	0

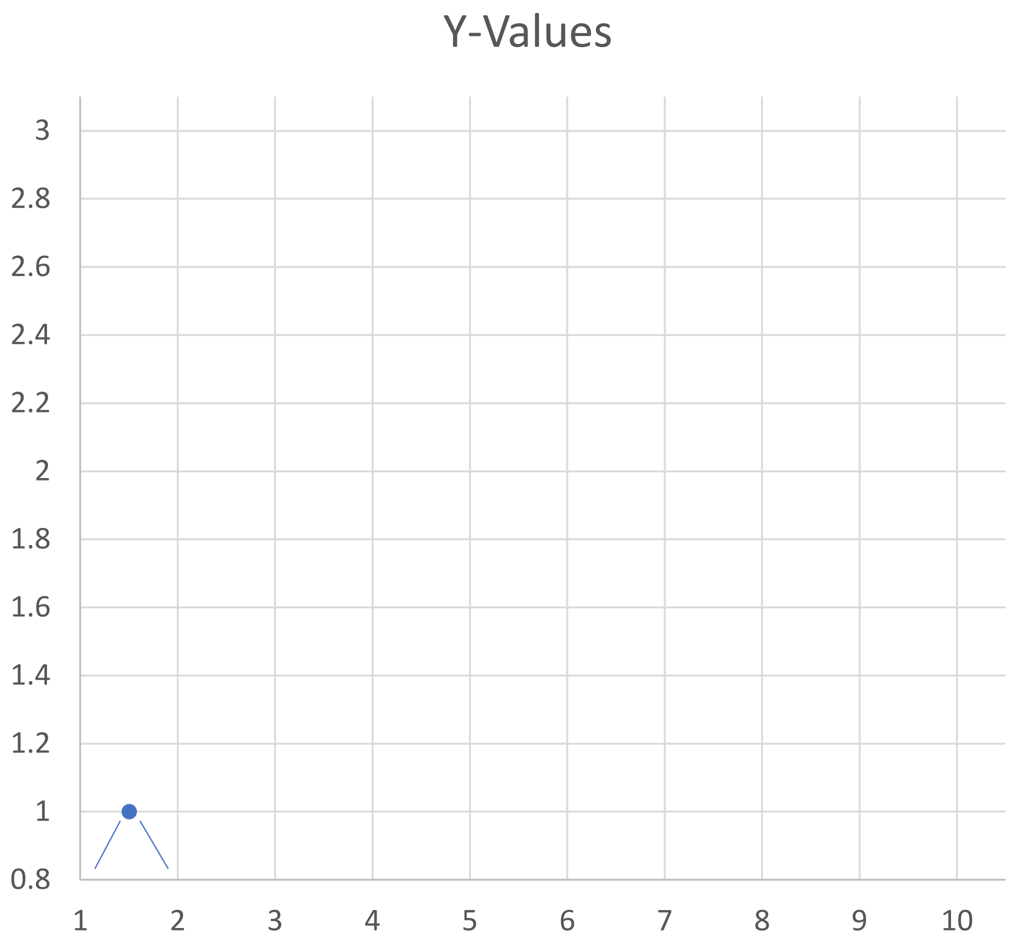
Inter-point distance Matrix

Step1: Calculate Distances between every pair of observation: Euclidean Distance

Dissimilarity Matrix

	1	2	3	4	5	6	7	8	9	10
1	0	1	2	3	4	5	6	7	8	9
2	1	0	1	2	3	4	5	6	7	8
3	2	1	0	1	2	3	4	5	6	7
4	3	2	1	0	1	2	3	4	5	6
5	4	3	2	1	0	1	2	3	4	5
6	5	4	3	2	1	0	1	2	3	4
7	6	5	4	3	2	1	0	1	2	3
8	7	6	5	4	3	2	1	0	1	2
9	8	7	6	5	4	3	2	1	0	1
10	9	8	7	6	5	4	3	2	1	0

Inter-point distance Matrix



Dendrogram Plot
X-axis → observations , Y-axis → distances

Step 2: Choose the most similar two observations to merge (i.e. Closest)

(i.e. pair with the minimum distance in Dissimilarity Matrix)

Dissimilarity Matrix

	1	2	3	4	5	6	7	8	9	10
1	0	1	2	3	4	5	6	7	8	9
2	1	0	1	2	3	4	5	6	7	8
3	2	1	0	1	2	3	4	5	6	7
4	3	2	1	0	1	2	3	4	5	6
5	4	3	2	1	0	1	2	3	4	5
6	5	4	3	2	1	0	1	2	3	4
7	6	5	4	3	2	1	0	1	2	3
8	7	6	5	4	3	2	1	0	1	2
9	8	7	6	5	4	3	2	1	0	1
10	9	8	7	6	5	4	3	2	1	0

Inter-point distance Matrix

	12	3	4	5	6	7	8	9	10
12	0	1							
3	1	0	1	2	3	4	5	6	7
4		1	0	1	2	3	4	5	6
5		2	1	0	1	2	3	4	5
6		3	2	1	0	1	2	3	4
7		4	3	2	1	0	1	2	3
8		5	4	3	2	1	0	1	2
9		6	5	4	3	2	1	0	1
10		7	6	5	4	3	2	1	0

Step 3: Update Dissimilarity Matrix: Calculate the distance between Cluster12 and all other observations (calculate linkage using min)

Dissimilarity Matrix

	1	2	3	4	5	6	7	8	9	10
1	0	1	2	3	4	5	6	7	8	9
2	1	0	1	2	3	4	5	6	7	8
3	2	1	0	1	2	3	4	5	6	7
4	3	2	1	0	1	2	3	4	5	6
5	4	3	2	1	0	1	2	3	4	5
6	5	4	3	2	1	0	1	2	3	4
7	6	5	4	3	2	1	0	1	2	3
8	7	6	5	4	3	2	1	0	1	2
9	8	7	6	5	4	3	2	1	0	1
10	9	8	7	6	5	4	3	2	1	0

Inter-point distance Matrix

	12	3	4	5	6	7	8	9	10
12	0	1	2	3	4	5	6	7	8
3	1	0	1	2	3	4	5	6	7
4	2	1	0	1	2	3	4	5	6
5	3	2	1	0	1	2	3	4	5
6	4	3	2	1	0	1	2	3	4
7	5	4	3	2	1	0	1	2	3
8	6	5	4	3	2	1	0	1	2
9	7	6	5	4	3	2	1	0	1
10	8	7	6	5	4	3	2	1	0

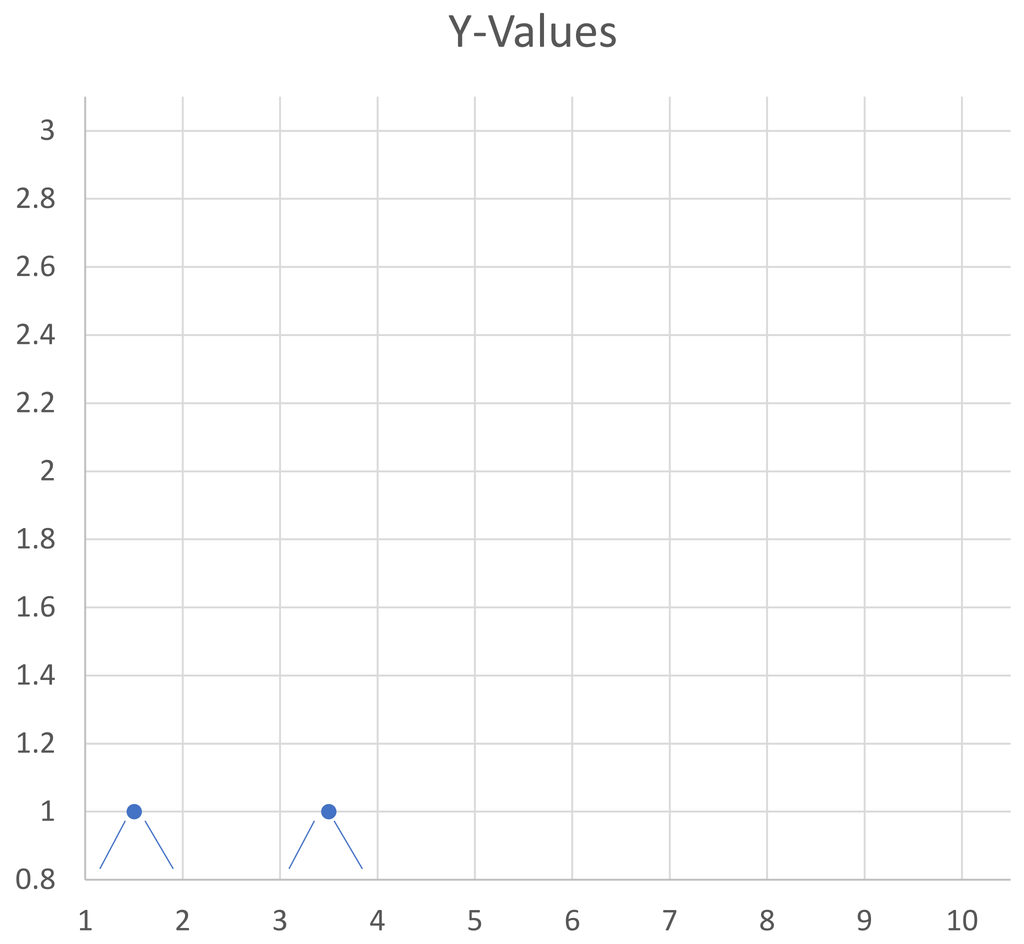
Step 3: Update Dissimilarity Matrix: Calculate the distance between Cluster12 and all other observations (calculate linkage using min)

How many clusters do we have now?

Updated Dissimilarity Matrix

	12	3	4	5	6	7	8	9	10
12	0	1	2	3	4	5	6	7	8
3	1	0	1	2	3	4	5	6	7
4	2	1	0	1	2	3	4	5	6
5	3	2	1	0	1	2	3	4	5
6	4	3	2	1	0	1	2	3	4
7	5	4	3	2	1	0	1	2	3
8	6	5	4	3	2	1	0	1	2
9	7	6	5	4	3	2	1	0	1
10	8	7	6	5	4	3	2	1	0

Updated distance Matrix



Extended Dendrogram Plot
X-axis → observations , Y-axis → distances

Repeat Step 2: Choose the most similar two observations to merge (i.e. Closest)
(i.e. pair with the minimum distance in Dissimilarity Matrix)

Dissimilarity Matrix

	12	34	5	6	7	8	9	10
12	0		3	4	5	6	7	8
34		0						
5	3		0	1	2	3	4	5
6	4		1	0	1	2	3	4
7	5		2	1	0	1	2	3
8	6		3	2	1	0	1	2
9	7		4	3	2	1	0	1
10	8		5	4	3	2	1	0

Inter-point distance Matrix

	12	3	4	5	6	7	8	9	10
12	0	1	2	3	4	5	6	7	8
3	1	0	1	2	3	4	5	6	7
4	2	1	0	1	2	3	4	5	6
5	3	2	1	0	1	2	3	4	5
6	4	3	2	1	0	1	2	3	4
7	5	4	3	2	1	0	1	2	3
8	6	5	4	3	2	1	0	1	2
9	7	6	5	4	3	2	1	0	1
10	8	7	6	5	4	3	2	1	0

Repeat Step 3: Update Dissimilarity Matrix: Calculate the distance between Cluster12 and all other observations (calculate single linkage using min)

Dissimilarity Matrix

	12	3	4	5	6	7	8	9	10
12	0	1	2	3	4	5	6	7	8
3	1	0	1	2	3	4	5	6	7
4	2	1	0	1	2	3	4	5	6
5	3	2	1	0	1	2	3	4	5
6	4	3	2	1	0	1	2	3	4
7	5	4	3	2	1	0	1	2	3
8	6	5	4	3	2	1	0	1	2
9	7	6	5	4	3	2	1	0	1
10	8	7	6	5	4	3	2	1	0

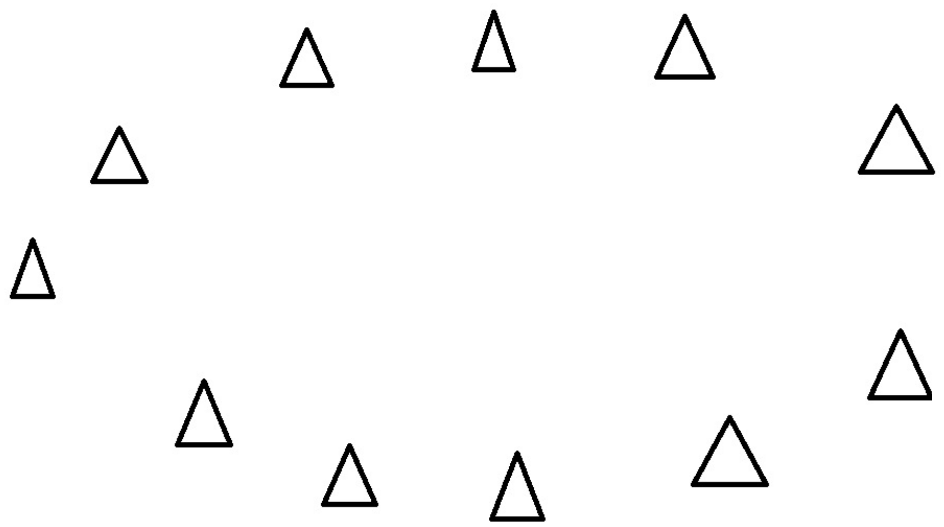
Inter-point distance Matrix

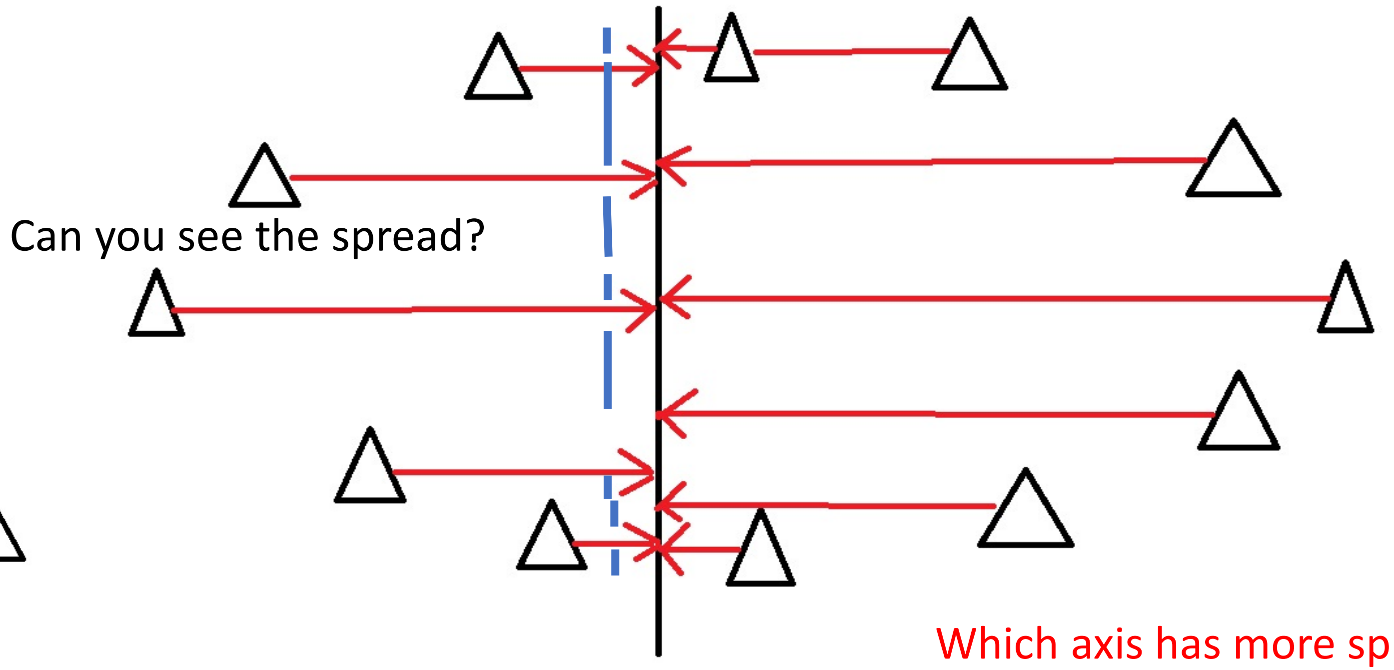
	12	34	5	6	7	8	9	10
12	0	1	3	4	5	6	7	8
34	1	0	1	2	3	4	5	6
5	3	1	0	1	2	3	4	5
6	4	2	1	0	1	2	3	4
7	5	3	2	1	0	1	2	3
8	6	4	3	2	1	0	1	2
9	7	5	4	3	2	1	0	1
10	8	6	5	4	3	2	1	0

Let’s see some python code

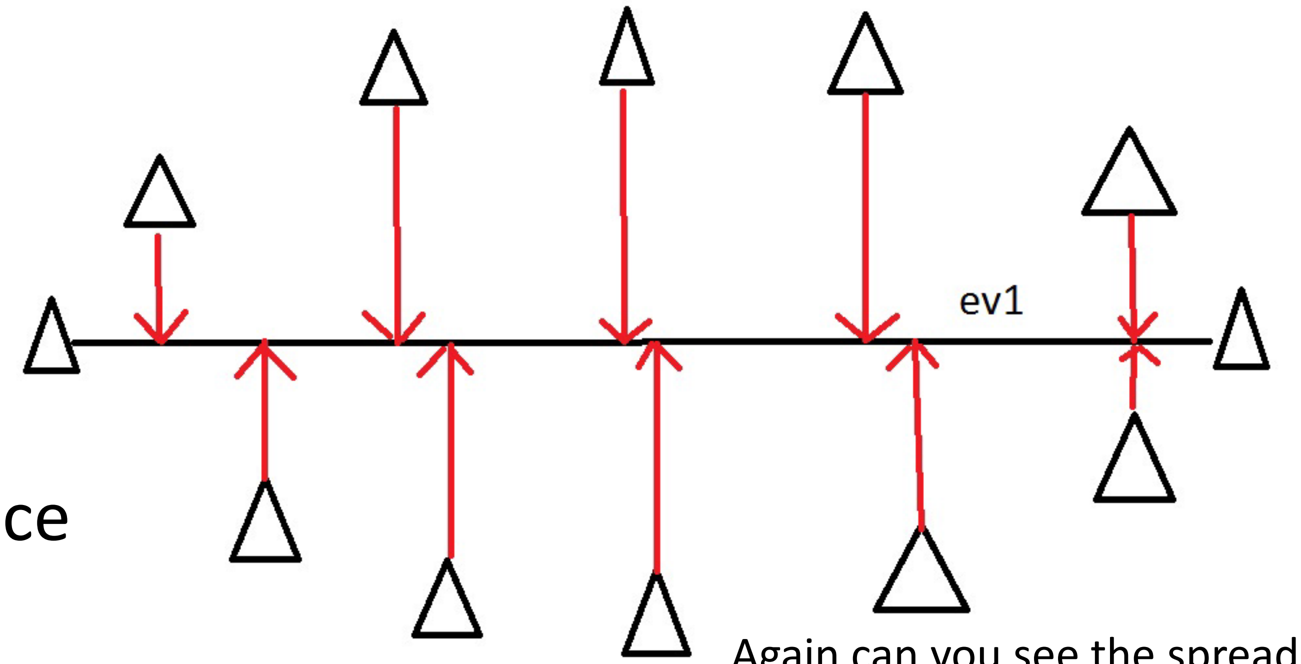
Repeat Step 3: Update Dissimilarity Matrix: Calculate the distance between Cluster12 and all other observations (calculate linkage using min)

Principal Component Analysis





Which axis has more spread, horizontal or vertical?



Principal Components:

- Directions with the most variance

- PCA Idea: Find the new axis lines (i.e. principal components) with the largest variance among data

- **2D example:**

http://setosa.io/ev/principal-component-analysis/

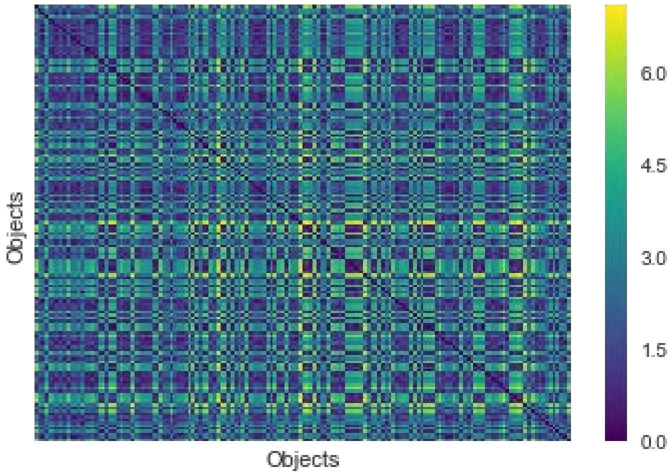
Key point: how much we will lose if we remove pc2?

- **3D example:**

Key point: visualization using pc1 and pc2

Visual Assessment for Clustering Tendency (VAT)

- From dissimilarity matrix to heatmap



- Reordering heatmap to make sense of how many cluster are there is the main idea for VAT