Tutorial exercises
Clustering – K-means, Nearest Neighbor and Hierarchical.

Exercise 1. ***K-means clustering***

Use the k-means algorithm and Euclidean distance to cluster the following 8 examples into 3 clusters:
A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9).
The distance matrix based on the Euclidean distance is given below:

	A1	A2	A3	A4	A5	A6	A7	A8
A1	0	$\sqrt{25}$	$\sqrt{36}$	$\sqrt{13}$	$\sqrt{50}$	$\sqrt{52}$	$\sqrt{65}$	$\sqrt{5}$
A2		0	$\sqrt{37}$	$\sqrt{18}$	$\sqrt{25}$	$\sqrt{17}$	$\sqrt{10}$	$\sqrt{20}$
A3			0	$\sqrt{25}$	$\sqrt{2}$	$\sqrt{2}$	$\sqrt{53}$	$\sqrt{41}$
A4				0	$\sqrt{13}$	$\sqrt{17}$	$\sqrt{52}$	$\sqrt{2}$
A5					0	$\sqrt{2}$	$\sqrt{45}$	$\sqrt{25}$
A6						0	$\sqrt{29}$	$\sqrt{29}$
A7							0	$\sqrt{58}$
A8								0

Suppose that the initial seeds (centers of each cluster) are A1, A4 and A7. Run the k-means algorithm for 1 epoch only. At the end of this epoch show:
a) The new clusters (i.e. the examples belonging to each cluster)
b) The centers of the new clusters
c) Draw a 10 by 10 space with all the 8 points and show the clusters after the first epoch and the new centroids.
d) How many more iterations are needed to converge? Draw the result for each epoch.

Solution:
a)
d(a,b) denotes the Eucledian distance between a and b. It is obtained directly from the distance matrix or calculated as follows: d(a,b)=sqrt($(x_b-x_a)^2+(y_b-y_a)^2$))
seed1=A1=(2,10), seed2=A4=(5,8), seed3=A7=(1,2)

epoch1 – start:

A1:
d(A1, seed1)=0 as A1 is seed1
d(A1, seed2)= $\sqrt{13}$ >0
d(A1, seed3)= $\sqrt{65}$ >0
➔A1 $\in$ cluster1

A2:
d(A2,seed1)= $\sqrt{25}$ = 5
d(A2, seed2)= $\sqrt{18}$ = 4.24
d(A2, seed3)= $\sqrt{10}$ = 3.16 ← smaller
➔ A2 $\in$ cluster3

A3:
d(A3, seed1)= $\sqrt{36}$ = 6
d(A3, seed2)= $\sqrt{25}$ = 5 ← smaller
d(A3, seed3)= $\sqrt{53}$ = 7.28
➔ A3 $\in$ cluster2

A4:
d(A4, seed1)= $\sqrt{13}$
d(A4, seed2)=0 as A4 is seed2
d(A4, seed3)= $\sqrt{52}$ >0
➔ A4 $\in$ cluster2

A5:
d(A5, seed1)= $\sqrt{50}$ = 7.07

A6:
d(A6, seed1)= $\sqrt{52}$ = 7.21

d(A5, seed2)= $\sqrt{13}$ = 3.60 ← smaller
d(A5, seed3)= $\sqrt{45}$ = 6.70
→ A5 $\in$ cluster2

d(A6, seed2)= $\sqrt{17}$ = 4.12 ← smaller
d(A6, seed3)= $\sqrt{29}$ = 5.38
→ A6 $\in$ cluster2

A7:
d(A7, seed1)= $\sqrt{65}$ >0
d(A7, seed2)= $\sqrt{52}$ >0
d(A7, seed3)=0 as A7 is seed3
→ A7 $\in$ cluster3

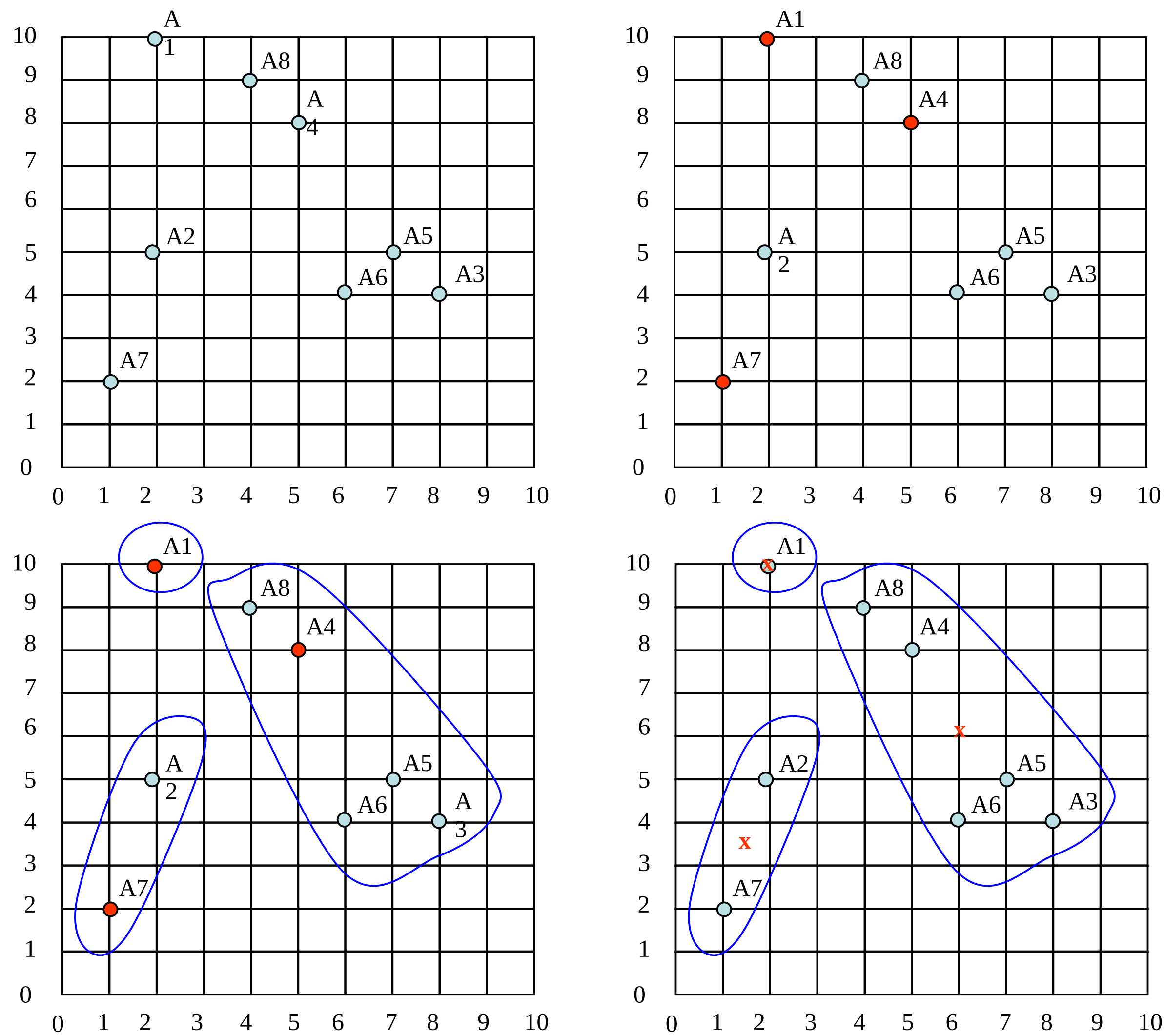
A8:
d(A8, seed1)= $\sqrt{5}$
d(A8, seed2)= $\sqrt{2}$ ← smaller
d(A8, seed3)= $\sqrt{58}$
→ A8 $\in$ cluster2

end of epoch1

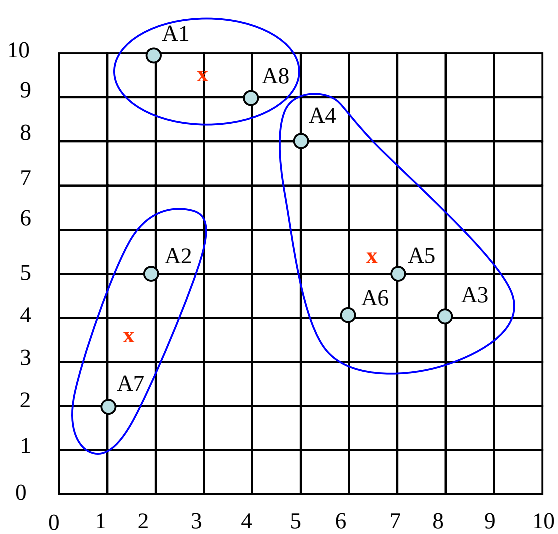
new clusters: 1: {A1}, 2: {A3, A4, A5, A6, A8}, 3: {A2, A7}

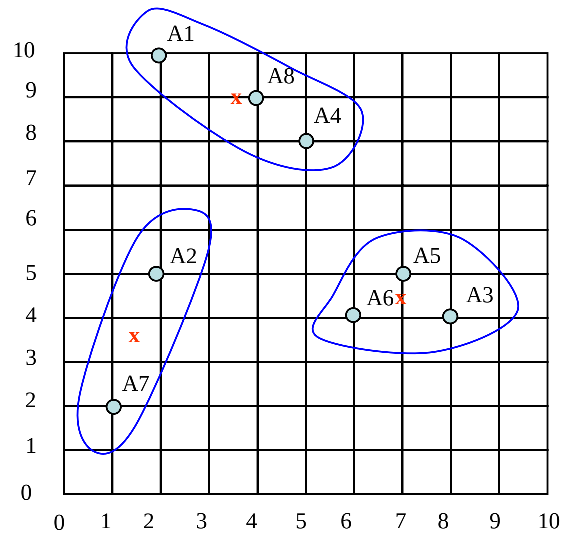
b) centers of the new clusters:
C1= (2, 10), C2= ((8+5+7+6+4)/5, (4+8+5+4+9)/5) = (6, 6), C3= ((2+1)/2, (5+2)/2) = (1.5, 3.5)

c)



d)
We would need two more epochs. After the 2nd epoch the results would be:
1: {A1, A8}, 2: {A3, A4, A5, A6}, 3: {A2, A7}
with centers C1=(3, 9.5), C2=(6.5, 5.25) and C3=(1.5, 3.5).
After the 3rd epoch, the results would be:
1: {A1, A4, A8}, 2: {A3, A5, A6}, 3: {A2, A7}
with centers C1=(3.66, 9), C2=(7, 4.33) and C3=(1.5, 3.5).





<u>Exercise 2.</u> Nearest Neighbor clustering

Use the Nearest Neighbor clustering algorithm and Euclidean distance to cluster the examples from the previous exercise: A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9). Suppose that the threshold t is 4.

Solution:
A1 is placed in a cluster by itself, so we have K1={A1}.

We then look at A2 if it should be added to K1 or be placed in a new cluster.
d(A1,A2)= $\sqrt{25} = 5 > t$ ➔ K2={A2}

A3: we compare the distances from A3 to A1 and A2.
A3 is closer to A2 and d(A3,A2)=$\sqrt{36} > t$ ➔ K3={A3}

A4: We compare the distances from A4 to A1, A2 and A3.
A1 is the closest object and d(A4,A1)= $\sqrt{13} < t$ ➔ K1={A1, A4}

A5: We compare the distances from A5 to A1, A2, A3 and A4.
A3 is the closest object and d(A5,A3)=$\sqrt{2} < t$ ➔ K3={A3, A5}

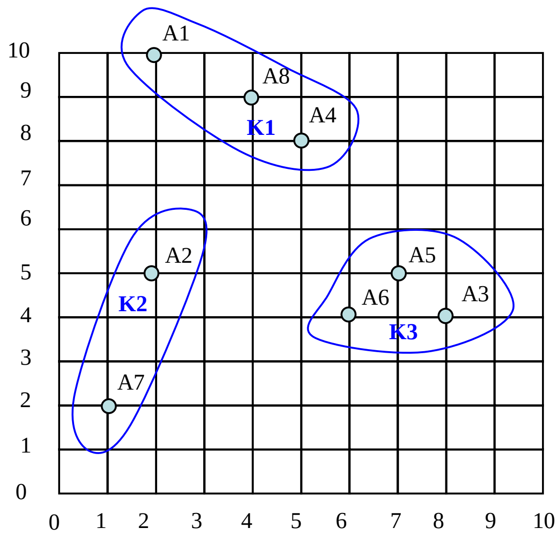
A6: We compare the distances from A6 to A1, A2, A3, A4 and A5.
A3 is the closest object and d(A6,A3)=$\sqrt{2} < t$ ➔ K3={A3, A5, A6}

A7: We compare the distances from A7 to A1, A2, A3, A4, A5, and A6.
A2 is the closest object and d(A7,A2)=$\sqrt{10} < t$ ➔ K2={A2, A7)

A8: We compare the distances from A8 to A1, A2, A3, A4, A5, A6 and A7.
A4 is the closest object and d(A8,A4)= $\sqrt{2}$ < t ➔ K1={A1, A4, A8)

Thus: K1={A1, A4, A8), K2={A2, A7), K3={A3, A5, A6)

Yes, it is the same result as with K-means.



Exercise 3. ***Hierarchical clustering***

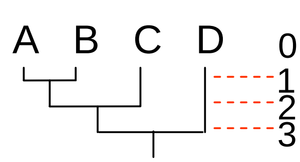
Use single and complete link agglomerative clustering to group the data described by the following distance matrix. Show the dendrograms.

	A	B	C	D
A	0	1	4	5
B		0	2	6
C			0	3
D				0

Solution:
Agglomerative ➔ initially every point is a cluster of its own and we merge cluster until we end-up with one unique cluster containing all points.

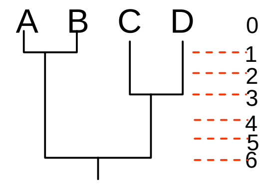
a) single link: distance between two clusters is the shortest distance between a pair of elements from the two clusters.

d	**k**	**K**	**Comments**
0	4	{A}, {B}, {C}, {D}	We start with each point = cluster
1	3	{A, B}, {C}, {D}	Merge {A} and {B} since A & B are the closest: d(A, B)=1
2	2	{A, B, C}, {D}	Merge {A, B} and {C} since B & C are the closest: d(B, C)=2
3	1	{A, B, C, D}	Merge D



b) complete link: distance between two clusters is the longest distance between a pair of elements from the two clusters.

d	k	K	Comments
0	4	{A}, {B}, {C}, {D}	We start with each point = cluster
1	3	{A, B}, {C}, {D}	d(A,B)=1<=1 ➔ merge {A} and {B}
2	3	{A, B}, {C}, {D}	d(A,C)=4>2 so we can't merge C with {A,B} d(A,D)=5>2 and d(B,D)=6>2 so we can't merge D with {A, B} d(C,D)=3>2 so we can't merge C and D
3	2	{A, B}, {C, D}	- d(A,C)=4>3 so we can't merge C with {A,B} - d(A,D)=5>3 and d(B,D)=6>3 so we can't merge D with {A, B} - d(C,D)=3 <=3 so merge C and D
4	2	{A, B}, {C, D}	{C,D} cannot be merged with {A, B} as d(A,D)= 5 >4 (and also d(B,D)= 6 >4) although d(A,C)= 4 <= 4, d(B,C)= 2<=4)
5	2	{A, B}, {C, D}	{C,D} cannot be merged with {A, B} as d(B,D)= 6 > 5
6	1	{A, B, C, D}	{C, D} can be merged with {A, B} since d(B,D)= 6 <= 6, d(A,D)= 5 <= 6, d(A,C)= 4 <= 6, d(B,C)= 2 <= 6



Exercise 4: **Hierarchical clustering <u>(to be done at your own time, not in class)</u>**

Use single-link, complete-link, average-link agglomerative clustering as well as medoid and centroid to cluster the following 8 examples:

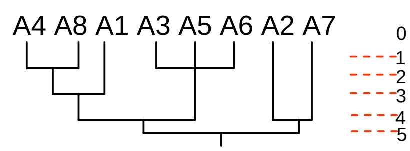
A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9).

The distance matrix is the same as the one in Exercise 1. Show the dendrograms.

Solution:

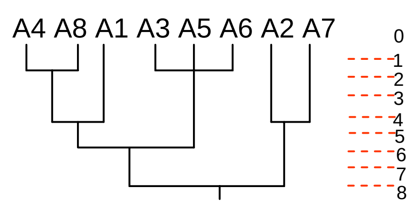
Single Link:

d	k	K
0	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
1	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
2	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
3	4	{A4, A8, A1}, {A3, A5, A6}, {A2}, {A7}
4	2	{A1, A3, A4, A5, A6, A8}, {A2, A7}
5	1	{A1, A3, A4, A5, A6, A8, A2, A7}



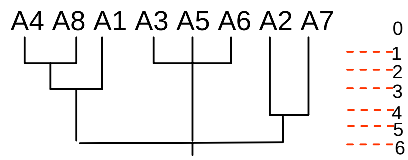
Complete Link

d	k	K
0	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
1	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
2	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
3	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
4	3	{A4, A8, A1}, {A3, A5, A6}, {A2, A7}
5	3	{A4, A8, A1}, {A3, A5, A6}, {A2, A7}
6	2	{A4, A8, A1, A3, A5, A6}, {A2, A7}
7	2	{A4, A8, A1, A3, A5, A6}, {A2, A7}
8	1	{A4, A8, A1, A3, A5, A6, A2, A7}



Average Link

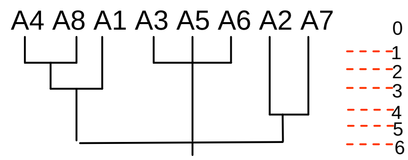
d	k	K
0	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
1	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
2	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
3	4	{A4, A8, A1}, {A3, A5, A6}, {A2}, {A7}
4	3	{A4, A8, A1}, {A3, A5, A6}, {A2, A7}
5	3	{A4, A8, A1}, {A3, A5, A6}, {A2, A7}
6	1	{A4, A8, A1, A3, A5, A6, A2, A7}



Average distance from {A3, A5, A6} to {A1, A4, A8} is 5.53 and is 5.75 to {A2, A7}

Centroid

D	k	K
0	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
1	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
2	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
3	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
4	3	{A4, A8, A1}, {A3, A5, A6}, {A2, A7}
5	3	{A4, A8, A1}, {A3, A5, A6}, {A2, A7}
6	1	{A4, A8, A1, A3, A5, A6, A2, A7}

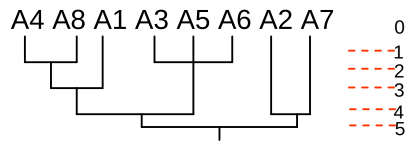


Centroid of {A4, A8} is B=(4.5, 8.5) and centroid of {A3, A5, A6} is C=(7, 4.33)
distance(A1, B) = 2.91 Centroid of {A1, A4, A8} is D=(3.66, 9) and of {A2, A7} is E=(1.5, 3.5)
distance(D,C)= 5.74 distance(D,E)= 5.90

Medoid

This is not deterministic. It can be different depending upon which medoid in a cluster we chose.

d	k	K
0	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
1	8	{A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8}
2	5	{A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7}
3	4	{A4, A8, A1}, {A3, A5, A6}, {A2}, {A7}
4	2	{A1, A3, A4, A5, A6, A8}, {A2, A7}
5	1	{A1, A3, A4, A5, A6, A8, A2, A7}



<u>Exercise 5:</u> DBScan

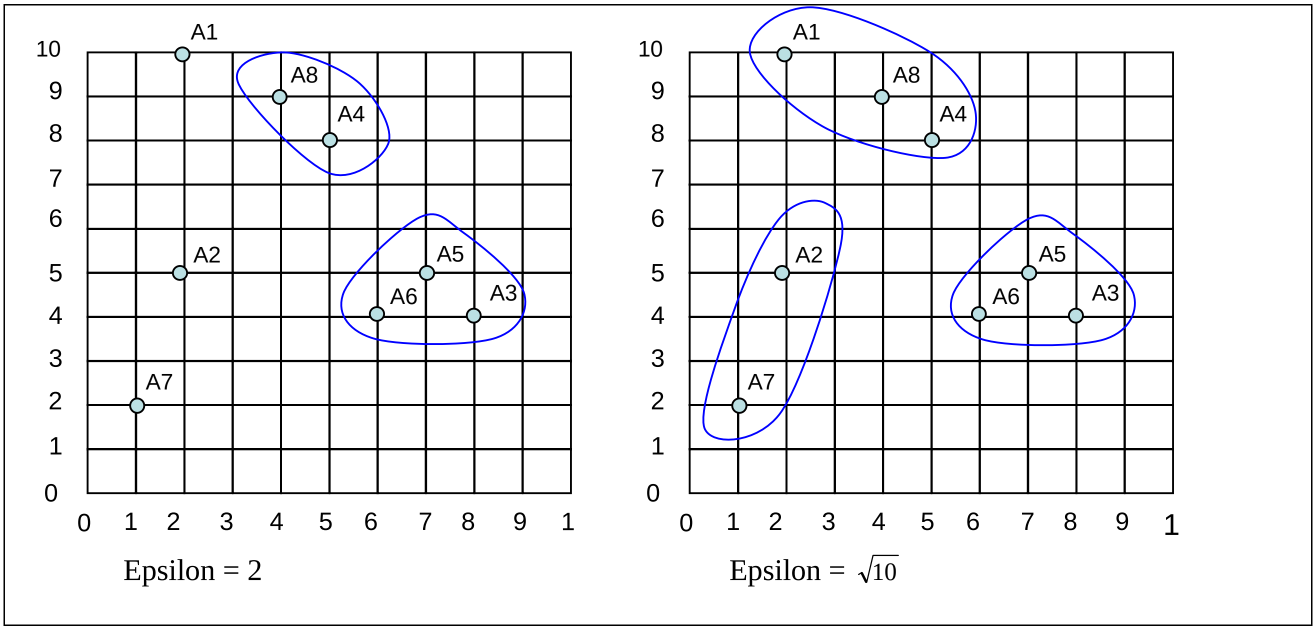
If Epsilon is 2 and minpoint is 2, what are the clusters that DBScan would discover with the following 8 examples: A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9).
The distance matrix is the same as the one in Exercise 1. Draw the 10 by 10 space and illustrate the discovered clusters. What if Epsilon is increased to $\sqrt{10}$?

Solution:

What is the Epsilon neighborhood of each point?
N_2(A1)={}; N_2(A2)={}; N_2(A3)={A5, A6}; N_2(A4)={A8}; N_2(A5)={A3, A6};
N_2(A6)={A3, A5}; N_2(A7)={}; N_2(A8)={A4}

So A1, A2, and A7 are outliers, while we have two clusters C1={A4, A8} and C2={A3, A5, A6}

If Epsilon is $\sqrt{10}$ then the neighborhood of some points will increase:
A1 would join the cluster C1 and A2 would joint with A7 to form cluster C3={A2, A7}.


A1
A8
A4
A2
A5
A6
A3
A7
Epsilon = 2
Epsilon = $\sqrt{10}$