

K-means

- Datasets

- Iris

- Iris_Initial_Centroids

	A	B
1	5.4,3.9,1.7,0.4	
2	6.4,3.1,5.5,1.8	
3	4.6,3.6,1.0,0.2	
4	5.5,4.2,1.4,0.2	
5	5.1,3.5,1.4,0.2	
6	4.3,3.0,1.1,0.1	
7	7.7,2.6,6.9,2.3	
8	6.4,2.7,5.3,1.9	
9	6.0,2.9,4.5,1.5	

	A	B
1	4.4,3,1.3,0.2	
2	5.9,3,5.1,1.8	
3	4,3,4,1.2	
4		

K-means

- assignCluster `def assignCluster(dataSet, k, centroids)`
- For each data point, the function is to assign it to the closest centroid.
- Input
 - dataSet: each row represents an observation and each column represents an attribute;
 - k: number of clusters
 - centroids: initial centroids or centroids of last iteration
- Output
 - clusterAssment: a list, which contains assigned cluster id for each data point

K-means

- assignCluster
- To implement this function, you can follow the following pseudo-code

for data in dataSet:

 minDist = Inf, minIndex = -1

 for center in centroids:

 d = distance(data, center)

 if d < minDist:

 minDist = d, minIndex = index of center

 clusterAssment.append(minIndex)

K-means

- getCentroid `def getCentroid(dataSet, k, clusterAssment)`
- The function is to recalculate centroids.
- Input
 - dataSet: each row represents an observation and each column represents an attribute
 - k: number of clusters
 - clusterAssment: a list, which contains assigned cluster id for each data point
- Output
 - centroids: cluster centroids

Hierarchical clustering

- Datasets
 - Example
 - Utilities

attribute

	A	B	C	D	E
1	0.88845	0.96682	0.93679	0.81723	0.88242
2	0.86257	0.85462	0.86419	0.84451	0.86159
3	0.9402	0.91072	0.93074	0.93317	0.94034
4	1.1151	0.00127	1.0215	1.2628	1.1573

	A	B	C	D	E	F	G	H
1	-0.29316	-0.68464	-0.41712	-0.57772	-0.52623	0.045903	-0.71463	-0.85368
2	-1.2145	-0.19445	0.821	0.20684	-0.33381	-1.0778	0.79205	0.8133
3	1.7121	2.0782	-1.3396	-0.89154	0.051019	0.083931	-0.71463	-0.080431
4	-0.50995	0.20661	-0.004414	-0.21906	-0.94313	-0.70171	1.328	-0.7242
5	2.0373	-0.86289	0.57823	-1.295	-0.71864	-1.5814	0.21439	1.6926
6	1.116	1.2315	-1.3882	0.67757	-1.7449	0.62337	0.6253	0.24865
7	0.574	0.65223	0.16552	2.3812	-0.33381	-0.35832	-0.71463	0.98773
8	-0.076369	-0.68464	1.8649	0.0050945	0.01895	1.1741	-0.71463	-1.4273
9	1.2244	1.0087	-0.004414	0.76723	1.2697	-0.14311	-0.71463	-0.43289
10	0.032026	0.74135	0.69962	-0.89154	-0.17347	-0.69269	1.6198	-0.86267
11	-1.9733	-1.4422	0.11697	-1.2278	1.0452	2.402	-0.71463	-0.60192
12	0.086223	0.07292	0.23836	1.1259	0.14723	-0.77748	-0.71463	1.4283
13	0.19462	0.87504	0.74817	-0.73463	1.0131	-0.48875	2.2749	-1.0353
14	-0.13057	0.56311	-1.7524	-1.6088	-0.59037	0.21379	-0.71463	-0.92561
15	-0.83513	-1.3976	-0.10152	1.1707	-1.0714	-0.68903	-0.66103	0.53457
16	0.24881	-0.3727	2.0348	-0.21906	1.911	1.9935	-0.71463	-0.86806
17	-1.9191	-1.9324	-0.78128	1.1035	1.8469	-0.90143	-0.22034	1.4697
18	-0.34736	0.83048	-0.4414	-0.062153	-0.17347	0.34534	-0.71463	0.0094816
19	0.24881	0.42942	-1.5581	-0.66738	-1.7128	1.2938	-0.71463	-0.83929

Hierarchical clustering

- merge_cluster
- The function is to merge two closest clusters according to min distances.
- Input
 - distance_matrix: a 2-D array distance matrix
 - cluster_candidate: a dictionary. Key is the cluster id, and value is point ids in the cluster.
 - T: current cluster index
- Output
 - cluster_candidate: a dictionary. We update cluster dictionary after merging two clusters. Key is the cluster id, and value is a list of point ids in the cluster
 - merge_list: list of tuples. It records the two old clusters' id and points that have just been merged.
 - [(cluster_one_id, point_ids_in_cluster_one),
(cluster_two_id, point_ids_in_cluster_two)]

Hierarchical clustering

- merge_cluster
- You can implement this function by two steps:
 - Find the smallest entry in the distance matrix—suppose the entry is i -th row and j -th column.
 - Merge the clusters that correspond to the i -th row and j -th column of the distance matrix as a new cluster with index T

Hierarchical clustering

- merge_cluster
- When you find minimum value indices in distance matrix, you may use the following methods in NumPy:
 - .flatten()
 - Return a copy of the array collapsed into one dimension.
 - np.unravel_index()
 - Converts a flat index or array of flat indices into a tuple of coordinate arrays

```
>>> a = np.array([[1,2], [3,4]])  
>>> a.flatten()  
array([1, 2, 3, 4])
```

```
>>> np.unravel_index([22, 41, 37], (7,6))  
(array([3, 6, 6]), array([4, 5, 1]))
```


Hierarchical clustering

- `merge_cluster`
- Merge the clusters that correspond to the i -th row and j -th column of the distance matrix as a new cluster with index T
- To implement this function, you may use the following method in python:
 - `.pop`
 - It can remove data in dictionary.

```
>>> a={1:2, 3:4, 5:6}
>>> a
{1: 2, 3: 4, 5: 6}
>>> a.pop(5)
6
>>> a
{1: 2, 3: 4}
>>>
```

Hierarchical clustering

- `update_distance`
- This function is to update the distance matrix.
- Input
 - `distance_matrix`: 2-D array
 - `cluster_candidate`: a dictionary. Key is the updated cluster id, value is point ids in the cluster.
 - `merge_list`: list of tuples. It records the two old clusters' id and points that have just been merged.
 `[(cluster_one_id, point_ids_in_cluster_one),`
 `(cluster_two_id, point_ids_in_cluster_two)]`
- Output
 - `distance_matrix`: 2-D array. Updated distance matrix.

Hierarchical clustering

- You need to mark all distance between points in two clusters in `merge_list` to be a large value.
- You can use “`merge_list[0][1]`” and “`merge_list[1][1]`” to get points indices in two clusters in `merge_list` .
- The large value can be set as 100000 or other big number.