K-Means Clustering

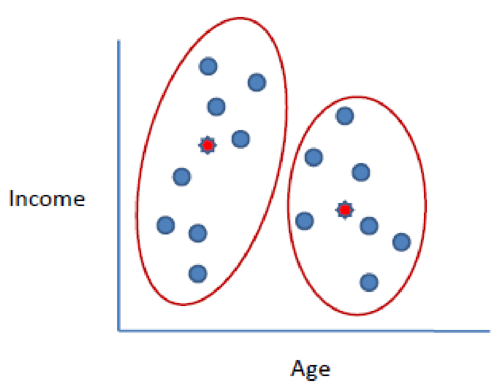
K-Means clustering intends to partition n objects into k clusters in which each object belongs to the cluster with the nearest mean. This method produces exactly k different clusters of greatest possible distinction. The best number of clusters k leading to the greatest separation (distance) is not known as a priori and must be computed from the data. The objective of K-Means clustering is to minimize total intra-cluster variance, or, the squared error function:

number of clusters, number of cases, case i, centroid for cluster j

$$\text{objective function} \leftarrow J = \sum_{j=1}^{k} \sum_{i=1}^{n} \underbrace{\left\| x_i^{(j)} - c_j \right\|^2}_{\text{Distance function}}$$

Algorithm

1. Clusters the data into k groups where k is predefined.
2. Select k points at random as cluster centers.
3. Assign objects to their closest cluster center according to the *Euclidean distance* function.
4. Calculate the centroid or mean of all objects in each cluster.
5. Repeat steps 2, 3 and 4 until the same points are assigned to each cluster in consecutive rounds.



K-Means is relatively an efficient method. However, we need to specify the number of clusters, in advance and the final results are sensitive to initialization and often terminates at a local optimum. Unfortunately there is no global theoretical method to find the optimal number of clusters. A practical approach is to compare the outcomes of multiple runs with different k and choose the best one based on a predefined criterion. In general, a large k probably decreases the error but increases the risk of overfitting.

Example:

Suppose we want to group the visitors to a website using just their age (one-dimensional space) as follows:

$$\boldsymbol{n} = \mathbf{19}$$

15,15,16,19,19,20,20,21,22,28,35,40,41,42,43,44,60,61,65

Initial clusters (random centroid or average):

$$\boldsymbol{k} = \mathbf{2}$$

$$c_1 = 16$$

$$c_2 = 22$$

$$\text{Distance } 1 = |x_i - c_1|$$

$$\text{Distance } 2 = |x_i - c_2|$$

Iteration 1:

$$c_1 = 15.33$$

$$c_2 = 36.25$$

x_i	c_1	c_2	Distance 1	Distance 2	Nearest Cluster	New Centroid
15	16	22	1	7	1	
15	16	22	1	7	1	**15.33**
16	16	22	0	6	1	
19	16	22	9	3	2	
19	16	22	9	3	2	
20	16	22	16	2	2	
20	16	22	16	2	2	
21	16	22	25	1	2	
22	16	22	36	0	2	
28	16	22	12	6	2	
35	16	22	19	13	2	
40	16	22	24	18	2	**36.25**
41	16	22	25	19	2	
42	16	22	26	20	2	
43	16	22	27	21	2	
44	16	22	28	22	2	
60	16	22	44	38	2	
61	16	22	45	39	2	
65	16	22	49	43	2	

Iteration 2:

$$c_1 = 18.56$$

$$c_2 = 45.90$$

x_i	c_1	c_2	Distance 1	Distance 2	Nearest Cluster	New Centroid
15	15.33	36.25	0.33	21.25	1	**18.56**
15	15.33	36.25	0.33	21.25	1	

16	15.33	36.25	0.67	20.25	1	
19	15.33	36.25	3.67	17.25	1	
19	15.33	36.25	3.67	17.25	1	
20	15.33	36.25	4.67	16.25	1	
20	15.33	36.25	4.67	16.25	1	
21	15.33	36.25	5.67	15.25	1	
22	15.33	36.25	6.67	14.25	1	
28	15.33	36.25	12.67	8.25	2	**45.9**
35	15.33	36.25	19.67	1.25	2	
40	15.33	36.25	24.67	3.75	2	
41	15.33	36.25	25.67	4.75	2	
42	15.33	36.25	26.67	5.75	2	
43	15.33	36.25	27.67	6.75	2	
44	15.33	36.25	28.67	7.75	2	
60	15.33	36.25	44.67	23.75	2	
61	15.33	36.25	45.67	24.75	2	
65	15.33	36.25	49.67	28.75	2	

Iteration 3:

$$c_1 = 19.50$$
$$c_2 = 47.89$$

x_i	c_1	c_2	Distance 1	Distance 2	Nearest Cluster	New Centroid
15	18.56	45.9	3.56	30.9	1	**19.50**
15	18.56	45.9	3.56	30.9	1	
16	18.56	45.9	2.56	29.9	1	
19	18.56	45.9	0.44	26.9	1	
19	18.56	45.9	0.44	26.9	1	
20	18.56	45.9	1.44	25.9	1	
20	18.56	45.9	1.44	25.9	1	
21	18.56	45.9	2.44	24.9	1	
22	18.56	45.9	3.44	23.9	1	
28	18.56	45.9	9.44	17.9	1	
35	18.56	45.9	16.44	10.9	2	**47.89**
40	18.56	45.9	21.44	5.9	2	
41	18.56	45.9	22.44	4.9	2	
42	18.56	45.9	23.44	3.9	2	
43	18.56	45.9	24.44	2.9	2	
44	18.56	45.9	25.44	1.9	2	
60	18.56	45.9	41.44	14.1	2	
61	18.56	45.9	42.44	15.1	2	
65	18.56	45.9	46.44	19.1	2	

Iteration 4:

$$c_1 = 19.50$$
$$c_2 = 47.89$$

x_i	c_1	c_2	Distance	Distance	Nearest	New

			1	2	Cluster	Centroid
15	19.5	47.89	4.50	32.89	1	
15	19.5	47.89	4.50	32.89	1	
16	19.5	47.89	3.50	31.89	1	
19	19.5	47.89	0.50	28.89	1	
19	19.5	47.89	0.50	28.89	1	**19.50**
20	19.5	47.89	0.50	27.89	1	
20	19.5	47.89	0.50	27.89	1	
21	19.5	47.89	1.50	26.89	1	
22	19.5	47.89	2.50	25.89	1	
28	19.5	47.89	8.50	19.89	1	
35	19.5	47.89	15.50	12.89	2	
40	19.5	47.89	20.50	7.89	2	
41	19.5	47.89	21.50	6.89	2	
42	19.5	47.89	22.50	5.89	2	
43	19.5	47.89	23.50	4.89	2	**47.89**
44	19.5	47.89	24.50	3.89	2	
60	19.5	47.89	40.50	12.11	2	
61	19.5	47.89	41.50	13.11	2	
65	19.5	47.89	45.50	17.11	2	

No change between iterations 3 and 4 has been noted. By using clustering, 2 groups have been identified 15-28 and 35-65. The initial choice of centroids can affect the output clusters, so the algorithm is often run multiple times with different starting conditions in order to get a fair view of what the clusters should be.

Exercise K Means Interactive