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Pattern Recognition

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Prototype Selection

- The nearest neighbor classifiers require time linear in the sample size for classification that goes up as the training data size goes up
- If the training dataset size can be reduced, the time required for classification can be reduced
- This reduction can be accomplished either by *reducing the number of training patterns*, *reducing the number of features*, or both
- Reducing the number of training patterns - *prototype selection.*
  - For example, Condensed Nearest Neighbor (CNN) method

Condensed Nearest Neighbor (CNN) algorithm

The CNN starts with a set of all patterns *Data* and a condensed set *Condensed* which is initially empty.

Data is scanned randomly, or better, using some method.

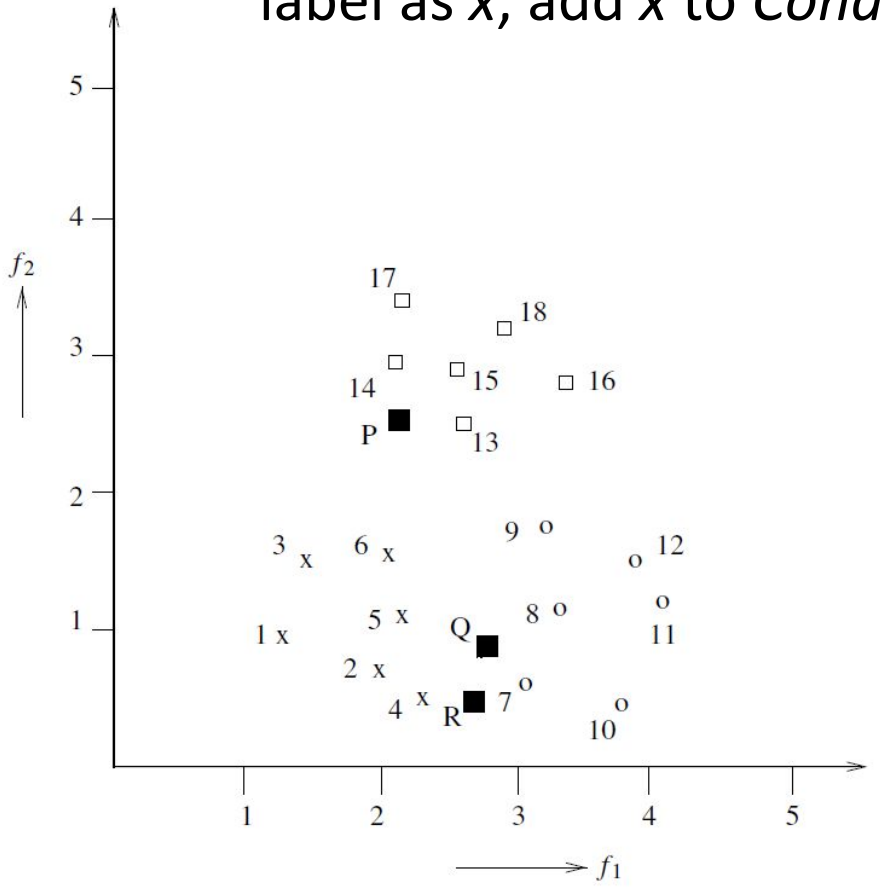
The first pattern in *Data* is put into *Condensed*. After this, the following set of statements are repeated until there is no change in *Condensed* in an iteration:

1. For every pattern *x* in *Data*, find its NN in *Condensed*
2. If the nearest neighbor does not have the same class label as *x*, remove x from Data and add it to *Condensed*

NOTE: Usually, there is an initial preprocessing step for outlier removal as we will see in an example.

Condensed Nearest Neighbor (CNN) algorithm

1. For every pattern *x* in *Data*, find its NN in *Condensed*
2. If the nearest neighbor does not have the same class label as *x*, add *x* to *Condensed*

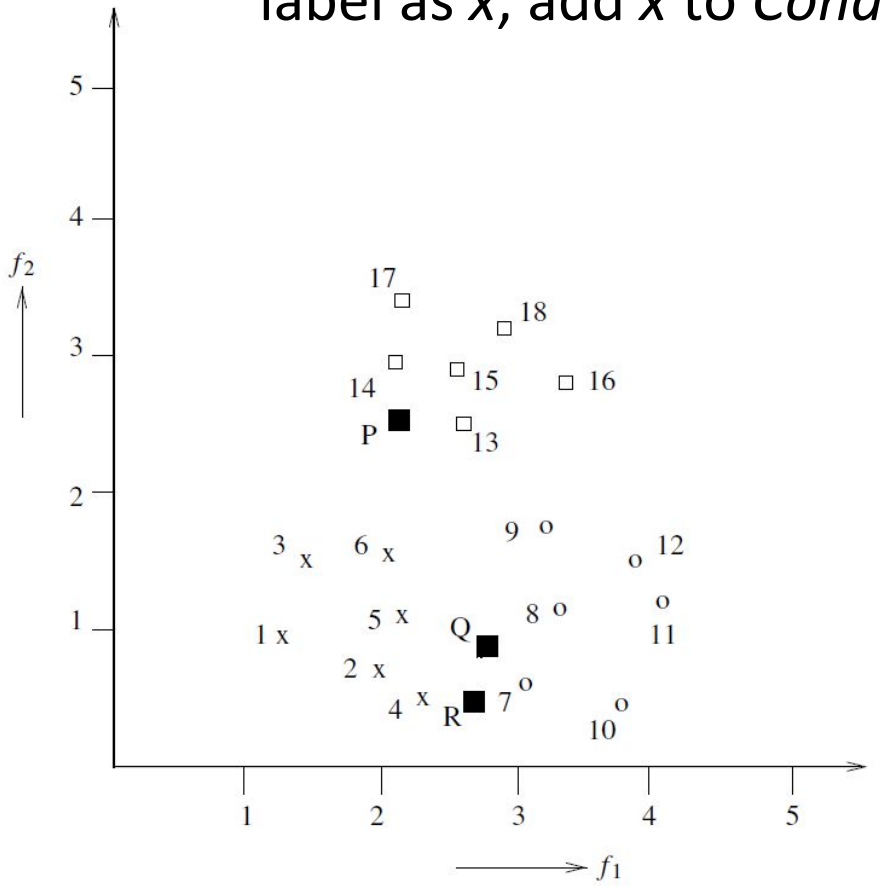


Example dataset.

- If the patterns are scanned by the algorithm in the order $x1$, $x2$, $x3$, $x4$, $x5$, $x6$, $x7$, . . . , pattern $x1$ belonging to class 'cross' will be first put into ***Condensed***.
- $x2$, $x3$, $x4$, $x5$, and $x6$ will be left out and $x7$ which belongs to class 'circle' will be put into ***Condensed***
- So in the first iteration, the first pattern presented to the algorithm from each class will be included in ***Condensed***, along with other patterns

Condensed Nearest Neighbor (CNN) algorithm

1. For every pattern *x* in *Data*, find its NN in *Condensed*
2. If the nearest neighbor does not have the same class label as *x*, add *x* to *Condensed*



Example dataset.

- Patterns put into *Condensed* depend on the order in which the patterns are presented to the algorithm. It is therefore an **order-dependent algorithm**

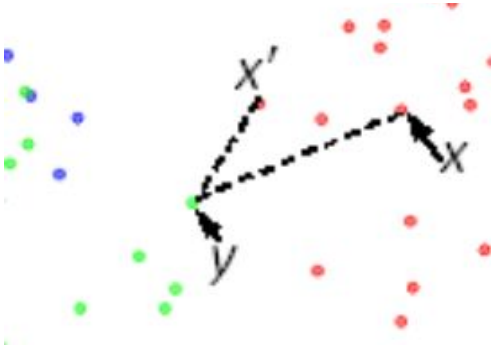
Condensed Nearest Neighbor (CNN) algorithm

1. For every pattern *x* in *Data*, find its NN in *Condensed*
2. If the nearest neighbor does not have the same class label as *x*, add *x* to *Condensed*

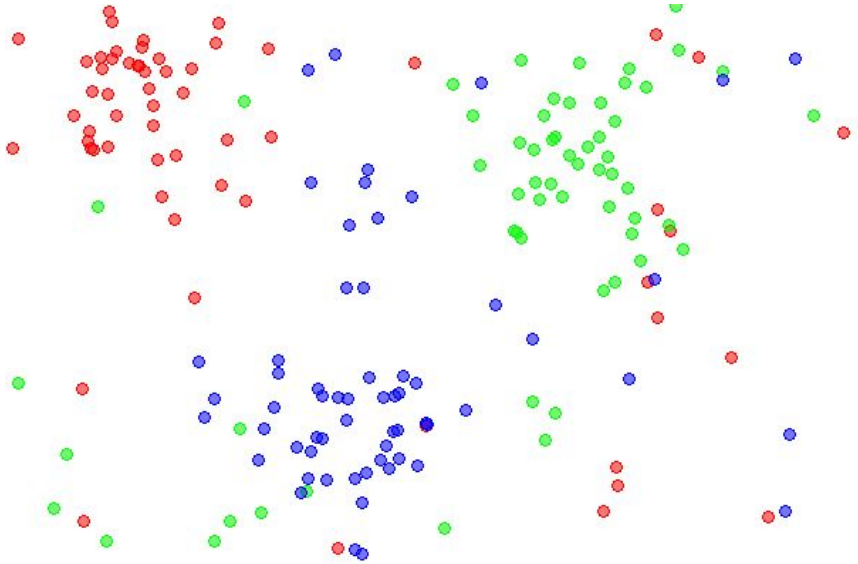
- Efficient to scan patterns in order of decreasing border ratio. Border ratio of point x is:

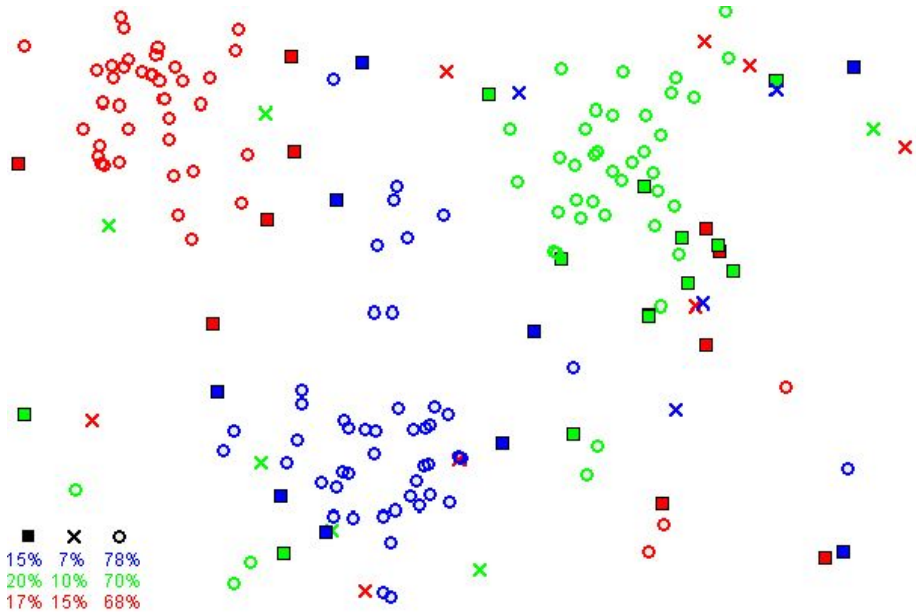
$$a(x) = \frac{||x'-y||}{||x-y||}$$

where $||x-y||$ is the distance to the closest example *y* having a different color than *x*, and $||x'-y||$ is the distance from *y* to its closest example *x'* with the same label as *x*.

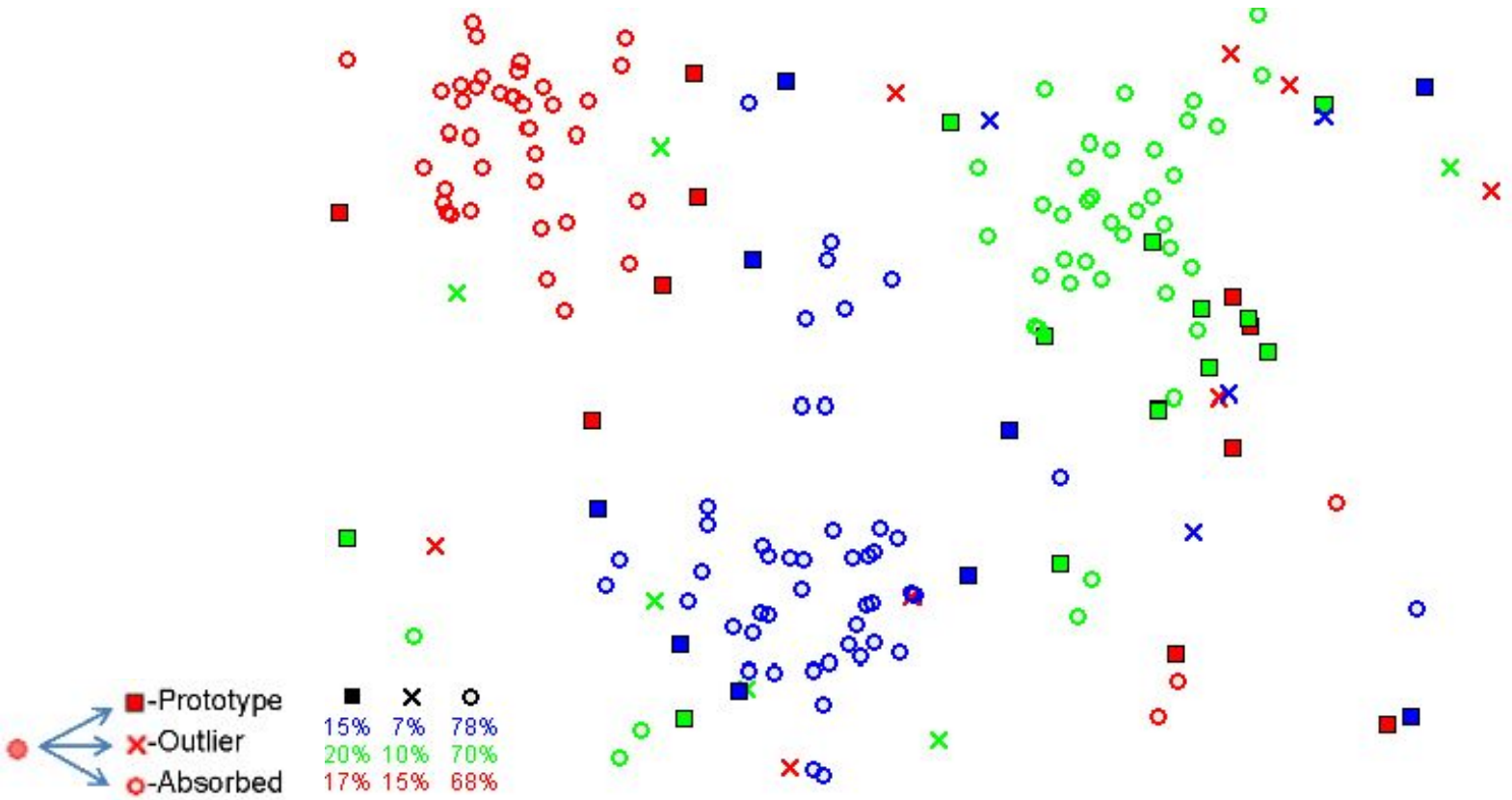


Condensed Nearest Neighbor - Example





Condensed Nearest Neighbor - Example



the class outliers selected by the (3,2)NN rule (all the three nearest neighbors of these instances belong to other classes)

*(k,r)*NN class-outlier: *k* nearest neighbors include more than *r* examples of other classes

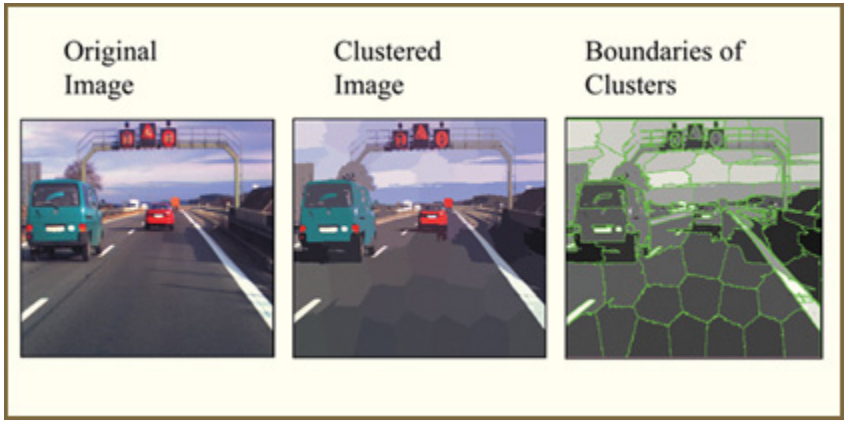
Cluster Analysis (Clustering)

Clustering

- Unsupervised learning
- No training labels available during clustering
  - However, some labels *may* be used during evaluation of clustering algorithms

Clustering

- Divide data into similar groups
- Goals of cluster analysis:
  - Clustering for understanding data (Information retrieval, climate, business)
  - Clustering as a utility (summarization, compression)



Clustering

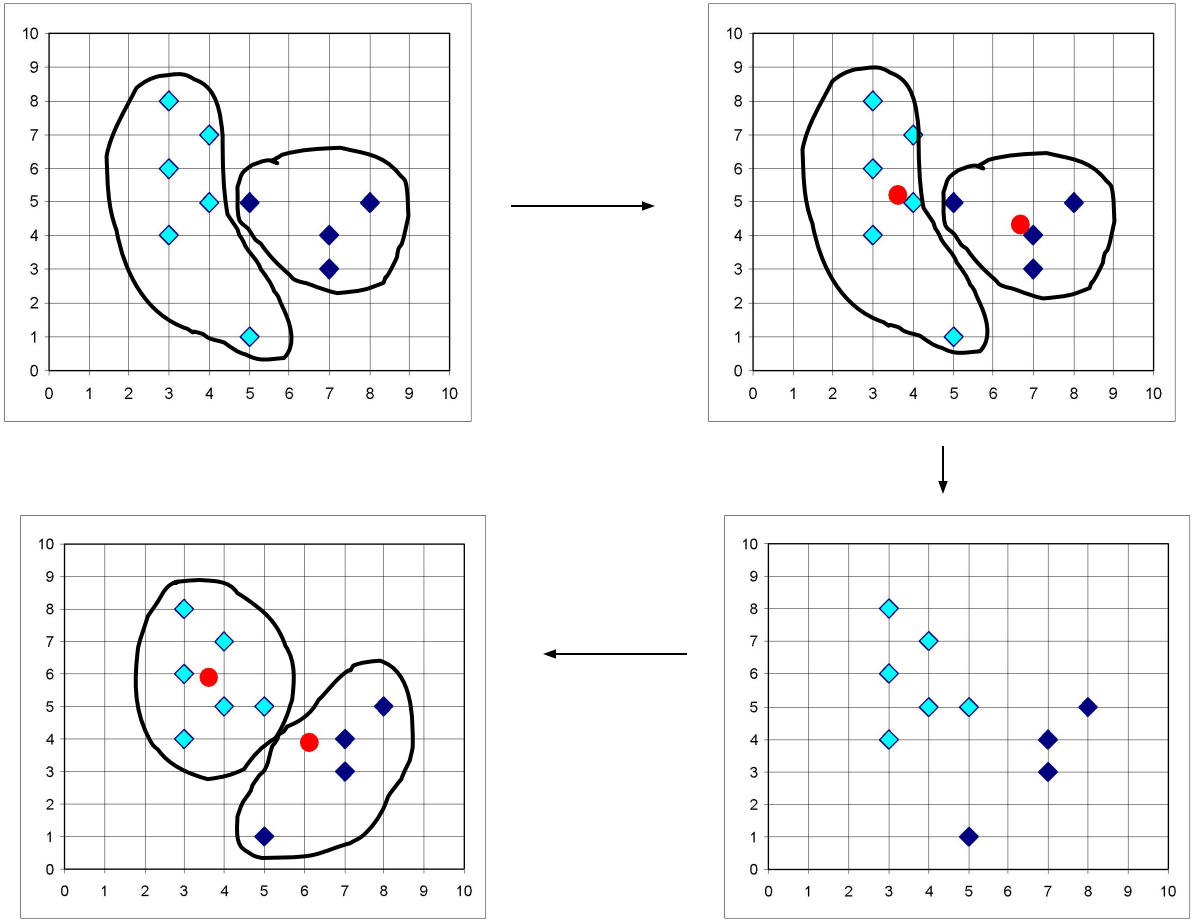
- Divide data into similar groups
- Goals of cluster analysis:
  - Clustering for understanding data (Info. retrieval, climate, business)
  - Clustering as a utility (summarization, compression)
- Examples of clustering algorithms: ***k-means, hierarchical agglomerative clustering***, DBSCAN

K-means Clustering

- Given *k*, the *k-means* algorithm consists of four steps:
  - Select initial centroids at random.
  - Assign each object to the cluster with the nearest centroid.
  - Compute each centroid as the mean of the objects assigned to it.
  - Repeat previous 2 steps until there is no change.

K-means Clustering

- Example



K-means example (K=2)

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

K-means example (K=2)

Initialization: Randomly we choose following two centroids (k=2) for two clusters.
In this case the 2 centroid are: m1=(1.0,1.0) and m2=(5.0,7.0).

Individual	Variable 1	Variable 2
1	1.0	1.0
2	1.5	2.0
3	3.0	4.0
4	5.0	7.0
5	3.5	5.0
6	4.5	5.0
7	3.5	4.5

	Individual	Mean Vector
Group 1	1	(1.0, 1.0)
Group 2	4	(5.0, 7.0)

K-means example (K=2)

- Thus, we obtain two clusters containing:
  {1,2,3} and {4,5,6,7}.
- Their new centroids are:

$$m_1 = \left(\frac{1}{3}(1.0+1.5+3.0), \frac{1}{3}(1.0+2.0+4.0)\right) = (1.83, 2.33)$$

$$m_2 = \left(\frac{1}{4}(5.0+3.5+4.5+3.5), \frac{1}{4}(7.0+5.0+5.0+4.5)\right)$$

$$= (4.12, 5.38)$$

Individual	Centroid 1	Centroid 2
1	0	7.21
2 (1.5, 2.0)	1.12	6.10
3	3.61	3.61
4	7.21	0
5	4.72	2.5
6	5.31	2.06
7	4.30	2.92

$$d(m_1, 2) = \sqrt{|1.0-1.5|^2 + |1.0-2.0|^2} = 1.12$$

$$d(m_2, 2) = \sqrt{|5.0-1.5|^2 + |7.0-2.0|^2} = 6.10$$

K-means example (K=2)

- Now using these centroids we compute the Euclidean distance of each object, as shown in table.

Individual	Centroid 1	Centroid 2
1	1.57	5.38
2	0.47	4.28
3	2.04	1.78
4	5.64	1.84
5	3.15	0.73
6	3.78	0.54
7	2.74	1.08

- Therefore, the new clusters are:

  {1,2} and {**3**,4,5,6,7}

- Next centroids are: m1=(1.25,1.5) and m2 = (3.9,5.1)

K-means example (K=2)

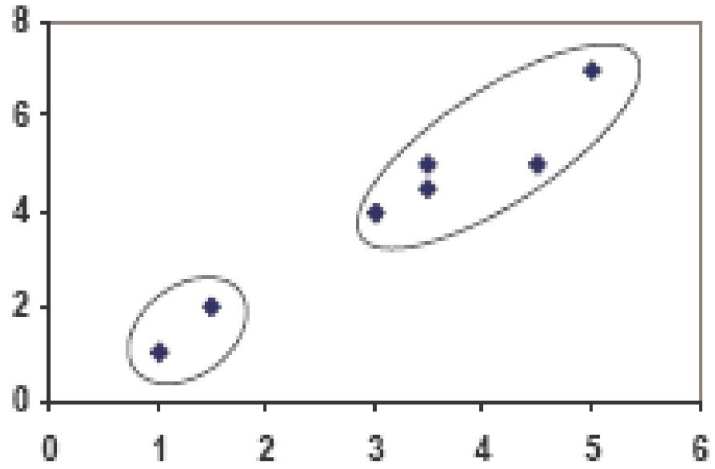
The clusters obtained are:

{1,2} and {3,4,5,6,7}

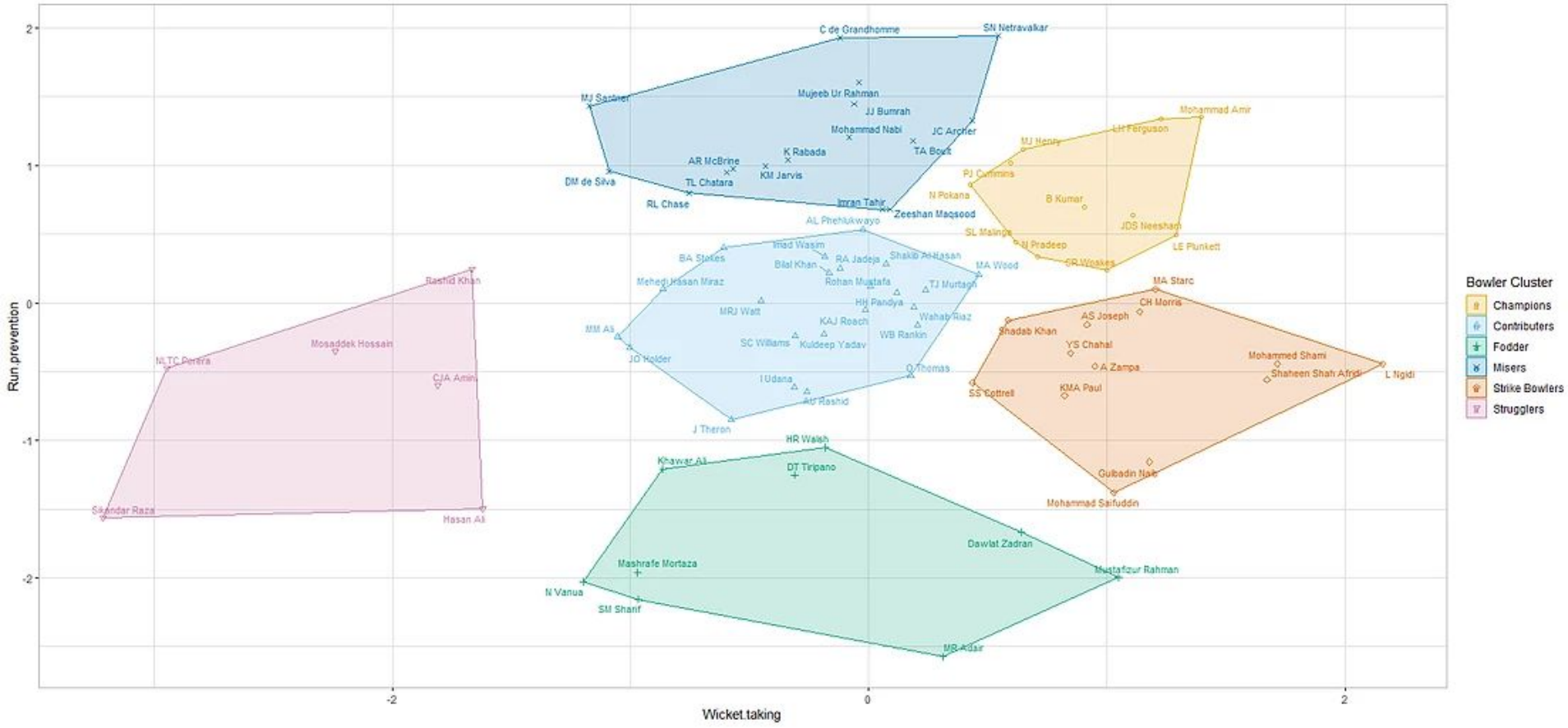
- Therefore, there is no change in the cluster.
- Thus, the algorithm comes to a halt
  - Final result consist of 2 clusters {1,2} and {3,4,5,6,7}

Individual	Centroid 1	Centroid 2
1	0.56	5.02
2	0. 56	3.92
3	3.05	1.42
4	6.66	2.20
5	4.16	0.41
6	4.78	0.61
7	3.75	0.72

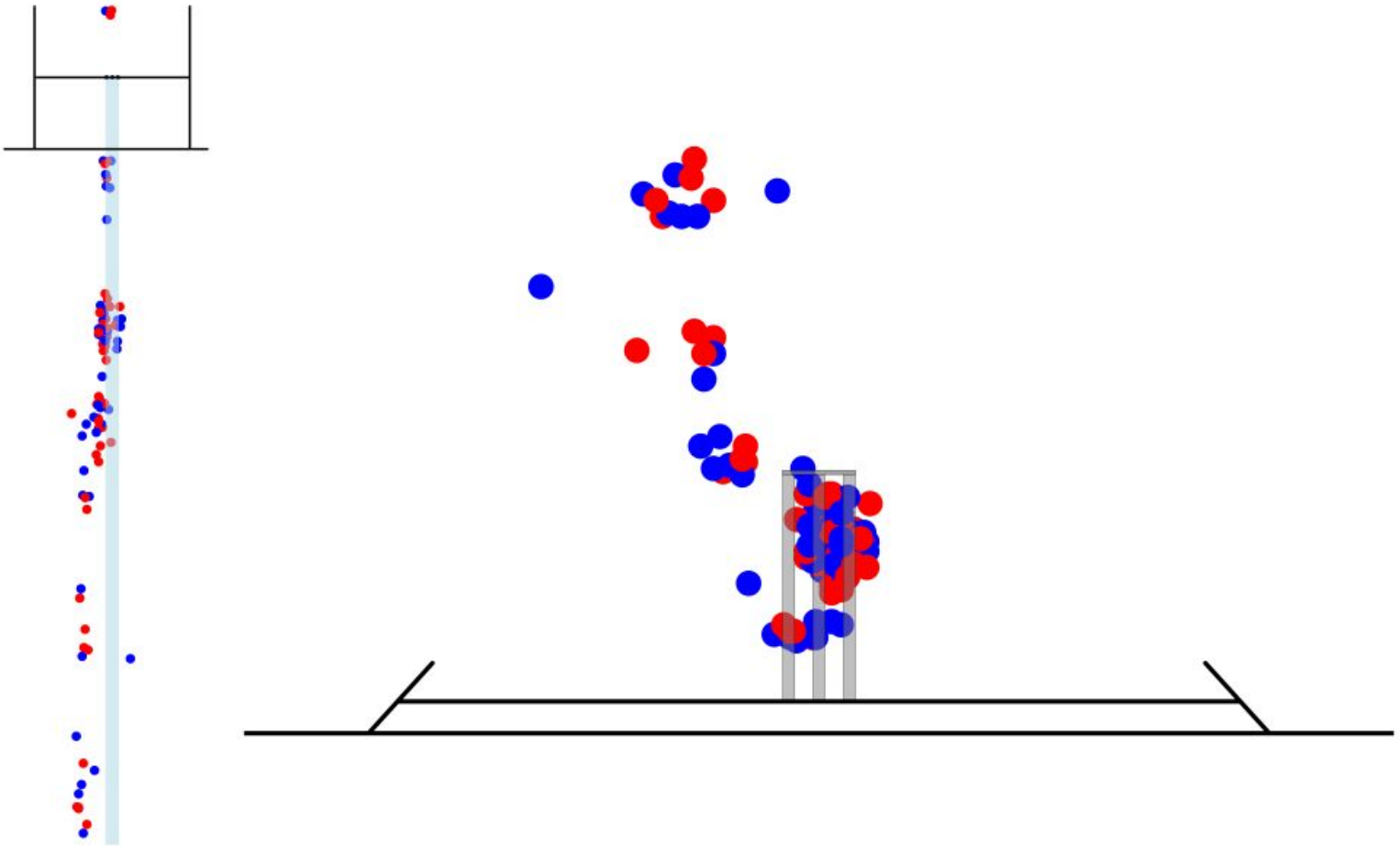
K-means example (K=2)



K-means real example

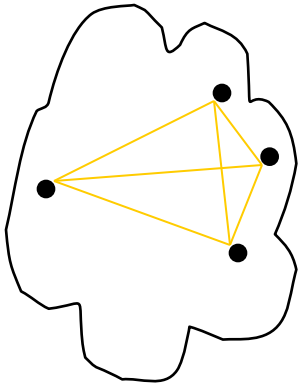


K-means real example

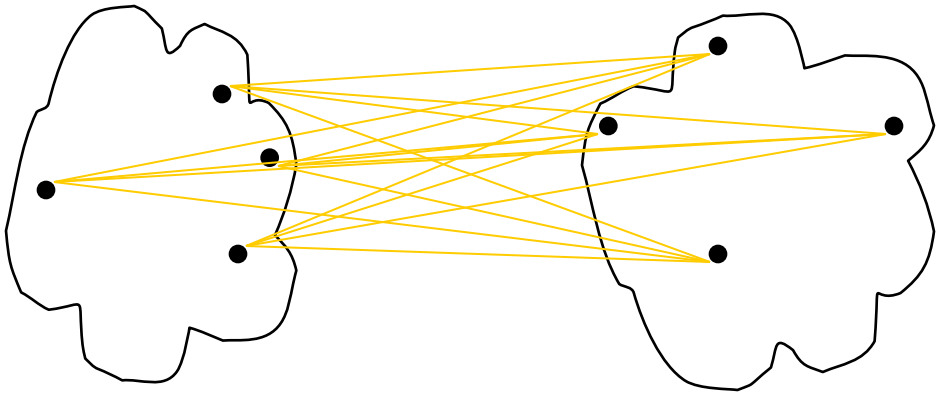


Measuring Cluster Quality: Cohesion and Separation

- A proximity graph based approach can be used for cohesion and separation.
  - Cluster cohesion is the sum of the weight of all links within a cluster.
  - Cluster separation is the sum of the weights between nodes in the cluster and nodes outside the cluster.



cohesion



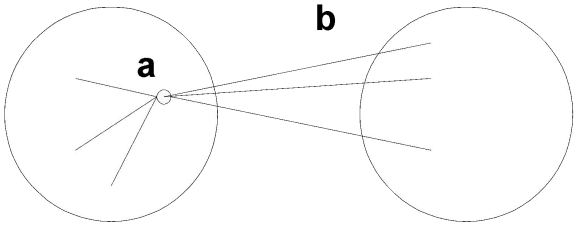
separation

Silhouette Coefficient

- Silhouette Coefficient combine ideas of both cohesion and separation, but for individual points, as well as clusters and clustering
- For an individual point *i*
  - Calculate ***a*** = average distance of *i* to the points in its cluster
  - Calculate ***b*** = min (average distance of *i* to points in another cluster)
  - The silhouette coefficient for a point is then given by

    s = (b – a)/max(a,b)

  - Varies between -1 and 1.
  - The closer to 1 the better.



- Can calculate the Average Silhouette coefficient for a cluster or a clustering

Example

Using the distance matrix in the following table, compute the **silhouette coefficient** for each point

	P1	P2	P3	P4
P1	0	0.10	0.65	0.55
P2	0.10	0	0.70	0.60
P3	0.65	0.70	0	0.30
P4	0.55	0.60	0.30	0

Cluster 1: {P1, P2}
Cluster 2: {P3, P4}

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Using the distance matrix in the following table, compute the **silhouette coefficient** for each point

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P4	0.55	0.60	0.30	0

Cluster 1: {P1, P2}
Cluster 2: {P3, P4}

Let a indicate the average distance of a point to other points in its cluster.
Let b indicate the minimum of the average distance of a point to points in another cluster.

Point P1: SC = 1- a/b = 1 - 0.1/((0.65+0.55)/2)= 5/6 = 0.833
Point P2: SC = 1- a/b = 1 - 0.1/((0.7+0.6)/2) = 0.846
Point P3: SC = 1- a/b = 1 - 0.3/((0.65+0.7)/2) = 0.556
Point P4: SC = 1- a/b = 1 - 0.3/((0.55+0.6)/2) = 0.478

Example

Using the distance matrix in the following table, compute the **silhouette coefficient** for each point **and each of the two clusters**

	P1	P2	P3	P4
P1	0	0.10	0.65	0.55
P2	0.10	0	0.70	0.60
P3	0.65	0.70	0	0.30
P4	0.55	0.60	0.30	0

Cluster 1: {P1, P2}
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Point P4: SC = 1- a/b = 1 - 0.3/((0.55+0.6)/2) = 0.478

Cluster 1 Average SC = (0.833+0.846)/2 = 0.84
Cluster 2 Average SC = (0.556+0.478)/2 = 0.52

Example

Using the distance matrix in the following table, compute the **silhouette coefficient** for each point, each of the two clusters, and **overall clustering**

	P1	P2	P3	P4
P1	0	0.10	0.65	0.55
P2	0.10	0	0.70	0.60
P3	0.65	0.70	0	0.30
P4	0.55	0.60	0.30	0

Cluster 1: {P1, P2}
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Cluster 1 Average SC = (0.833+0.846)/2 = 0.84
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Cluster 1: {P1, P2}
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Cluster 1 Average SC = (0.833+0.846)/2 = 0.84
Cluster 2 Average SC = (0.556+0.478)/2 = 0.52

Overall Average SC = (0.840+0.517)/2 = 0.68

K-means with scikit-learn

```
from sklearn import datasets
import matplotlib.pyplot as plt
import pandas as pd
from sklearn.cluster import KMeans
from sklearn import metrics

iris = datasets.load_iris()
X = iris.data
y = iris.target
plt.scatter(X[:,0], X[:,2], c=y, cmap='spring', s=100)
plt.title('Actual',fontsize=25, fontweight='bold')
plt.xlabel('Sepal Length',fontsize=20)
plt.ylabel('Petal Length',fontsize=20)
plt.figure()

cls = KMeans(n_clusters = 3, random_state=42)
cls.fit(X)
print 'Final centroids:'
print cls.cluster_centers_

km_labels = cls.labels_
print metrics.silhouette_score(X, km_labels)
plt.scatter(X[:,0], X[:,2],c=km_labels, cmap='spring',  s=100)
plt.xlabel('Sepal Length',fontsize=20)
plt.ylabel('Petal Length',fontsize=20)
plt.title('Predicted clusters',fontsize=25, fontweight='bold')
plt.show()
```

Thank You!