

# **Unsupervised Learning**

Machine Learning

#### **Contents**

- K-means clustering
  - K-means
  - K-means++
  - Distortion, Silhouette: Quantifying the quality of cluster
- DBSCAN(Density-Based Spatial Clustering of Application with Noise)
  - DBSCAN
  - K-means vs DBSCAN
  - Outlier Detection

# Machine Learning

- Types of learning
  - Supervised learning
  - Unsupervised learning
  - Reinforcement learning

Using unlabeled data Find hidden structure Unsupervised Learning Supervised Learning

Using labeled data Predict outcome/future

Reinforcement Learning

Using reward from actions Learn action policy



# **Machine Learning**

- Types of learning
  - Supervised learning
  - Unsupervised learning
  - Reinforcement learning

Using unlabeled data Find hidden structure Unsupervised Learning Supervised Learning

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Reinforcement Learning

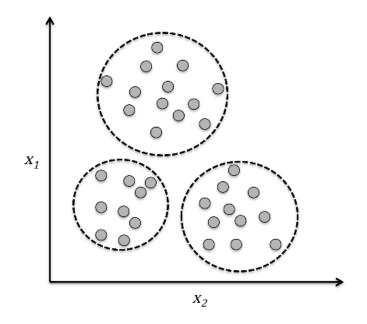
Using reward from actions Learn action policy



# **Unsupervised Learning**

- Finding subgroups with clustering
  - Given: <data> examples
  - Learning: <groups> of data

Н	W
185	65
160	90
180	70
165	95



- K-means clustering
  - Our goal is to group the samples based on their feature similarities
  - Algorithm
    - 1. Randomly pick k centroids from the sample points as initial clusters
    - 2. Assign each sample to the nearest centroid  $\mu^{(j)}$ ,  $j \in \{1, ..., k\}$
    - 3. Move the centroids to the center of the samples that were assigned to it
    - 4. Repeat steps 2 and 3 until the cluster assignments do not change or a user-defined tolerance or a maximum number of iterations is reached

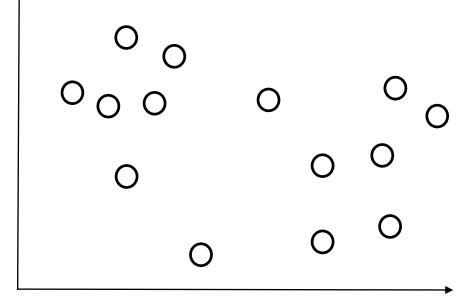
- K-means clustering
  - We can define similarity as the opposite of distance, "square Euclidean distance" between 2 points x and y in m-dimensional space

$$d(x,y) = \sum_{j=1}^{m} (x_j - y_j)^2 = ||x - y||_2^2$$

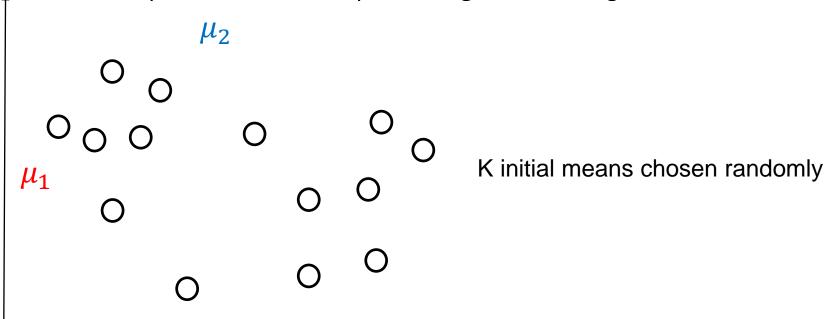
- Based on this Euclidean distance metric, we can describe the k-means algorithm as a simple optimization problem
- An iterative approach for minimizing the within-cluster sum of squared errors(SSE)

$$SSE = \sum_{i=1}^{n} \sum_{j=1}^{k} w^{(i,j)} \|x^{(i)} - \mu^{(j)}\|_{2}^{2}$$

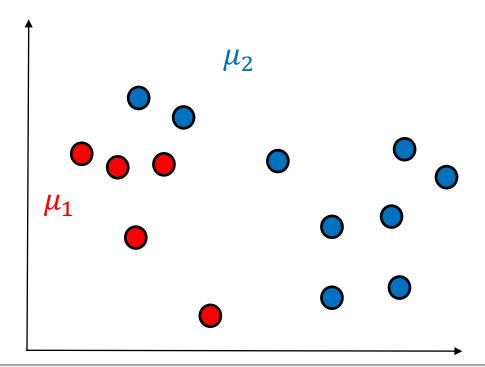
- EM(Expectation and Maximization) algorithm for K-means
  - Expectation
    - Assign the data points to the nearest centroid
  - Maximization
    - Update the centroid positions given the assignments



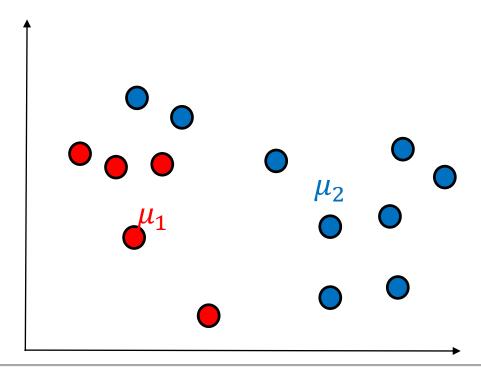
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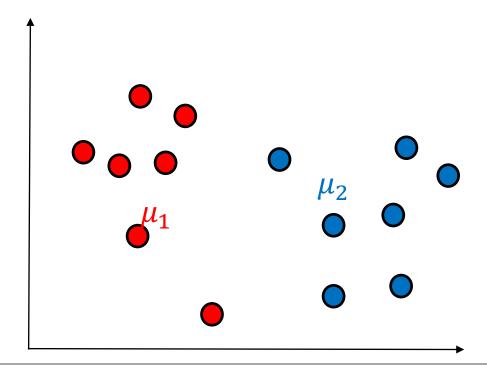
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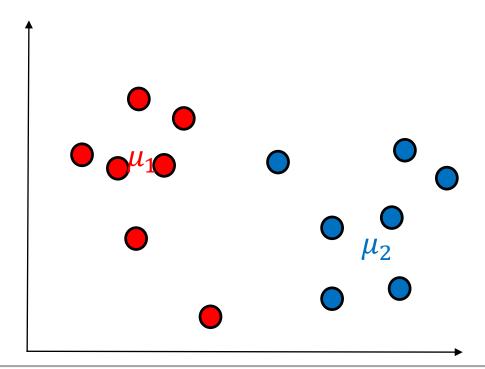
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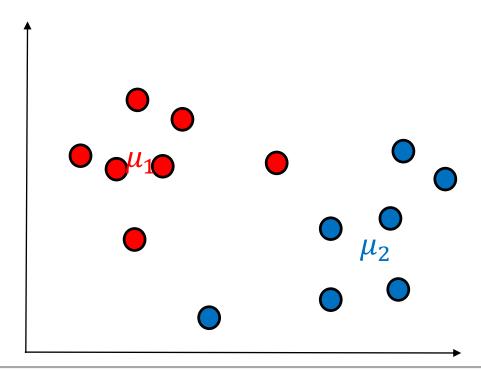
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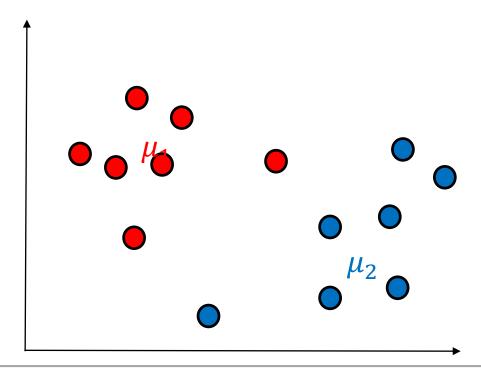
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  - Maximization
    - Update the centroid positions given the assignments



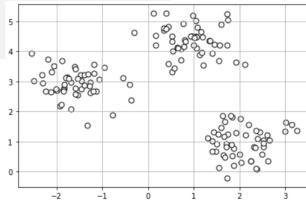
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  - Expectation
    - Assign the data points to the nearest centroid



- EM(Expectation and Maximization) algorithm for K-means
  - Maximization
    - Update the centroid positions given the assignments

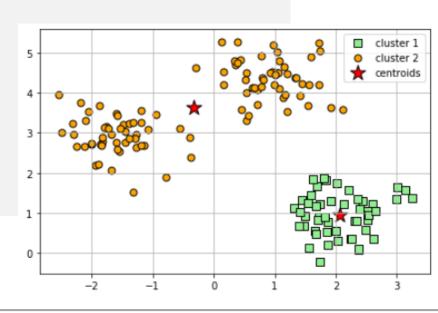


#### Make simple data and plotting



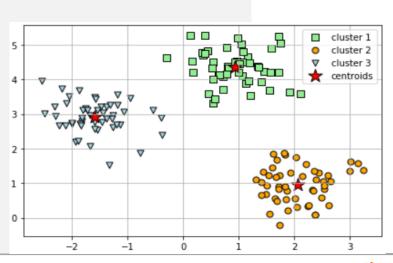
```
from sklearn.cluster import KMeans
# KMeans with k = 2
km = KMeans(n clusters=2,
         init='random',
         max iter=300,
         random state=0)
# cluster assignment
y km = km.fit predict(X)
y km
1, 1, 0, 0, 1, 1, 0, 1, 1, 1, 1, 1, 0, 0, 0, 1, 1, 1, 1, 1, 0, 0, 0,
      1, 1, 1, 1, 0, 1, 1, 0, 0, 1, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 1,
      1, 1, 0, 0, 1, 0, 1, 1, 1, 1, 0, 0, 1, 1, 0, 0, 0, 1, 1, 0, 0, 1,
      0, 1, 0, 1, 1, 1, 0, 0, 0, 0, 1, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
      1, 1, 1, 1, 1, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1, 1, 1, 0, 1, 1, 1, 1, 1,
      0, 1, 1, 1, 0, 0, 1, 1, 1, 1, 0, 0])
# cluster centers
print('<Cluster centers>\n', km.cluster centers )
<Cluster centers>
 [[ 2.06521743  0.96137409]
 [-0.33088235 3.63828839]]
```

```
plt.scatter(X[y km == 0, 0],
            X[y km == 0, 1],
            s=50, c='lightgreen',
            marker='s', edgecolor='black',
            label='cluster 1')
plt.scatter(X[y km == 1, 0],
            X[y km == 1, 1],
            s=50, c='orange',
            marker='o', edgecolor='black',
            label='cluster 2')
plt.scatter(km.cluster centers [:, 0],
            km.cluster centers [:, 1],
            s=250, marker='*',
            c='red', edgecolor='black',
            label='centroids')
plt.legend(scatterpoints=1)
plt.grid()
plt.tight layout()
plt.show()
```



```
from sklearn.cluster import Kmeans
km = KMeans(n clusters=3,
            init='random',
            max iter=300,
            random state=0)
y km = km.fit predict(X)
y km
array([2, 1, 1, 1, 2, 1, 1, 2, 0, 1, 2, 0, 0, 1, 1, 0, 0, 2, 0, 2, 1, 2,
       1, 1, 0, 2, 2, 1, 0, 2, 0, 0, 0, 0, 1, 2, 2, 2, 1, 1, 0, 0, 1, 2,
       2, 2, 0, 1, 0, 1, 2, 1, 1, 2, 2, 0, 1, 2, 0, 1, 0, 0, 0, 0, 1, 0,
       1, 2, 1, 1, 1, 2, 2, 1, 2, 1, 1, 0, 0, 1, 2, 2, 1, 1, 2, 2, 2, 0,
       0, 2, 2, 1, 2, 1, 2, 1, 0, 0, 2, 2, 2, 2, 0, 2, 2, 1, 0, 1, 1, 1,
       0, 1, 2, 0, 1, 0, 1, 1, 0, 0, 1, 2, 1, 1, 2, 2, 0, 2, 0, 0, 0, 0,
       2, 0, 0, 0, 1, 0, 2, 0, 1, 1, 2, 2, 0, 0, 0, 0, 2, 2])
# cluster centers
print('<Cluster centers>\n', km.cluster centers )
<Cluster centers>
 [[ 0.9329651 4.35420712]
 [ 2.06521743  0.96137409]
 [-1.5947298 2.92236966]]
```

```
plt.scatter(X[y km == 0, 0],
            X[v km == 0, 1],
            s=50, c='lightgreen',
            marker='s', edgecolor='black',
            label='cluster 1')
plt.scatter(X[y km == 1, 0],
            X[y km == 1, 1],
            s=50, c='orange',
            marker='o', edgecolor='black',
            label='cluster 2')
plt.scatter(X[y km == 2, 0],
            X[y km == 2, 1],
            s=50, c='lightblue',
            marker='v', edgecolor='black',
            label='cluster 3')
plt.scatter(km.cluster centers_[:, 0],
            km.cluster centers [:, 1],
            s=250, marker='*',
            c='red', edgecolor='black',
            label='centroids')
plt.legend(scatterpoints=1)
plt.grid()
plt.tight layout()
plt.show()
```

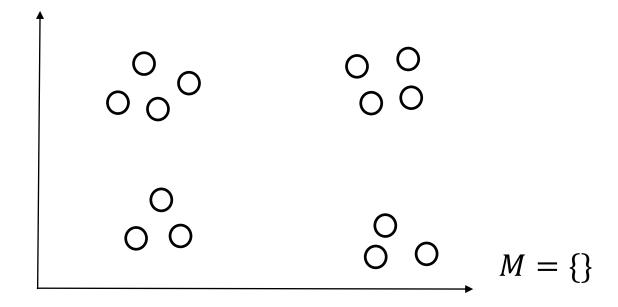


#### Concept

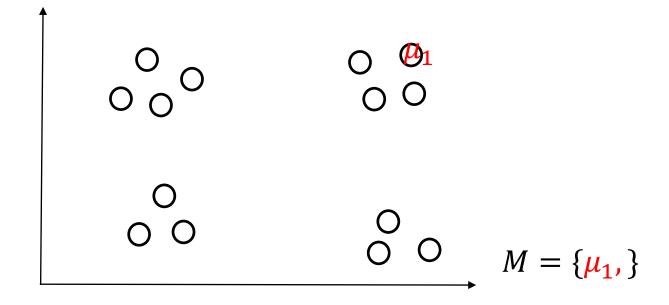
- Classic K-means
  - It can sometimes result in bad clustering or slow convergence if the initial centroids are chosen poorly
- Algorithm of K-means++
  - 1. Initialize an empty set M to store the k centroids being selected
  - 2. Randomly choose the first centroid  $\mu^{(j)}$  from the input samples and assign it to M
  - 3. For each sample  $x^{(i)}$  that is not in M, find the minimum squared distance  $d(x^{(i)}, M)^2$  to any of the centroids in M
  - 4. To randomly select the next centroid  $\mu^{(p)}$ , use a weighted probability distribution equal to  $\frac{d(x^{(p)},M)^2}{\sum_i d(x^{(i)},M)^2}$
  - 5. Repeat steps 2 and 3 until k centroids are chosen
  - 6. Proceed with the classic K-means algorithm



Algorithm of K-means++



Algorithm of K-means++



Algorithm of K-means++

select the next centroid using weight probability

Algorithm of K-means++

select the next centroid using weight probability

$$\frac{a(x^{(r)}, M)^{2}}{\sum_{i} d(x^{(i)}, M)^{2}}$$

$$0$$

$$0$$

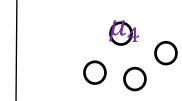
$$0$$

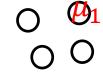
$$M = \{\mu_{1}, \mu_{2}, \mu_{3}\}$$

Algorithm of K-means++

select the next centroid using weight probability

$$\frac{d(x^{(p)}, M)^2}{\sum_i d(x^{(i)}, M)^2}$$

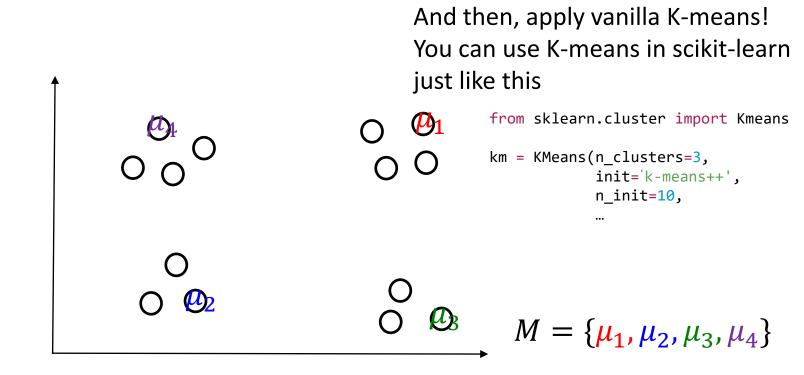






$$M = \{\mu_1, \mu_2, \mu_3, \mu_4\}$$

Algorithm of K-means++



#### Distortion

 Using the elbow method to find the optimal number of clusters

```
print('Distortion: %.2f' % km.inertia )
                                                           Distortion: 72.48
# plotting distortions for k = 1 to 11
distortions = []
for i in range(1, 11):
      km = KMeans(n_clusters=i,
                 init='k-means++',
                 max iter=300,
                 random state=0)
     km.fit(X)
     distortions.append(km.inertia )
                                                          700
plt.plot(range(1, 11), distortions, marker='o')
plt.xlabel('Number of clusters')
                                                          600
plt.ylabel('Distortion')
                                                          500
plt.tight_layout()
                                                        Distortion
300
plt.show()
                                                                          k = 3
                                                          200
                                                          100
                                                                           Number of clusters
```

### Silhouette Analysis

#### Silhouette Analysis

- One of intrinsic metric to evaluate the quality of a clustering
  - Can be used as a graphical tool to plot a measure of how tightly grouped the samples in the clusters are
- Algorithm
  - 1. Calculate **the cluster cohesion**  $a^{(i)}$  as the average distance between a sample  $x^{(i)}$  and all other points in the same cluster
  - 2. Calculate **the cluster separation**  $b^{(i)}$  from the next closest cluster as the average distance between the sample  $x^{(i)}$  and all samples in the nearest cluster
  - 3. Calculate the silhouette  $s^{(i)}$  as the difference between cluster cohesion and separation divided by the greater of the two, as shown here:

$$s^{(i)} = \frac{b^{(i)} - a^{(i)}}{max\{b^{(i)}, a^{(i)}\}}$$



### Silhouette Analysis

- Silhouette Analysis
  - Average Silhouette Width
    - Average of  $s^{(i)}$
    - How to use the value

Range of SC	Interpretation
0.71-1.0	A strong structure has been found
0.51-0.70	A reasonable structure has been found
0.26-0.50	The structure is weak and could be artificial
< 0.25	No substantial structure has been found

https://www.stat.berkeley.edu/~spector/s133/Clus.html

# Silhouette Analysis using scikit-learn

Measuring the quality of clustering via silhouette plots

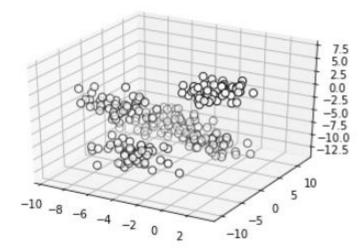
```
from sklearn.metrics import silhouette score
# plotting silhouette scores for k = 2 to 11
silhouette scores = []
for i in range(2, 11):
     km = KMeans(n clusters=i,
                  init='k-means++',
                  max iter=300,
                  random state=0)
     y km = km.fit predict(X)
      silhouette scores.append(silhouette score(X, y km, metric='euclidean'))
plt.plot(range(2, 11), silhouette scores, marker='o')
                                                               0.70
plt.xlabel('Number of clusters')
plt.ylabel('Silhouette score')
                                                               0.65
plt.tight layout()
                                                               0.60
                                                             Silhouette score
plt.show()
                                                               0.55
                                                               0.50
                                                               0.45
                                                               0.40
                                                               0.35
                                                                                 Number of clusters
```

#### Make simple 3D data and plotting

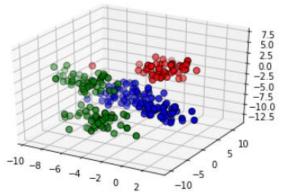
```
from sklearn.datasets import make blobs
# make simple 3D data
X, y = make blobs(n samples=250,
                n features=3,
                centers=5,
                cluster std=1.5,
                shuffle=True,
                random state=1)
X
array([[ -3.53629743e+00,
                          -6.02983465e+00, -9.53019216e+00],
         1.81801027e+00,
                          -9.91484955e-01, 3.15589155e+00],
        -4.32462107e+00,
                          -7.40257340e+00, -7.58369028e+00],
         1.85916632e+00,
                          -9.24290830e-01, 1.72209806e+00],
        -2.78149052e+00,
                          3.53529403e+00, -1.01638435e+01],
       -4.67636968e+00,
                          -2.97755645e+00, 4.29766489e-01],
       [ -8.02808319e+00,
                          -1.20932028e+00, -2.57803932e+00],
        -9.97923558e-01,
                          -2.52376196e+00, 2.57342840e+00],
        -4.84489985e+00,
                          -3.74014658e+00,
                                           -1.87979408e-01],
       [ -1.38773851e+00,
                          5.25300717e+00,
                                           -1.08474778e+01],...
```

#### Make simple 3D data and plotting

```
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
# plotting simple 3D data
fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')
ax.scatter(X[:, 0], X[:, 1], X[:, 2], s=50, c='white', edgecolor='black')
plt.show()
```



```
from sklearn.cluster import KMeans
# KMeans with k = 3
km = KMeans(n clusters=3,
           init='random',
           max iter=300,
           random state=0)
# cluster assignment
y km = km.fit predict(X)
y km
array([2, 0, 2, 0, 1, 2, 2, 0, 2, 1, 1, 2, 1, 1, 1, 1, 2, 2, 1, 1, 1, 2, 2,
       2, 2, 1, 2, 0, 2, 1, 1, 0, 0, 1, 2, 0, 1, 0, 1, 2, 2, 2, 2, 2, 0, 0,
       2, 2, 0, 2, 0, 2, 1, 2, 2, 1, 0, 2, 2, 1, 1, 0, 1, 1, 0, 0, 2, 2, 1,
       2, 2, 1, 0, 1, 1, 2, 0, 0, 0, 2, 1, 2, 1, 1, 2, 1, 0, 2, 1, 2, 2, 0,
       1, 0, 2, 1, 2, 2, 2, 1, 2, 0, 1, 0, 1, 0, 2, 1, 2, 1, 0, 1, 1, 1, 2,
       1, 1, 1, 0, 2, 1, 1, 1, 2, 1, 2, 2, 1, 2, 1, 0, 1, 2, 2, 0, 2, 2, 2,
       1, 2, 1, 1, 0, 2, 1, 2, 0, 0, 1, 0, 2, 2, 0, 2, 2, 2, 0, 1, 1, 1, 1,
       1, 0, 2, 2, 2, 2, 1, 1, 2, 1, 1, 0, 0, 1, 2, 1, 1, 2, 2, 0, 0, 2, 1,
       2, 0, 1, 1, 2, 1, 2, 0, 1, 1, 2, 2, 0, 1, 2, 0, 2, 1, 0, 2, 1, 1, 2,
       1, 2, 1, 1, 0, 1, 1, 2, 2, 2, 1, 1, 1, 1, 0, 1, 2, 1, 1, 1, 1, 1, 1,
       0, 2, 2, 2, 0, 2, 2, 1, 2, 1, 2, 2, 0, 2, 2, 1, 1, 2, 1, 1]
```



 Using the elbow method to find the optimal number of clusters

```
# plotting distortions for k = 1 to 11
distortions = []
for i in range(1, 11):
      km = KMeans(n clusters=i,
                  init='k-means++',
                 max iter=300,
                  random state=0)
     km.fit(X)
                                                      18000
     distortions.append(km.inertia )
                                                      16000
plt.plot(range(1, 11), distortions, marker='o')
                                                      14000
plt.xlabel('Number of clusters')
plt.ylabel('Distortion')
                                                      12000
plt.tight layout()
                                                      10000
plt.show()
                                                       8000
                                                       6000
                                                       4000
                                                       2000
                                                                  2
                                                                                                       10
                                                                            Number of clusters
```

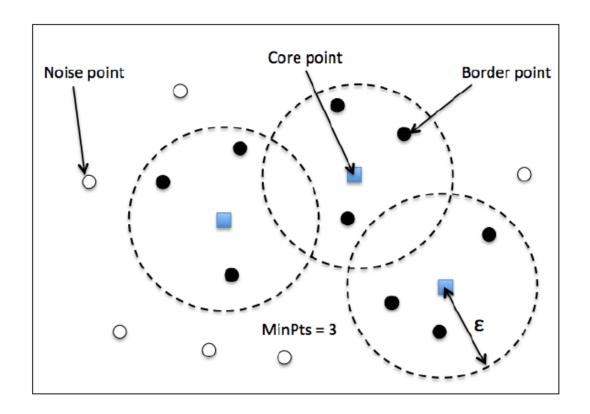
### Example

Measuring the quality of clustering via silhouette plots

```
# plotting silhouette scores for k = 1 to 11
silhouette scores = []
for i in range(2, 11):
      km = KMeans(n clusters=i,
                  init='k-means++',
                  max iter=300,
                  random state=0)
      y km = km.fit predict(X)
      silhouette scores.append(silhouette_score(X, y_km, metric='euclidean'))
plt.plot(range(2, 11), silhouette scores, marker='o')
plt.xlabel('Number of clusters')
plt.ylabel('Silhouette score')
                                                            0.60
plt.tight layout()
                                                            0.55
plt.show()
                                                          Silhouette score
                                                            0.50
                                                            0.45
                                                            0.35
                                                            0.30
                                                                               Number of clusters
```

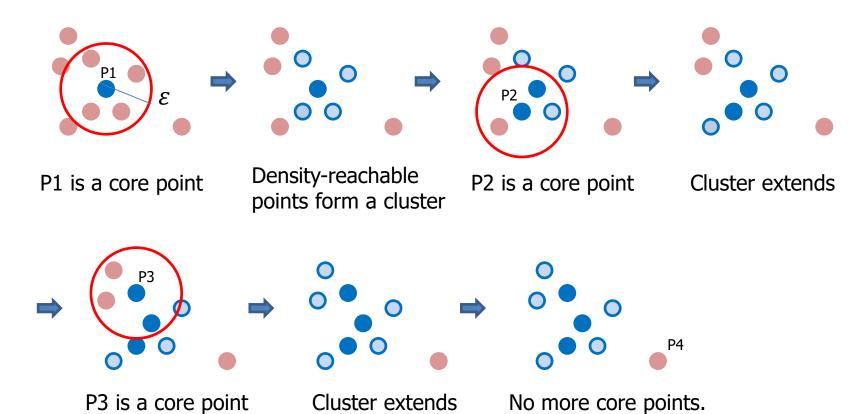
- Density-Based Spatial Clustering of Applications with Noise
  - DBSCAN groups data in dense region
  - Density parameters
    - Radius  $\varepsilon$ : Distance to determine the neighborhood
    - MinPts: Minimum number of points in neighborhood
- In DBSCAN, a special label is assigned to each sample (point)
  - Core point: It contains *MinPts* of neighboring points within *radius*  $\varepsilon$
  - **Border point**: It has fewer neighbors than MinPts within  $\varepsilon$ , but lies within the  $\varepsilon$  radius of a core point
  - Noise points(outliers): All other points that are neither core nor border points are considered as noise points

- Density-Based Spatial Clustering of Applications with Noise
  - MinPts = 4



- DBSCAN algorithm
  - A cluster a maximal set of density-connected points
  - Discovers clusters of arbitrary shape in databases with noise
  - 1. Arbitrary select a point **p**
  - 2. Retrieve all  $\varepsilon$ -neighborhood of  $\boldsymbol{p}$
  - 3. If **p** is a core object, a cluster is formed
  - 4. From each core object **p**, iteratively collects density-reachable objects (may merge clusters)
  - 5. Continue the process until no new points can be added

- DBSCAN algorithm example
  - MinPts = 4 (example)



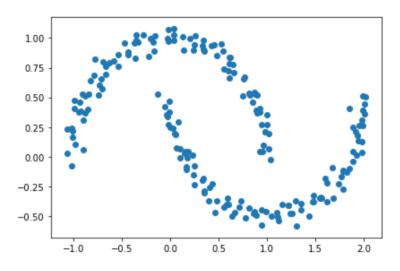
P4 is an outlier

### Make simple data and plotting

```
from sklearn.datasets import make_moons
import matplotlib.pyplot as plt

X, y = make_moons(n_samples=200, noise=0.05, random_state=0)
plt.scatter(X[:, 0], X[:, 1])
plt.tight_layout()

plt.show()
```



#### Problem of K-means clustering

#### Problem of K-means clustering

```
# plotting clusters
f, (ax1)= plt.subplots(1, 1, figsize=(6, 4))
ax1.scatter(X[y \ km == 0, 0], X[y_km == 0, 1],
            c='blue', marker='o', s=40, label='cluster 1')
ax1.scatter(X[y \ km == 1, 0], X[y \ km == 1, 1],
           c='red', marker='s', s=40, label='cluster 2')
ax1.set title('K-means clustering')
plt.legend()
                                                                      K-means clustering
plt.tight layout()
                                                                                                cluster 1
                                                 1.00
                                                                                                cluster 2
plt.show()
                                                 0.75
                                                 0.50
                                                 0.25
                                                 0.00
                                                -0.25
```

2.0

1.5

-0.50

-1.0

-0.5

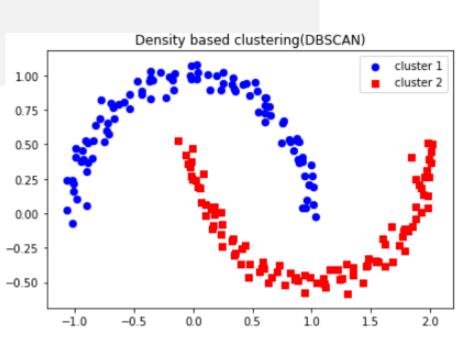
0.0

0.5

1.0

#### Density based clustering

### Density based clustering



#### Outlier Detection

```
# make outliers
X[0] = [1, 1]
X[1] = [-0.5, -0.5]
# DBSCAN with eps = 0.2, min samples = 5
db = DBSCAN(eps=0.2, min samples=5, metric='euclidean')
y_db = db.fit_predict(X)
y db
                        0,
                                            0,
array([-1, -1,
                            0,
                                0, 1,
                                            0,
                                            0,
                        1,
                        0,
                                            1,
                        1,
                                                        0], dtype=int64)
```

#### Outlier Detection

```
# find data that is not clustered (-1) - outlier
outlier idxs = (y db == -1)
X[outlier idxs]
array([[ 1. , 1. ],
       [-0.5, -0.5]
# plotting outliers
plt.scatter(X[~outlier idxs, ∅],
           X[~outlier idxs, 1],
           alpha=0.5, color='b', label='normal')
                                                                  Detecting outliers using DBSCAN
plt.scatter(X[outlier idxs, 0],
           X[outlier idxs, 1],
                                                     1.00
           color='r', label='outliers')
plt.legend()
                                                     0.75
plt.title("Detecting outliers using DBSCAN")
                                                     0.50
plt.show()
                                                     0.25
                                                     0.00
                                                    -0.25
                                                    -0.50
```

2.0

1.5

1.0

normal

outliers

-1.0

-0.5

0.0

### Submit

- To make sure if you have completed this practice,
   Submit your practice file(Week11 givencode.ipynb) to e-class.
- Deadline : tomorrow 11:59pm
- Modify your ipynb file name as "Week11\_StudentNum\_Name.ipynb"
   Ex) Week11\_2020123456\_홍길동.ipynb
- You can upload this file without taking the quiz, but homework will be provided like a quiz every three weeks, so it is recommended to take the quiz as well.

## Quiz1: K-means Clustering

- Figure out the data structure of unlabeled data
- Motor Trend Dataset
  - The data was extracted from the 1974 Motor Trend US magazine, and comprises fuel consumption and 10 aspects of automobile design and performance for 32 automobiles (1973–74 models).

#### Goal

- We would like to recommend the products that meet the needs of customers by classifying the cars in the list into several clusters according to their features.
- After clustering, Explain each cluster based on its features



### Quiz2: DBSCAN

- Detecting outliers using DBSCAN
- Iris Dataset
- Goal
  - Detect & Remove outliers from the iris dataset

