03ClusteringTheory

March 18, 2019

1 分群 (Clustering)

1. 目標:
    - 群內相似度很高
    - 群間相似度很低
2. 主要影響因子:
    - 相似度的衡量與實作
    - 「群」的定義
    - 演算法
3. 應用面:
    - 市場區隔
    - 生物分群
    - 新聞分群

2 距離的定義

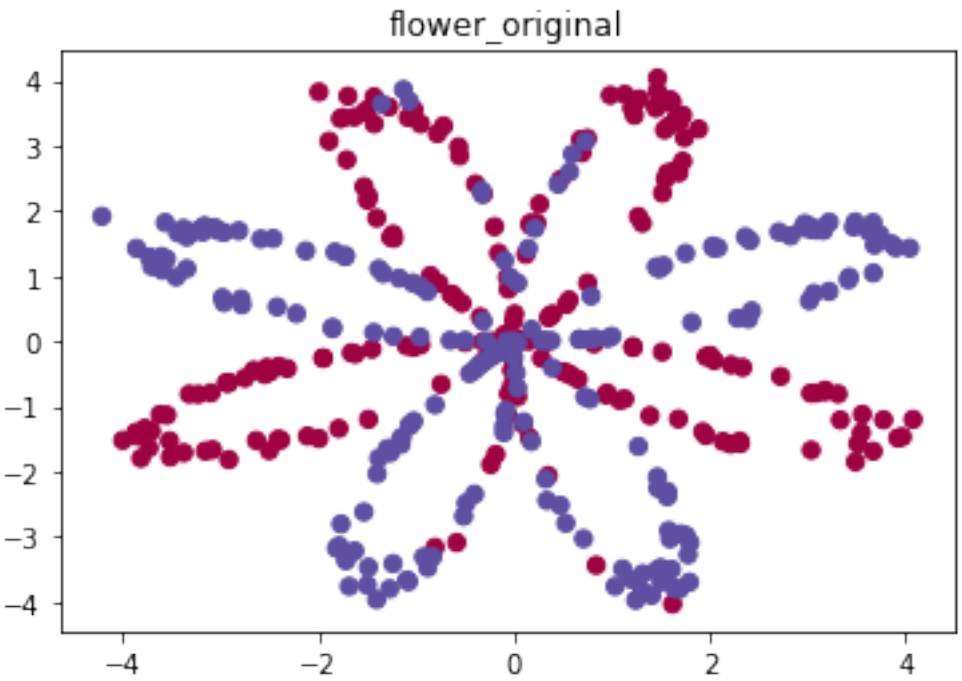
1. Euclidean distance(歐基里德距離)
    - $d(i,j) = \sqrt{|x_{i1} - x_{j1}|^2 + |x_{i2} - x_{j2}|^2 + \cdots + |x_{in} - x_{jn}|^2}$
2. Manhattan (city block) distance(曼哈頓距離)
    - $d(i,j) = |x_{i1} - x_{j1}| + |x_{i2} - x_{j2}| + \cdots + |x_{in} - x_{jn}|$
3. Minkowski distance
    - $d(i,j) = \sqrt[q]{|x_{i1} - x_{j1}|^q + |x_{i2} - x_{j2}|^q + \cdots + |x_{in} - x_{jn}|^q}$
4. Weighted Manhattan distance(加權曼哈頓距離)
    - $d(i,j) = \sqrt[q]{w1|x_{i1} - x_{j1}|^q + w2|x_{i2} - x_{j2}|^q + \cdots + w3|x_{in} - x_{jn}|^q}$

3 IMPORT & DATA

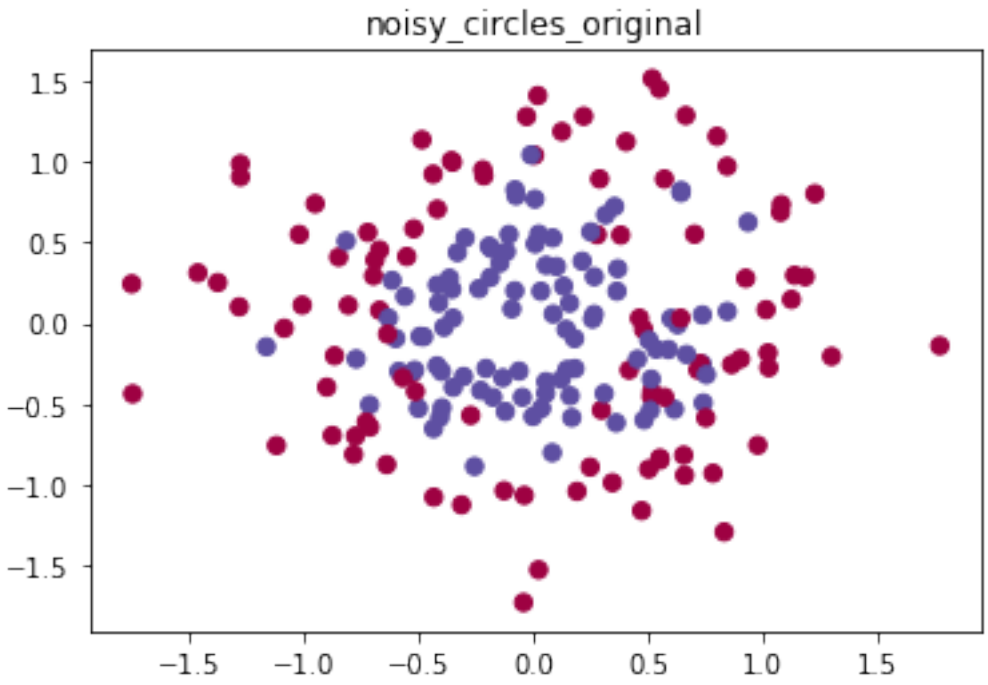
In [1]:
```
import matplotlib.pyplot as plt
from planar_utils import plot_decision_boundary, sigmoid, load_planar_dataset, load_ex
import numpy as np
np.random.seed(1212)

import os
from collections import Counter
import pandas as pd

from load_all_datasets import load
from sklearn.cluster import KMeans, AgglomerativeClustering, DBSCAN

from mpl_toolkits.mplot3d import Axes3D
from sklearn import datasets
from sklearn.decomposition import PCA
```

In [2]:
```
# demo 用資料
datas = load()

for name, X, Y in datas:
    print(name)
    plt.scatter(X[:, 0], X[:, 1], c=Y , s=40, cmap=plt.cm.Spectral);
    plt.title(name+'_original')
    plt.show()
```

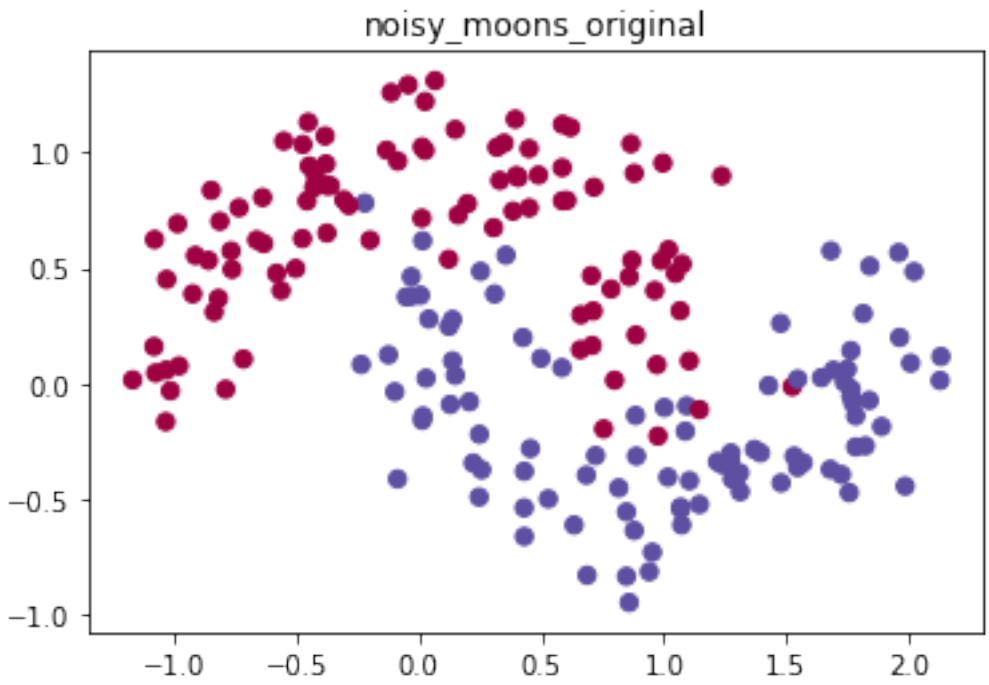
```
flower
```



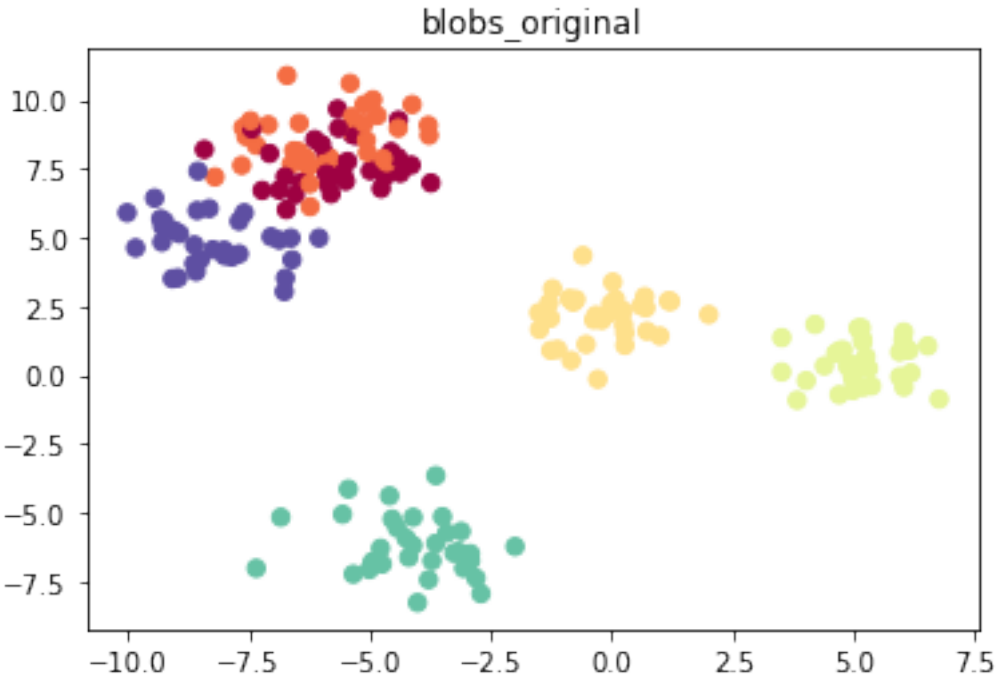
noisy_circles



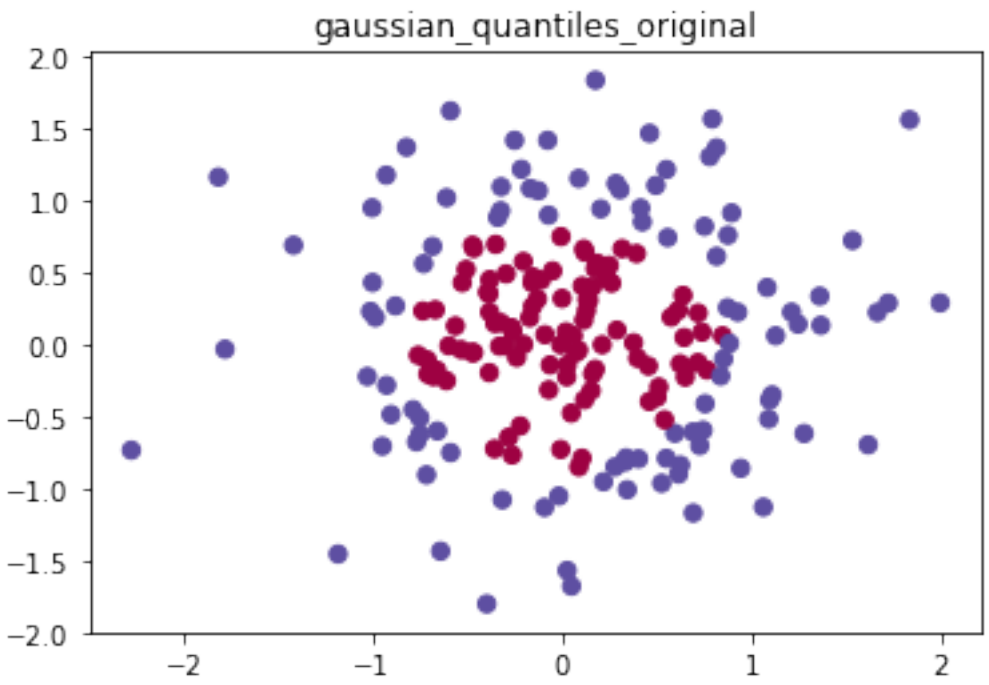
noisy_moons


noisy_moons_original
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0

blobs


blobs_original
10.0
7.5
5.0
2.5
0.0
−2.5
−5.0
−7.5
−10.0
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5

gaussian_quantiles



In [3]:
```
# 練習用資料
iris = datasets.load_iris()
df_iris = pd.DataFrame(iris.data, columns=iris['feature_names'])
df_iris['target'] = list(map(lambda x:iris.target_names[x], iris.target))
df_iris.head()
```

Out[3]:

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
0	5.1	3.5	1.4	0.2	setosa
1	4.9	3.0	1.4	0.2	setosa
2	4.7	3.2	1.3	0.2	setosa
3	4.6	3.1	1.5	0.2	setosa
4	5.0	3.6	1.4	0.2	setosa

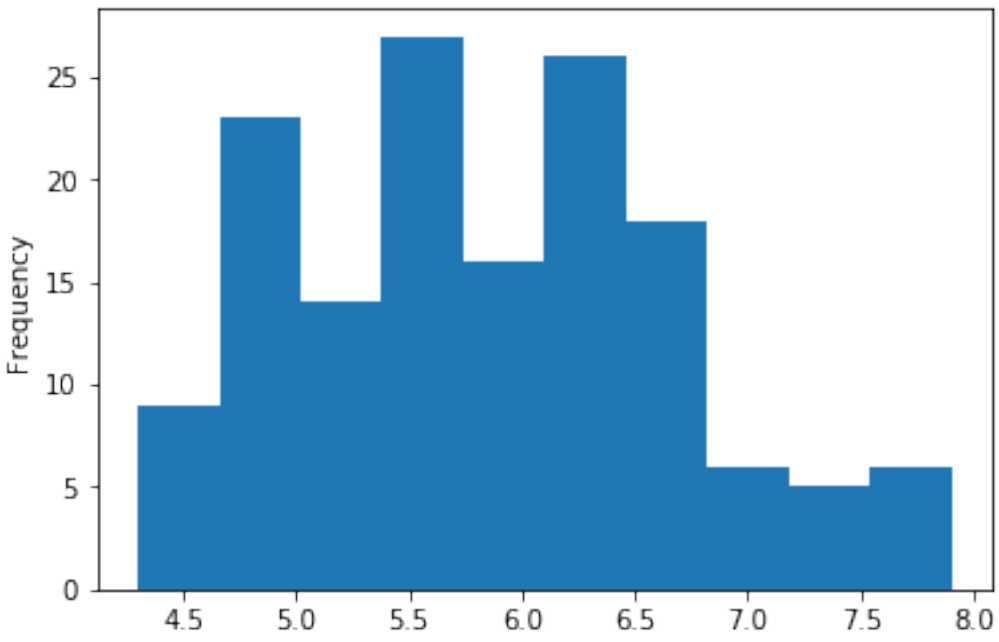
In [4]:
```
# 簡單資料探索
# 請找出每一個 target(花的類別) 的種類各有幾筆資料 (hint: groupby)
```

```
        #!=============your works starts===============!#

        #!=============your works ends================!#
```

Out[4]:

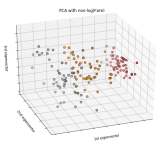
target	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)
setosa	50	50	50	50
versicolor	50	50	50	50
virginica	50	50	50	50

```
In [5]: # 請畫出 ['sepal length (cm)'] 的分布狀況
        #!=============your works starts===============!#

        #!=============your works ends================!#

        plt.show()
```




```
In [6]: iris_X = df_iris[["sepal length (cm)", "sepal width (cm)", "petal length (cm)", "petal
        iris_Y = iris.target
        X = iris_X
```

```
Y = iris_Y

# 請使用 PCA 畫出不同花在三維空間中的分布位置 (請上網尋找 PCA 的程式碼，並複製過來)
#!=============your works starts===============!#









#!==============your works ends================!#

plt.show()
```



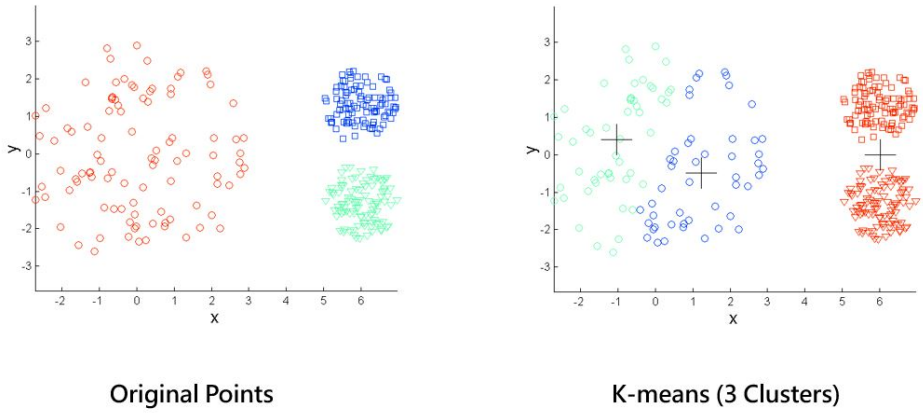
4 ALGORITHM

4.1 1. K-means

4.1.1 steps

1. 設定重心:
   - 決定要分幾個群 (e.g. K 群)
   - 隨機產生 K 個重心
2. 分群:
   - 找到所有資料點歸屬的重心: 找到分別最靠近這三個點的所有資料點，並做第一個迴圈的分群
3. 尋找重心:
   - 重新計算所有資料點的重心 (element-wise 的平均)
4. ....
5. 停止:
   - 重複上述方法，只到不會有資料點因為重新尋找重心而改變群組

kmeans



KmeansCon1.JPG

4.1.2 visualize

1. web:

   game

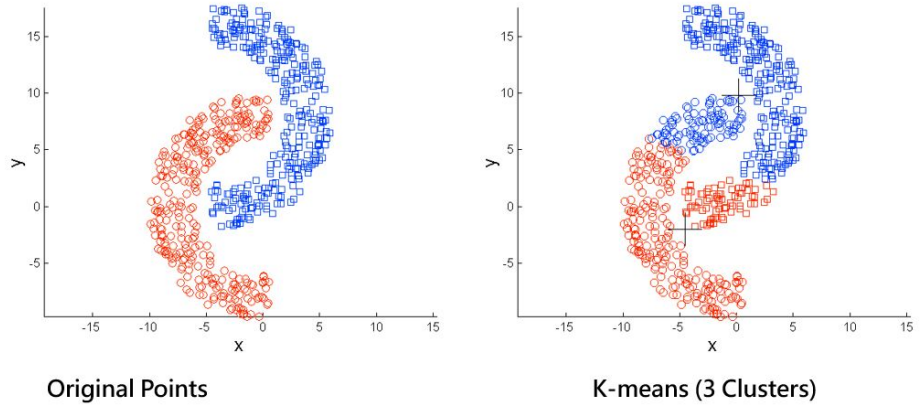
2.

4.1.3 parameters

參數	意義
n_cluster	要分成幾個群
random_state	決定初始點的隨機 seed

4.1.4 pros & cons

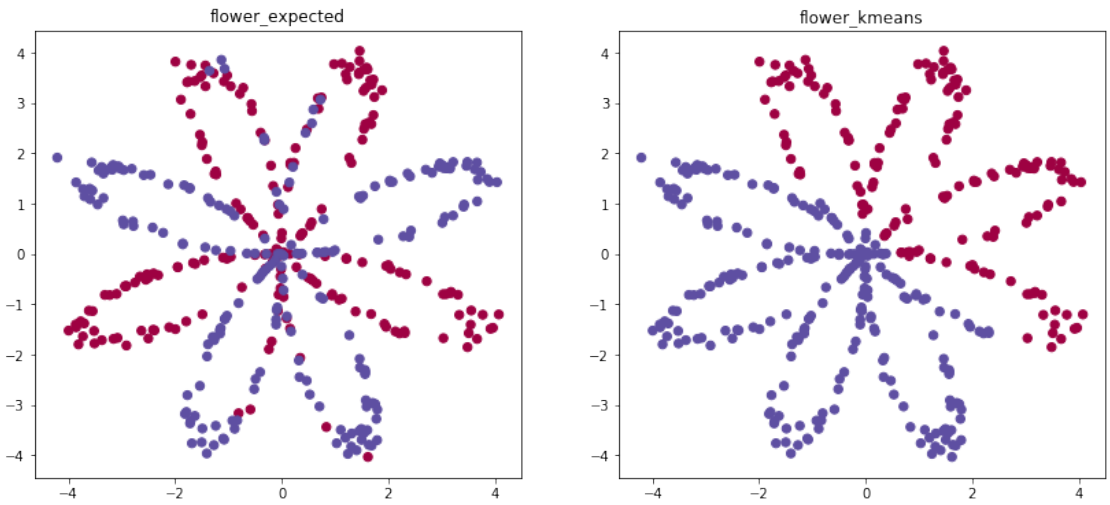
1. 一開始需要決定要分成幾個群
2. 優點
   - 效率: 時間複雜度 O(tkn)。n 是資料點的個數，k 是群的個數，t 是迴圈的個數，一班來說: k, t << n。
3. 缺點
   - 需要指定分成幾群
   - 無法處理具有雜訊 (noisy) 的資料及離群值 (outliers)
   - 無法處理不同大小及不同密度的群
   - 無法發現凸多邊形 (non-convex) 以外的群

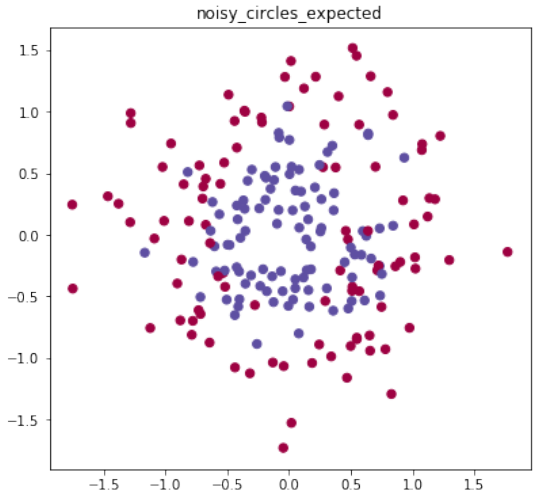


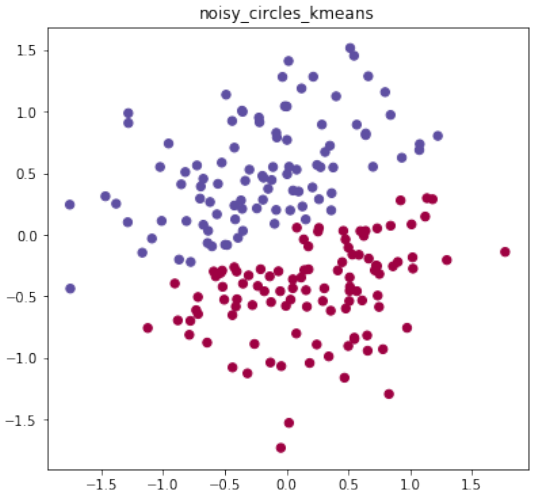
KmeansCon2.JPG

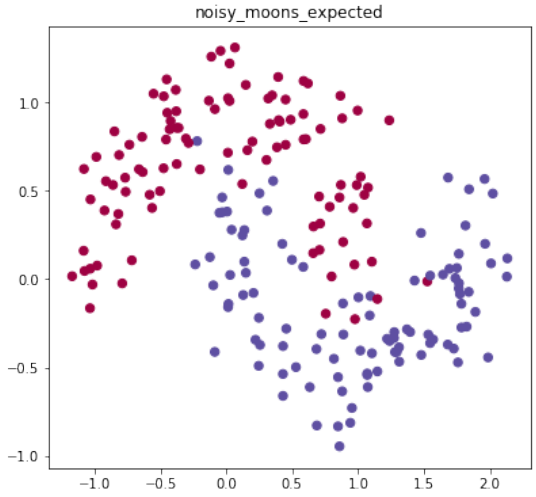
- 通常在 local optimum 停止

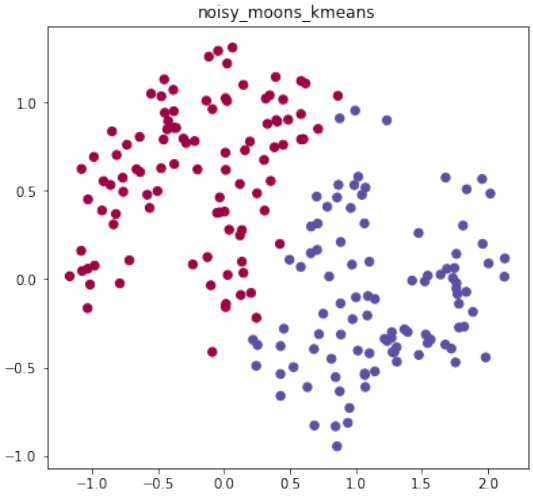
```
In [7]: for name, X, Y in datas:
            plt.figure(figsize=(14,6))


            axes1 = plt.subplot(1, 2, 1)
            axes1.scatter(X[:, 0], X[:, 1], c=Y, s=40, cmap=plt.cm.Spectral)
            plt.title(name + "_expected")

            axes2 = plt.subplot(1, 2, 2)
            n_clusters = len(set(Y))
            kmeans = KMeans(n_clusters=n_clusters, random_state=0).fit_predict(X)
            axes2.scatter(X[:, 0], X[:, 1], c=kmeans, s=40, cmap=plt.cm.Spectral);
            plt.title(name+'_kmeans')

            plt.show()
```

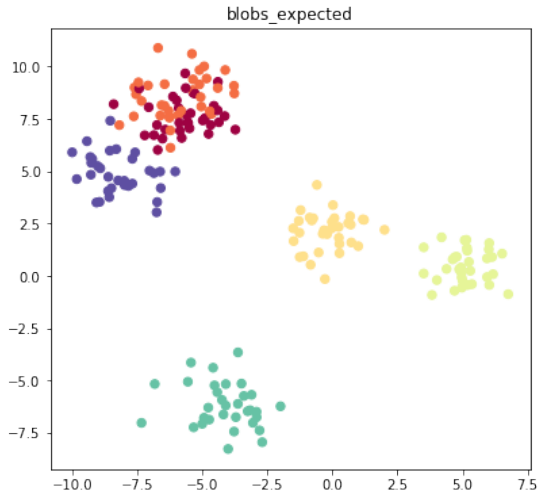


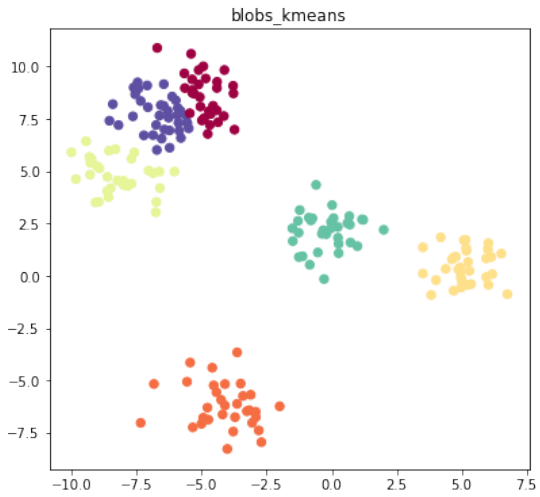

noisy_circles_expected
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

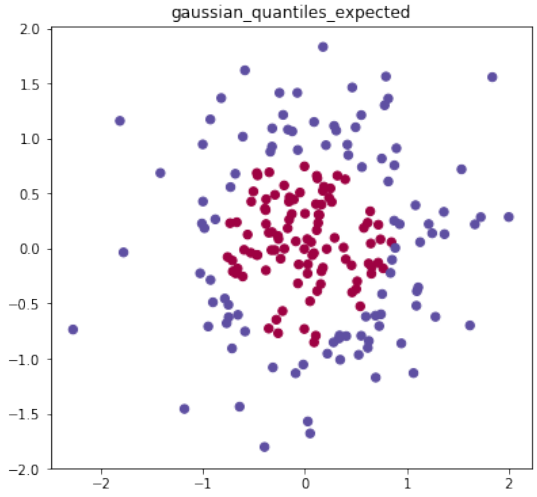

noisy_circles_kmeans
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5

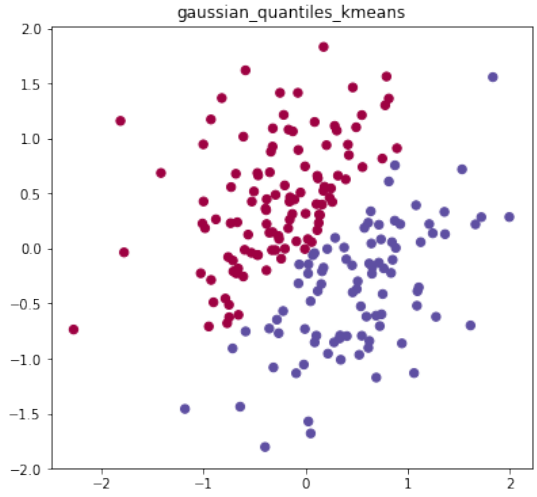

noisy_moons_expected
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0


noisy_moons_kmeans
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0









In [8]:
```
# 解釋 fit_predict
# from  sklearn.model_selection import train_test_split
# iris_X_train, iris_X_test, iris_Y_train ,iris_Y_test = train_test_split(iris_X, iris_
# kmeans_clf.fit(iris_X_train)
# predict_Y = kmeans_clf.predict(iris_X_test)


# X = iris_X_test
# Y = iris_Y_test
# print(len(X))
# print(len(Y))
# fig = plt.figure(1, figsize=(16, 6))
```

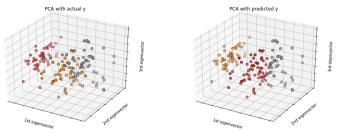
```
        # ax = fig.add_subplot(1, 2, 1, projection='3d')
        # X_reduced = PCA(n_components=3).fit_transform(X)
        # ax.scatter(X_reduced[:, 0], X_reduced[:, 1], X_reduced[:, 2], c=Y,
        #            cmap=plt.cm.Set1, edgecolor='k', s=40)
        # ax.set_title("PCA with non-log(Fare)")
        # ax.set_xlabel("1st eigenvector")
        # ax.w_xaxis.set_ticklabels([])
        # ax.set_ylabel("2nd eigenvector")
        # ax.w_yaxis.set_ticklabels([])
        # ax.set_zlabel("3rd eigenvector")
        # ax.w_zaxis.set_ticklabels([])

        # # predict
        # X = iris_X_test
        # Y = predict_Y
        # print(len(X))
        # print(len(Y))
        # fig = plt.figure(1, figsize=(16, 6))
        # ax = fig.add_subplot(1, 2, 2, projection='3d')
        # X_reduced = PCA(n_components=3).fit_transform(X)
        # ax.scatter(X_reduced[:, 0], X_reduced[:, 1], X_reduced[:, 2], c=Y,
        #            cmap=plt.cm.Set1, edgecolor='k', s=40)
        # ax.set_title("PCA with non-log(Fare)")
        # ax.set_xlabel("1st eigenvector")
        # ax.w_xaxis.set_ticklabels([])
        # ax.set_ylabel("2nd eigenvector")
        # ax.w_yaxis.set_ticklabels([])
        # ax.set_zlabel("3rd eigenvector")
        # ax.w_zaxis.set_ticklabels([])

        # plt.show()
```

In [9]:
```
        # 請使用 kmeans 將 iris_X 進行分群 (注意:random_state=0)
        #=============your works starts===============#
        n_clusters =
        kmeans_Y =
        #==============your works ends================#

        np.random.seed(1212)
        print(kmeans_Y[np.random.randint(149, size=10)])
        # # [2 0 0 2 2 1 1 1 1 0]
```

```
[2 0 0 2 2 1 1 1 1 0]
```

In [10]:
```
        # actual
         def plot_iris_predict_acc(predict_Y):
             X = iris_X
```

```
    Y = iris_Y
    fig = plt.figure(1, figsize=(16, 6))
    ax = fig.add_subplot(1, 2, 1, projection='3d')
    X_reduced = PCA(n_components=3).fit_transform(X)
    ax.scatter(X_reduced[:, 0], X_reduced[:, 1], X_reduced[:, 2], c=Y,
               cmap=plt.cm.Set1, edgecolor='k', s=40)
    ax.set_title("PCA with actual y")
    ax.set_xlabel("1st eigenvector")
    ax.w_xaxis.set_ticklabels([])
    ax.set_ylabel("2nd eigenvector")
    ax.w_yaxis.set_ticklabels([])
    ax.set_zlabel("3rd eigenvector")
    ax.w_zaxis.set_ticklabels([])

    # predict
    X = iris_X
    Y = predict_Y
    fig = plt.figure(1, figsize=(16, 6))
    ax = fig.add_subplot(1, 2, 2, projection='3d')
    X_reduced = PCA(n_components=3).fit_transform(X)
    ax.scatter(X_reduced[:, 0], X_reduced[:, 1], X_reduced[:, 2], c=Y,
               cmap=plt.cm.Set1, edgecolor='k', s=40)
    ax.set_title("PCA with predicted y")
    ax.set_xlabel("1st eigenvector")
    ax.w_xaxis.set_ticklabels([])
    ax.set_ylabel("2nd eigenvector")
    ax.w_yaxis.set_ticklabels([])
    ax.set_zlabel("3rd eigenvector")
    ax.w_zaxis.set_ticklabels([])

    plt.show()

np.random.seed(1212)
plot_iris_predict_acc(kmeans_Y)
```



```
In [11]: # curve the k-means algorithm
         from sklearn.metrics.pairwise import euclidean_distances
         np.random.seed(2424)
         n_samples = 40
         n_features = 100
         n_means = 3
```

```
        # initialize your X and means using np.random.random()
        #=============your works starts===============#
        X =
        means =
        #==============your works ends================#

        print(X.shape)
        print(means.shape)
        # (40, 100)
        # (3, 100)
```

```
(40, 100)
(3, 100)
```

In [12]:
```
        # find the distance between each sample and mean(hint: euclidean_distances)
        #=============your works starts===============#
        distances =
        #==============your works ends================#

        print(distances.shape)
        # (40, 3)
```

```
(40, 3)
```

In [13]:
```
        # get the nearest mean index(0,1,2) for each sample (hint: np.argmin)
        #=============your works starts===============#
        nearest_mean_index =
        #==============your works ends================#

        print(nearest_mean_index.shape)
        # (40,)
```

```
(40,)
```

In [37]:
```
        # find the X belong to each cluster
        # find new mean for each cluster
        # and reshape into (3, 100)
        #=============your works starts===============#
        X_belong_cluster_n =
        new_means =
        new_means =
        #==============your works ends================#

        print(len(X_belong_cluster_n))
        print(X_belong_cluster_n[0].shape)
```

```
        print(X_belong_cluster_n[1].shape)
        print(X_belong_cluster_n[2].shape)
        print(new_means.shape)
        # 3
        # (17, 100)
        # (9, 100)
        # (14, 100)
        # (3, 100)
```

```
3
(17, 100)
(9, 100)
(14, 100)
(3, 100)
```

4.2 2. Hierarchical Clustering

4.2.1 steps

hierarchical 的分群方法，步驟簡述如下，可參考下圖 (取自維基百科):

1. 把每一個點當作一個群組
2. 透過掃描過整個資料及尋找出最近的兩個群組，並把這兩個點榜再一起變成一個群組
3. 尋找下一個最近的的兩個群組，再綁再一起變成一個群組
4. ....
5. 停止：直到所有資料都被分成一群，或是透過設定參數到分到幾個群時自動停止

4.2.2 parameters

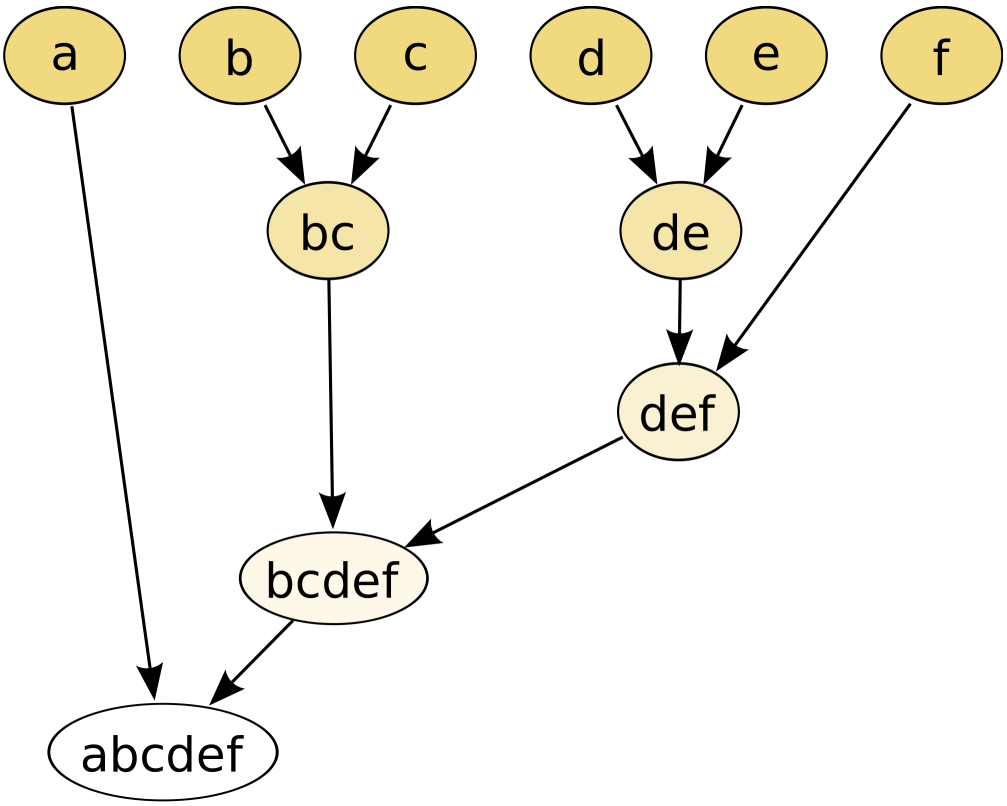
1. table

參數	意義
linkage	如何衡量群與群之間的距離。(註解)
n_clusters	分成幾個群

2. 註解:
    - ward(single): 兩個群中最近的點。
    - complete: 兩個群中最遠的點。
    - average: 兩個群的重心。

4.2.3 pros & cons

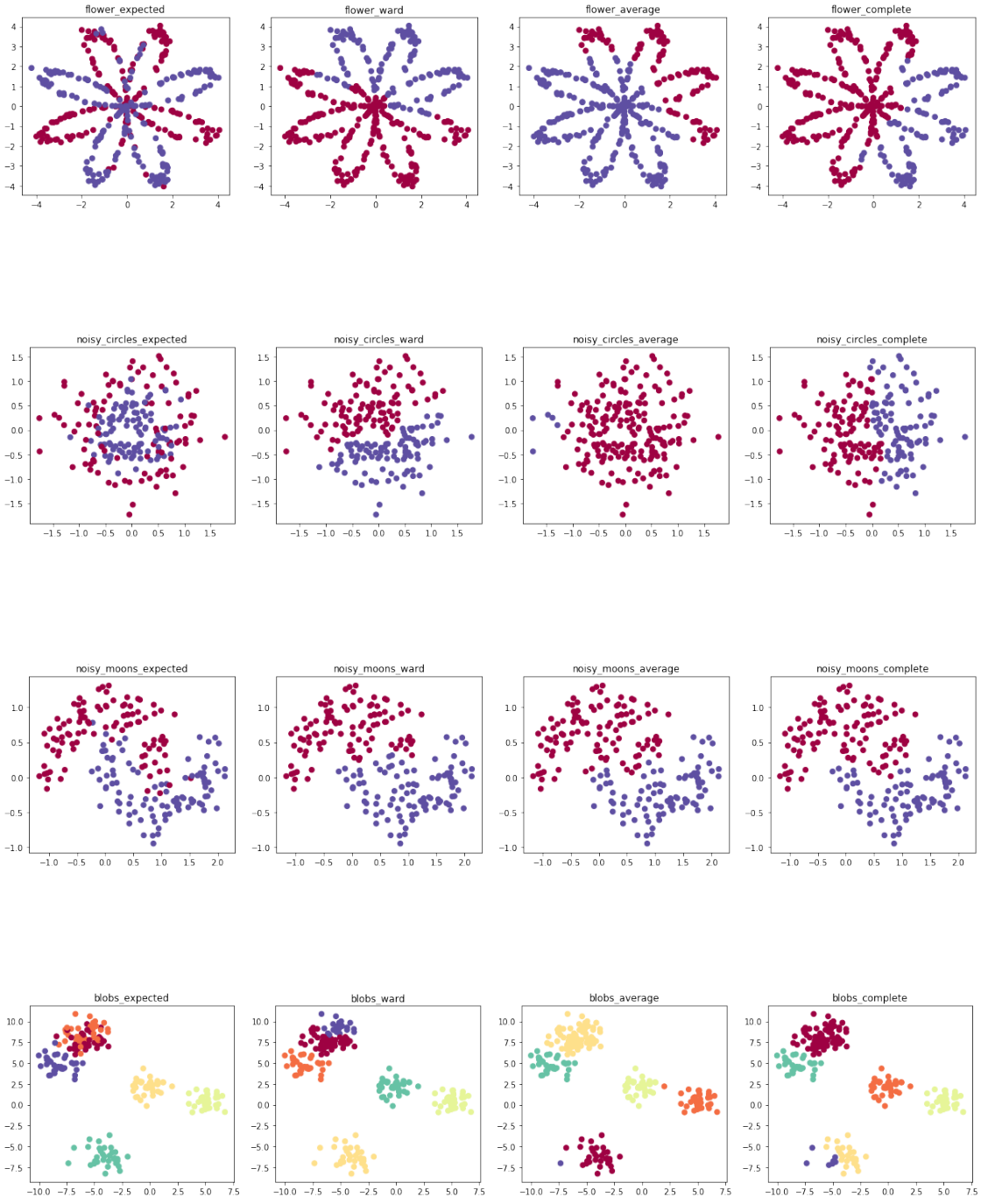
1. 比較耗效能: 因為有 100 萬筆資料，就要跑 100 萬次迴圈，每一次迴圈都要掃描過每一筆資料，才能跑完。
2. 很適合用來做生物分類，因為它可以完整畫出分類樹狀圖。

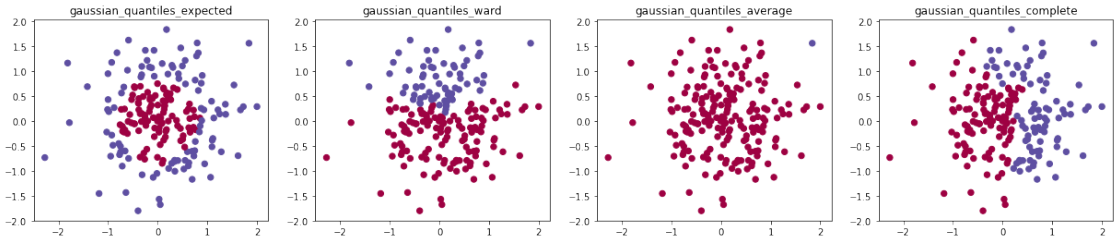


hierarchical

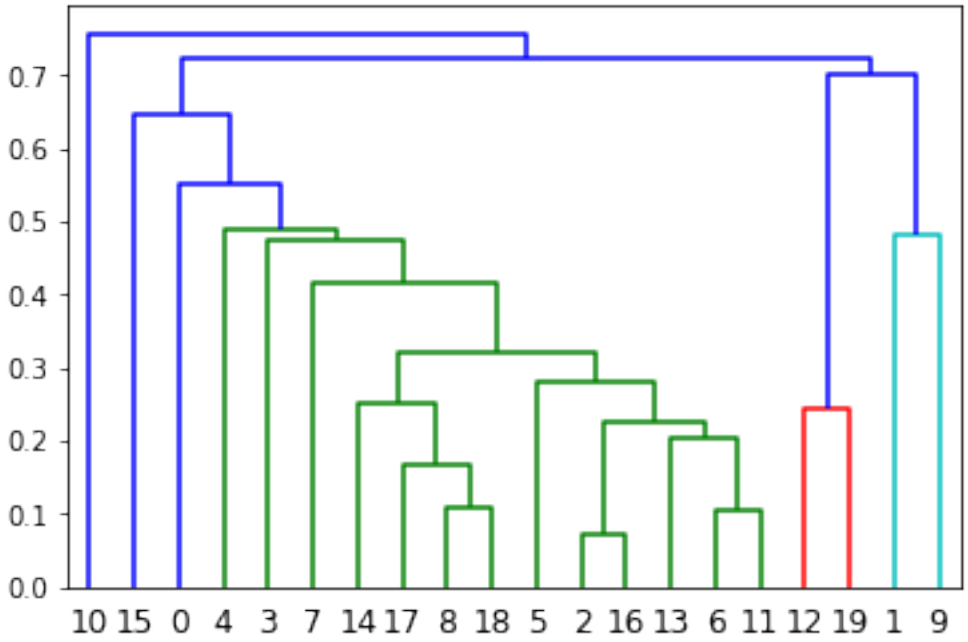
```
In [38]: linkage = ['ward', 'average', 'complete']
         for name, X, Y in datas:

             plt.figure(figsize=(21,4))

             axes1 = plt.subplot(1, 4, 1)
             axes1.scatter(X[:, 0], X[:, 1], c=Y, s=40, cmap=plt.cm.Spectral)
             plt.title(name+'_expected')

             axes2 = plt.subplot(1, 4, 2)
             n_clusters = len(set(Y))
             hierarchy = AgglomerativeClustering(linkage=linkage[0], n_clusters=n_clusters).fi
             axes2.scatter(X[:, 0], X[:, 1], c=hierarchy, s=40, cmap=plt.cm.Spectral);
             plt.title(name+'_' + linkage[0])

             axes3 = plt.subplot(1, 4, 3)
             n_clusters = len(set(Y))
             hierarchy = AgglomerativeClustering(linkage=linkage[1], n_clusters=n_clusters).fi
             axes3.scatter(X[:, 0], X[:, 1], c=hierarchy, s=40, cmap=plt.cm.Spectral);
             plt.title(name+'_' + linkage[1])
```

```
    axes4 = plt.subplot(1, 4, 4)
    n_clusters = len(set(Y))
    hierarchy = AgglomerativeClustering(linkage=linkage[2], n_clusters=n_clusters).fit
    axes4.scatter(X[:, 0], X[:, 1], c=hierarchy, s=40, cmap=plt.cm.Spectral);
    plt.title(name+'_' + linkage[2])


    plt.show()
```

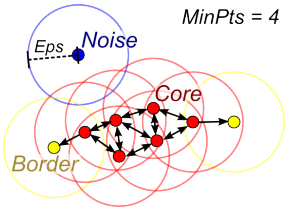




In [39]:
```
# Other Method (參考就好)
from scipy.cluster.hierarchy import dendrogram, linkage
Z = linkage(X[:20], 'single')
plt.figure()
dn = dendrogram(Z)
plt.show()
```

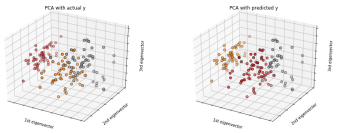


In [40]:
```
# 請用 AgglomerativeClustering(linkage='average') 將 iris_X 進行分群
#=============your works starts===============#
n_clusters =
hierarchy_Y =
#==============your works ends================#
```



DBSCAN

```
plot_iris_predict_acc(hierarchy_Y)
```



4.3 3. Density Based Clustering (DBSCAN)

4.3.1 steps

顧名思義，這種分群演算法計算的是密度，透過設定多長的半徑內，有出現幾個點，不斷延伸，延伸到無法延伸，所有出現在前面延伸範圍的點分成一個群組，請見下圖 (取自stackexchange)。

4.3.2 parameters

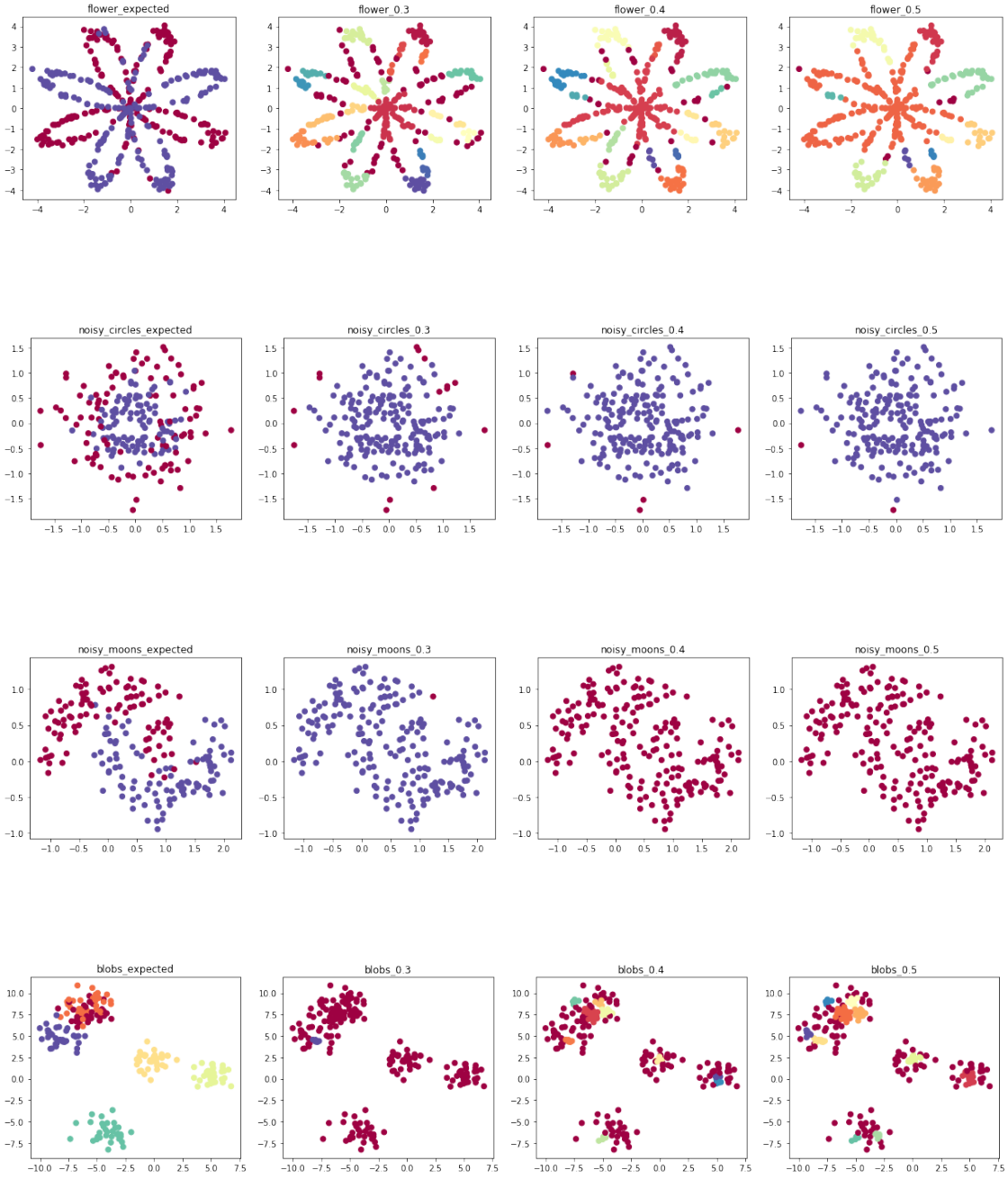
參數	意義
eps	半徑

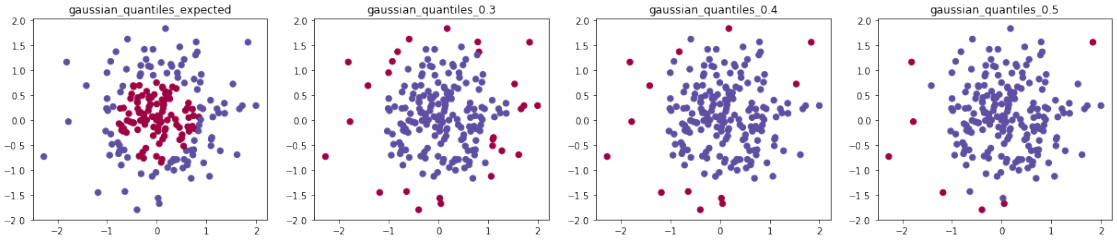
4.3.3 pros & cons

1. 常常用來偵測 Noisy Data。
2. 無法設定要分成幾個群。

```
In [15]: epss = [0.3, 0.4, 0.5]
         for name, X, Y in datas:

             plt.figure(figsize=(21,4))


             axes1 = plt.subplot(1, 4, 1)
             axes1.scatter(X[:, 0], X[:, 1], c=Y, s=40, cmap=plt.cm.Spectral)
             plt.title(name+'_expected')


             axes2 = plt.subplot(1, 4, 2)
             dbscan = DBSCAN(eps=epss[0]).fit_predict(X)
             axes2.scatter(X[:, 0], X[:, 1], c=dbscan, s=40, cmap=plt.cm.Spectral)
             plt.title(name+'_'+str(epss[0]))
```

```
axes3.scatter(X[:, 0], X[:, 1], c=dbscan, s=40, cmap=plt.cm.Spectral)
plt.title(name+'_'+str(epss[1]))


axes3 = plt.subplot(1, 4, 4)
dbscan = DBSCAN(eps=epss[2]).fit_predict(X)
axes3.scatter(X[:, 0], X[:, 1], c=dbscan, s=40, cmap=plt.cm.Spectral)
plt.title(name+'_'+str(epss[2]))


plt.show()
```





In [16]:
```
# 請用 DBSCAN(eps=0.3) 將 iris_X 進行分群
#=============your works starts===============#
dbscan_Y =
#==============your works ends================#

plot_iris_predict_acc(dbscan_Y)
```