# 1 Clustering

```
In [1]: # Install additional libraries
#!pip install fastcluster
```

# 2 Import Libraries ¶

```
In [2]: # Import libraries
        '''Main'''
        import numpy as np
        import pandas as pd
        import os, time
        import pickle, gzip
        '''Data Viz'''
        import matplotlib.pyplot as plt
        import matplotlib as mpl
        import seaborn as sns
        color = sns.color palette()
        %matplotlib inline
        '''Data Prep and Model Evaluation'''
        from sklearn import preprocessing as pp
        from sklearn.model_selection import train_test_split
        from sklearn.metrics import precision_recall_curve, average_precision_score
        from sklearn.metrics import roc_curve, auc, roc_auc_score
        '''Algorithms'''
        from sklearn.decomposition import PCA
        from sklearn.cluster import KMeans
        import fastcluster
        from scipy.cluster.hierarchy import dendrogram, cophenet, fcluster
        from scipy.spatial.distance import pdist
```

### 3 Load Data

```
In [3]: # Load the datasets
    current_path = os.getcwd()
    file = os.path.sep.join(['', 'datasets', 'mnist_data', 'mnist.pkl.gz'])

f = gzip.open(current_path+file, 'rb')
    train_set, validation_set, test_set = pickle.load(f, encoding='latin1')
    f.close()

X_train, y_train = train_set[0], train_set[1]
    X_validation, y_validation = validation_set[0], validation_set[1]
    X_test, y_test = test_set[0], test_set[1]
```

```
In [4]: | # Create Pandas DataFrames from the datasets
        train_index = range(0,len(X_train))
        validation_index = range(len(X_train), \
                                 len(X_train)+len(X_validation))
        test_index = range(len(X_train)+len(X_validation), \
                           len(X_train)+len(X_validation)+len(X_test))
        X_train = pd.DataFrame(data=X_train,index=train_index)
        y_train = pd.Series(data=y_train,index=train_index)
        X_validation = pd.DataFrame(data=X_validation,index=validation_index)
        y_validation = pd.Series(data=y_validation,index=validation_index)
        X_test = pd.DataFrame(data=X_test,index=test_index)
        y_test = pd.Series(data=y_test,index=test_index)
        print('train:',X_train.shape)
        print('validation:',X_validation.shape)
        print('test:',X_test.shape)
        train: (50000, 784)
        validation: (10000, 784)
        test: (10000, 784)
In [5]: |np.bincount(y_train)
Out[5]: array([4932, 5678, 4968, 5101, 4859, 4506, 4951, 5175, 4842, 4988],
              dtype=int64)
In [6]: print(sum(np.bincount(y_train)))
        50000
```

# 4 Dimensionality Reduction

```
In [7]:
        # Principal Component Analysis
        from sklearn.decomposition import PCA
        n_{components} = 784
        pca = PCA(n_components=n_components)
        X_train_PCA = pca.fit_transform(X_train)
        X_train_PCA = pd.DataFrame(data=X_train_PCA, index=train_index)
        X train PCA.head()
Out[7]:
                           1
                                   2
                                                                                7
                  0
                                             3
                                                              5
                                                                       6
           0.461484 -1.246856 0.046275 -2.151944 -0.247284 -0.925426 0.889320 0.507180 -1.54
         1 3.921805 -1.252039 2.335258 -1.340842 -3.421519 -0.725720 -0.206354 -0.345258 0.13
         2 -0.203586    1.547886    -0.980333    2.039061    -1.079858
                                                        0.112944 -3.312401
                                                                         1.403132 -0.59
         3 -3.148331 -2.296074
                             4 -1.442694 2.872064 0.175669 -0.976944 0.302754 0.120619 -0.376697 -1.478133 1.00
        5 rows × 784 columns
                                                                                     \blacktriangleright
In [8]: # # Log data
        # cwd = os.getcwd()
        # log_dir = cwd+"/logs/05_clustering/"
        # y_train[0:2000].to_csv(log_dir+'labels.tsv', sep = '\t', index=False, head
In [9]: # # Write dimensions to CSV
        # X_train_PCA.iloc[0:2000,0:3].to_csv(log_dir+'pca_data.tsv', sep = '\t', ir
```

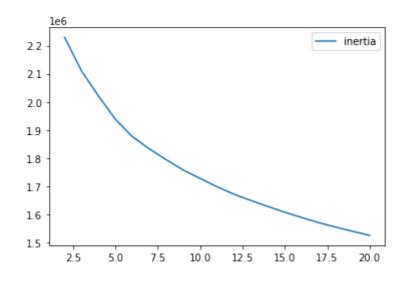
### 5 K-means

### 5.1 Inertia

- MNIST只取前cutoff(=99)個的PCA特徵,進行k-means 並將得到的inertia存於DataFrame
- Cluster數量從2到20個, 觀察k-means inertia

```
In [68]: # Plot inertia relative to k # of clusters
kMeans_inertia.plot()
```





## 5.2 Accuracy

### 5.2.1 如何設計分群好壞的評分指標

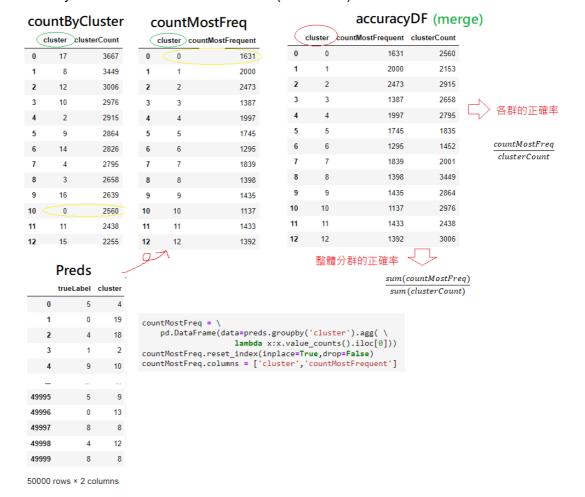
單群精確度:每一群內的同質性愈高,表示分群的愈好.同質性=該群內類別出現最多次的數量/該群的總數 若值為1,表示該群內為均為同一種類別,若為0.5表示只有最多有一半是相同類別.

整體的精確度=sum(各群內類別出現最多次的數量)/全部資料數

群的數量是為k (k=2~20)

- countByCluster:記錄了預測k群, 各群的數量分佈
- countMostFreq:記錄預測的每一群中,出現最多次數字的數量
- accuracyDF: 為countMostFreq和countByCluster的合併

• countByLabel 記錄了Ground Truth在各群(即數字0~9)的數量分佈



```
In [13]: # Define analyze cluster function
         def analyzeCluster(clusterDF, labelsDF):
             countByCluster = pd.DataFrame(data=clusterDF['cluster'].value_counts())
             countByCluster.reset_index(inplace=True,drop=False) #drop = False : the d
             countByCluster.columns = ['cluster','clusterCount']
             preds = pd.concat([labelsDF,clusterDF], axis=1) #merge horizontally
             preds.columns = ['trueLabel','cluster']
             countMostFreq = \
                 pd.DataFrame(data=preds.groupby('cluster').agg( \
                                 lambda x:x.value_counts().iloc[0]))
             countMostFreq.reset_index(inplace=True, drop=False)
             countMostFreq.columns = ['cluster', 'countMostFrequent']
             accuracyDF = countMostFreq.merge(countByCluster, \
                                 left_on="cluster", right_on="cluster")
             overallAccuracy = accuracyDF.countMostFrequent.sum()/ \
                                 accuracyDF.clusterCount.sum()
             accuracyByLabel = accuracyDF.countMostFrequent/ \
                                 accuracyDF.clusterCount
             countByLabel = pd.DataFrame(data=preds.groupby('trueLabel').count())
             return countByCluster, countByLabel, countMostFreq, \
                     accuracyDF, overallAccuracy, accuracyByLabel
```

### 5.2.2 Review: Pandas functoin

DataFrame.agg(func=None, axis=0, *args,* \*kwargs)
Aggregate using one or more operations over the specified axis.

https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.agg.html (https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.agg.html)

```
In [71]: XClustered = kmeans.predict(X_train_PCA.loc[:,0:cutoff])
    XClustered = pd.DataFrame(data=XClustered, index=X_train.index,columns=['clustered_tbl = pd.concat([y_train,XClustered], axis=1)
    XClustered_tbl.columns = ['trueLabel','cluster']
    XClustered_tbl
```

	trueLabel	cluster
0	5	17
1	0	16
2	4	0
3	1	12
4	9	8
49995	5	14
49996	0	18
49997	8	11
49998	4	19
49999	8	11
50000	rows × 2 co	olumns

In [82]: countByLabel = pd.DataFrame(data=XClustered\_tbl.groupby('trueLabel').count()
countByLabel

#### Out[82]:

#### cluster

```
trueLabel
       0
            4932
       1
            5678
       2
            4968
       3
            5101
       4
            4859
       5
            4506
       6
            4951
       7
            5175
       8
            4842
       9
            4988
```

```
In [83]: np.bincount(y_train)
```

Out[83]: array([4932, 5678, 4968, 5101, 4859, 4506, 4951, 5175, 4842, 4988], dtype=int64)

# In [78]: #分群後每一群的數量 countByCluster = pd.DataFrame(XClustered\_tbl['cluster'].value\_counts()) countByCluster.reset\_index(inplace=True,drop=False) #drop=False: the old i countByCluster.columns = ['cluster','clusterCount'] countByCluster

### Out[78]:

	cluster	clusterCount
0	10	3668
1	11	3480
2	19	3089
3	8	2936
4	12	2918
5	14	2893
6	9	2839
7	17	2804
8	1	2683
9	6	2588
10	0	2390
11	4	2377
12	3	2350
13	2	2254
14	7	2111
15	15	1997
16	13	1845
17	18	1741
18	16	1593
19	5	1444

```
#groupby 'cluster', 顯示每一群的Label
         XClustered_tbl.groupby('cluster').agg(lambda x: print(x))
         49976
                  2
         49993
                  2
         Name: trueLabel, Length: 2254, dtype: int64
         54
         89
                  4
         115
                  4
         139
                  4
         167
                  9
         49874
                 4
         49904
                 9
         49940
                 4
                 4
         49982
         49988
         Name: trueLabel, Length: 2350, dtype: int64
         15
                  7
         19
                  9
         22
                  9
                  9
         33
In [74]: #groupby 'cluster', 計算每一群的Label數量(預設由大小到小排序輸出)
         XClustered_tbl.groupby('cluster').agg(lambda x: print(x.value_counts()))
         4
              1082
         9
               780
         7
               255
         2
                73
         5
                71
         8
                44
                43
         6
         3
                22
                20
         Name: trueLabel, dtype: int64
         5
              1406
         4
               292
         8
               254
         0
               176
         2
               173
         6
               166
         3
                99
         7
                50
                41
```

### 

### Out[75]:

	cluster	countMostFrequent
0	0	1082
1	1	1406
2	2	2127
3	3	1394
4	4	1486
5	5	1293
6	6	2061
7	7	1961
8	8	1106
9	9	2495
10	10	3093
11	11	1408
12	12	2474
13	13	1756
14	14	1447
15	15	1839
16	16	1487
17	17	1996
18	18	1665
19	19	1421

In [79]: accuracyDF = countMostFreq.merge(countByCluster,left\_on="cluster",right\_on=" accuracyDF

### Out[79]:

	cluster	countMostFrequent	clusterCount
0	0	1082	2390
1	1	1406	2683
2	2	2127	2254
3	3	1394	2350
4	4	1486	2377
5	5	1293	1444
6	6	2061	2588
7	7	1961	2111
8	8	1106	2936
9	9	2495	2839
10	10	3093	3668

### In [81]: #*各群的正確率*

accuracyByLabel = accuracyDF.countMostFrequent/accuracyDF.clusterCount accuracyByLabel

```
Out[81]: 0
               0.452720
         1
```

- 0.524040
- 2 0.943656
- 3 0.593191
- 4 0.625158
- 5 0.895429
- 6 0.796368
- 7 0.928944
- 8 0.376703
- 9 0.878831
- 10 0.843239 0.404598 11
- 12 0.847841
- 13 0.951762
- 14 0.500173
- 15 0.920881
- 16 0.933459
- 17 0.711840
- 18 0.956347
- 19 0.460019
- dtype: float64

In [80]: overallAccuracy = accuracyDF.countMostFrequent.sum()/accuracyDF.clusterCount print('overallAccuracy',overallAccuracy)

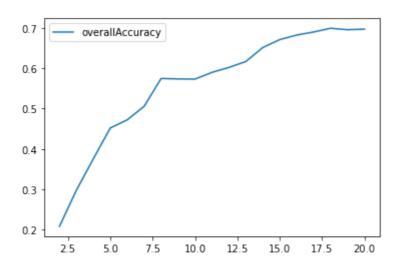
overallAccuracy 0.69994

# 5.3 K-means - Accuracy as the number of clusters varies

```
In [19]:
         n_{init} = 10
         max_iter = 300
         tol = 0.0001
         random_state = 2018
         kMeans_inertia = \
             pd.DataFrame(data=[],index=range(2,21),columns=['inertia'])
         overallAccuracy_kMeansDF = \
             pd.DataFrame(data=[],index=range(2,21),columns=['overallAccuracy'])
         for n clusters in range(2,21):
             kmeans = KMeans(n_clusters=n_clusters, n_init=n_init, \
                         max_iter=max_iter, tol=tol, random_state=random_state)
             cutoff = 99
             kmeans.fit(X_train_PCA.loc[:,0:cutoff])
             kMeans_inertia.loc[n_clusters] = kmeans.inertia_
             X_train_kmeansClustered = kmeans.predict(X_train_PCA.loc[:,0:cutoff])
             X_train_kmeansClustered = \
                 pd.DataFrame(data=X_train_kmeansClustered, index=X_train.index, \
                              columns=['cluster'])
             countByCluster_kMeans, countByLabel_kMeans, countMostFreq_kMeans, \
                 accuracyDF_kMeans, overallAccuracy_kMeans, accuracyByLabel_kMeans \
                 = analyzeCluster(X_train_kmeansClustered, y_train)
             overallAccuracy_kMeansDF.loc[n_clusters] = overallAccuracy_kMeans
```

```
In [20]: # Plot accuracy #分群愈多,accuracy愈高(理所當然. 因為群愈多,群內的同質性就會愈高) overallAccuracy_kMeansDF.plot()
```

### Out[20]: <Axes: >



```
In [21]: # Accuracy by cluster
         accuracyByLabel_kMeans
Out[21]: 0
                0.634156
          1
                0.923767
         2
                0.389366
         3
                0.905002
         4
                0.463787
         5
                0.941964
         6
                0.928007
         7
                0.856261
         8
                0.954465
         9
                0.596520
         10
                0.823661
                0.711253
         11
          12
                0.526414
         13
                0.950378
          14
                0.489108
         15
                0.838684
          16
                0.802189
         17
                0.385685
         18
                0.451670
         19
                0.864761
         dtype: float64
In [22]: # View cluster labels
         X_train_kmeansClustered
Out[22]:
                 cluster
                    11
              0
              1
                     6
              2
                    18
              3
                    10
```

```
0 11
1 6
2 18
3 10
4 17
...
49995 14
49996 8
49997 2
49998 4
49999 2
```

50000 rows × 1 columns

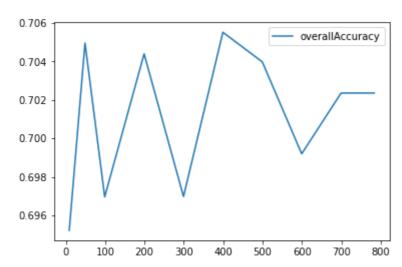
```
In [23]: # Save cluster labels
X_train_kmeansClustered[0:2000].to_csv('kmeans_cluster_labels.tsv', sep = ''
```

# 5.4 Accuracy as the number of principal components varies

```
In [85]: # K-means - Accuracy as the number of components varies
         n_{clusters} = 20
         n_{init} = 10
         max_iter = 300
         tol = 0.0001
         random_state = 2018
         kMeans_inertia = pd.DataFrame(data=[],index=[9, 49, 99, 199, \
                             299, 399, 499, 599, 699, 783],columns=['inertia'])
         overallAccuracy_kMeansDF = pd.DataFrame(data=[],index=[9, 49, \
                             99, 199, 299, 399, 499, 599, 699, 783], \
                             columns=['overallAccuracy'])
         for cutoffNumber in [9, 49, 99, 199, 299, 399, 499, 599, 699, 783]:
             kmeans = KMeans(n_clusters=n_clusters, n_init=n_init, \
                         max_iter=max_iter, tol=tol, random_state=random_state)
             cutoff = cutoffNumber
             kmeans.fit(X_train_PCA.loc[:,0:cutoff])
             kMeans_inertia.loc[cutoff] = kmeans.inertia_
             X_train_kmeansClustered = kmeans.predict(X_train_PCA.loc[:,0:cutoff])
             X train kmeansClustered = pd.DataFrame(data=X train kmeansClustered, \
                                          index=X_train.index, columns=['cluster'])
             countByCluster_kMeans, countByLabel_kMeans, countMostFreq_kMeans, \
                 accuracyDF_kMeans, overallAccuracy_kMeans, accuracyByLabel_kMeans \
                 = analyzeCluster(X_train_kmeansClustered, y_train)
             overallAccuracy kMeansDF.loc[cutoff] = overallAccuracy kMeans
```

# In [87]: # Accuracy relative to number of principal components overallAccuracy\_kMeansDF.plot()





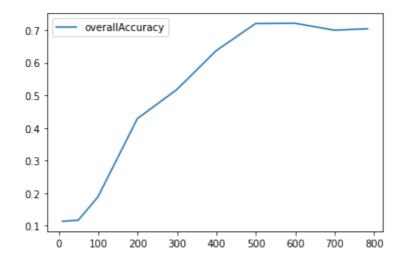
# 5.5 Accuracy as the number of original dimensions varies

```
In [88]: # K-means - Accuracy as the number of components varies
         # On the original MNIST data (not PCA-reduced)
         n_{clusters} = 20
         n_{init} = 10
         max iter = 300
         tol = 0.0001
         random_state = 2018
         kMeans_inertia = pd.DataFrame(data=[],index=[9, 49, 99, 199, \
                              299, 399, 499, 599, 699, 783], columns=['inertia'])
         overallAccuracy_kMeansDF = pd.DataFrame(data=[],index=[9, 49, \
                              99, 199, 299, 399, 499, 599, 699, 783], \
                              columns=['overallAccuracy'])
         for cutoffNumber in [9, 49, 99, 199, 299, 399, 499, 599, 699, 783]:
             kmeans = KMeans(n_clusters=n_clusters, n_init=n_init, \
                          max_iter=max_iter, tol=tol, random_state=random_state)
             cutoff = cutoffNumber
             kmeans.fit(X_train.loc[:,0:cutoff])
             kMeans_inertia.loc[cutoff] = kmeans.inertia_
             X train kmeansClustered = kmeans.predict(X train.loc[:,0:cutoff])
             X_train_kmeansClustered = pd.DataFrame(data=X_train_kmeansClustered, \
                                           index=X_train.index, columns=['cluster'])
             countByCluster_kMeans, countByLabel_kMeans, countMostFreq_kMeans, \
                  accuracy DF\_k Means, \ overall Accuracy\_k Means, \ accuracy By Label\_k Means \ \setminus \\
                 = analyzeCluster(X_train_kmeansClustered, y_train)
             overallAccuracy_kMeansDF.loc[cutoff] = overallAccuracy_kMeans
```

```
C:\Users\joseph\anaconda3\lib\site-packages\sklearn\base.py:1152: Converge
nceWarning: Number of distinct clusters (1) found smaller than n_clusters
(20). Possibly due to duplicate points in X.
  return fit_method(estimator, *args, **kwargs)
```

In [89]: # Accuracy relative to number of original dimensions
 overallAccuracy\_kMeansDF.plot()

Out[89]: <Axes: >



### 5.6 Conculsion:

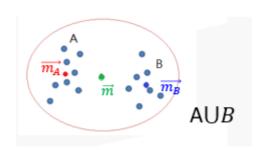
使用原始資料·資料維度在784維時的正確率是0.7左右, 而若使用PCA時, 在少於100個維度的情況下, 就可以達到0.7的正確率。

# 6 Hierarchical clustering

https://jbhender.github.io/Stats506/F18/GP/Group10.html (https://jbhender.github.io/Stats506/F18/GP/Group10.html)

**Ward's method** says that the distance between two clusters, A and B, is how much the sum of squares will increase when we merge them.

$$\Delta(A, B) = \sum_{i \in A \cup B} ||\overrightarrow{x_i} - \overrightarrow{m}_{A \cup B}||^2 - \sum_{i \in A} ||\overrightarrow{x_i} - \overrightarrow{m}_{A}||^2 - \sum_{i \in B} ||\overrightarrow{x_i} - \overrightarrow{m}_{B}||^2 = \frac{n_A n_B}{n_A + n}$$



4

In [29]: # Show Leaves
Z\_dataFrame.iloc[:20]

### Out[29]:

	clusterOne	clusterTwo	distance	newClusterSize
0	42194.0	43025.0	0.562811	2.0
1	28350.0	37674.0	0.590923	2.0
2	26696.0	44705.0	0.621491	2.0
3	12634.0	32823.0	0.627762	2.0
4	24707.0	43151.0	0.637646	2.0
5	20465.0	24483.0	0.662483	2.0
6	466.0	42098.0	0.664151	2.0
7	46542.0	49961.0	0.665527	2.0
8	2301.0	5732.0	0.671081	2.0
9	37564.0	47668.0	0.675107	2.0
10	3375.0	26243.0	0.685899	2.0
11	15722.0	30368.0	0.686326	2.0
12	21247.0	21575.0	0.694369	2.0
13	14900.0	42486.0	0.696735	2.0
14	30100.0	41908.0	0.699287	2.0
15	12040.0	13254.0	0.701116	2.0
16	10508.0	25434.0	0.708619	2.0
17	30695.0	30757.0	0.710044	2.0
18	31019.0	31033.0	0.712045	2.0
19	36264.0	37285.0	0.713133	2.0

```
In [30]: # Show Leaves higher on the tree
Z_dataFrame.iloc[49980:]
```

### Out[30]:

	clusterOne	clusterTwo	distance	newClusterSize
49980	99938.0	99959.0	152.158499	3544.0
49981	99953.0	99974.0	177.594230	5680.0
49982	99961.0	99976.0	179.132302	3379.0
49983	99942.0	99972.0	180.320587	4781.0
49984	99962.0	99980.0	189.535103	6051.0
49985	99971.0	99979.0	198.547538	6364.0
49986	99968.0	99969.0	202.903316	4246.0
49987	99954.0	99973.0	205.242622	6070.0
49988	99956.0	99982.0	222.401645	4872.0
49989	99966.0	99987.0	246.573179	9119.0
49990	99978.0	99986.0	247.756736	7000.0
49991	99975.0	99977.0	262.852446	6133.0
49992	99984.0	99985.0	265.504907	12415.0
49993	99983.0	99990.0	267.704777	11781.0
49994	99981.0	99989.0	293.502476	14799.0
49995	99992.0	99993.0	390.062843	24196.0
49996	99991.0	99995.0	419.196650	30329.0
49997	99988.0	99996.0	469.343025	35201.0
49998	99994.0	99997.0	497.511872	50000.0

```
In [31]: # Create clusters
from scipy.cluster.hierarchy import fcluster

distance_threshold = 160
clusters = fcluster(Z, distance_threshold, criterion='distance')
X_train_hierClustered = \
    pd.DataFrame(data=clusters,index=X_train_PCA.index,columns=['cluster'])
```

Number of distinct clusters: 19

Accuracy by cluster for hierarchical clustering

accuracyByLabel\_hierClust

```
Out[34]: 0
               0.917068
         1
               0.505117
         2
               0.503444
         3
               0.559322
         4
               0.969558
         5
               0.990623
         6
               0.986610
         7
               0.982719
         8
               0.860870
         9
               0.984424
         10
               0.960112
         11
               0.526806
         12
               0.402222
         13
               0.906386
         14
               0.952848
         15
               0.946633
         16
               0.982934
         17
               0.965486
               0.701881
         18
```

dtype: float64

```
In [35]: # View cluster Labels
X_train_hierClustered
```

### Out[35]:

	cluster
0	14
1	7
2	3
3	10
4	4
49995	14
49996	7
49997	12
49998	4
49999	13

50000 rows × 1 columns

```
In [36]: # Save cluster labels
X_train_hierClustered[0:2000].to_csv('hierarchical_cluster_labels.tsv', sep
```

## 7 DBSCAN

Out[37]: 0.22434

```
In [38]: # Print overall accuracy
          print("Overall accuracy from DBSCAN: ",overallAccuracy_dbscan)
          Overall accuracy from DBSCAN: 0.22434
In [39]: # View cluster labels
          {\tt X\_train\_PCA\_dbscanClustered}
Out[39]:
                 cluster
              0
                     -1
              1
                     -1
              2
                     -1
              3
                      0
                     -1
                     ...
           49995
                     -1
           49996
                     -1
           49997
                     -1
           49998
                     -1
           49999
                     -1
          50000 rows × 1 columns
In [40]:
          # Show cluster results
          print("Cluster results for DBSCAN")
          countByCluster_dbscan
          Cluster results for DBSCAN
Out[40]:
              cluster clusterCount
           0
                  -1
                           42073
            1
                   0
                            7259
           2
                   5
                             184
           3
                             100
                   1
            4
                   4
                              66
            5
                  11
                              36
           6
                  12
                              31
           7
                  16
                              29
```

8

9

3

13

21

21

In [41]: accuracyDF\_dbscan

### Out[41]:

	cluster	countMostFrequent	clusterCount
0	-1	5095	42073
1	0	5455	7259
2	1	100	100
3	2	14	14
4	3	21	21
5	4	65	66
6	5	184	184
7	6	9	9
8	7	9	9
9	8	10	10
10	9	10	10
11	10	7	7
12	11	36	36
13	12	31	31
14	13	21	21
15	14	12	12
16	15	9	9
17	16	29	29
18	17	8	8
19	18	8	8
20	19	5	5
21	20	11	11
22	21	10	10
23	22	8	8
24	23	10	10
25	24	10	10
26	25	10	10
27	26	10	10
28	27	10	10

```
In [42]: # Save cluster labels
X_train_PCA_dbscanClustered[0:2000].to_csv('dbscan_cluster_labels.tsv', sep
```

### 7.1 Conclusion:

DBSCAN 在處理MNIST 資料集表現比k-means差很多, 因為找不到 Density 的關係, 超過80%以上資料都被歸類成outlier. 扣除群0其他群僅僅是零星數量。

# 7.2 Conslusion

HDBSCAN 效果只有比 DBSCAN 好一點而己

In [ ]:		
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