Comparative Clustering of Shape and S-Set Datasets:

S-sets:

Synthetic 2-d data with N=5000 vectors and k=15 Gaussian clusters with different degree of cluster overlap

P. Fränti and O. Virmajoki, "Iterative shrinking method for clustering problems", Pattern Recognition, 39 (5), 761-765, May 20

Shape Sets:

Pathbased

N=300, k=3, D=2 Pathbased: txt H. Chang and D.Y. Yeung, Robust path-based spectral clustering. Pattern Recognition, 2008. 41(1): p. 191-2

Spiral

N=312, k=3, D=2 Spiral: txt H. Chang and D.Y. Yeung, Robust path-based spectral clustering. Pattern Recognition, 2008. 41(1): p. 191-2

Jain

N=373, k=2, D=2 Jain: txt A. Jain and M. Law, Data clustering: A user's dilemma. Lecture Notes in Computer Science, 2005. 3776: p. 1-

Flame

N=240, k=2, D=2 Flame: txt L. Fu and E. Medico, FLAME, a novel fuzzy clustering method for the analysis of DNA microarray data. BMC bioinformatics, 2007. 8(1): p. 3.10.03.03.06

Importing modules and datasets

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
```

```
S1 = pd.read_csv("s1.txt",sep="\s+",header=None)
S4 = pd.read_csv("s4.txt",sep="\s+",header=None)
```

```
#Third row is label
pathbased = pd.read_csv("pathbased.txt",sep="\s+",header=None)
spiral = pd.read_csv("spiral.txt",sep="\s+",header=None)
jain = pd.read_csv("jain.txt",sep="\s+",header=None)
flame = pd.read_csv("flame.txt",sep="\s+",header=None)
spiral
```

	0	1	2
0	31.95	7.95	3
1	31.15	7.30	3
2	30.45	6.65	3
3	29.70	6.00	3
4	28.90	5.55	3
...	...	...	...
307	15.75	13.85	2
308	15.65	14.05	2
309	15.65	14.25	2
310	15.65	14.50	2
311	15.65	14.60	2

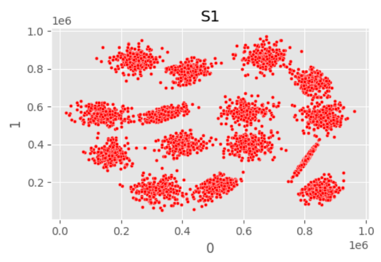
```
dfs= {"S1":[S1,15],
      "S4":[S4,15],
        "pathbased":[pathbased,3],
        "spiral":[spiral,3],
        "jain":[jain,2],
        "flame":[flame,2]


}
for df_name in dfs.keys():
    if df_name=="S1" or df_name=="S4":
        pass
    else:
        df=dfs[df_name][0]
        df.rename(columns={2:"true_cluster"},inplace=True)
        df['true_cluster']=df['true_cluster']-1 # Changing the labeling from 1...k to 0..
```

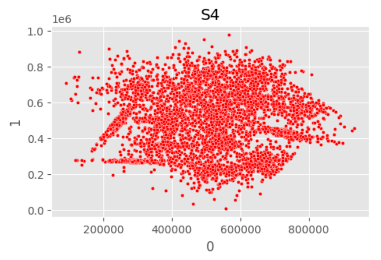
```
flame.true_cluster.unique()
```

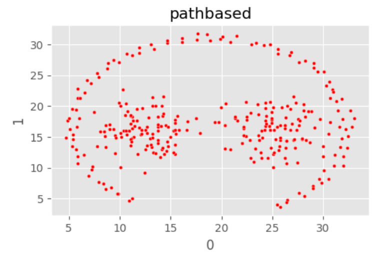
```
array([0, 1], dtype=int64)
```

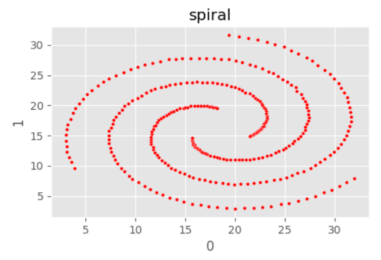
Visualization

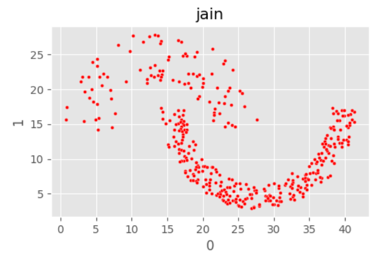
```
plt.style.use('ggplot')

fig,axs=plt.subplots(6,1,figsize=(5,20))
axs=axs.ravel()
i=0
for df in dfs.keys():
    axs[i].set_title(f'{df}')

    sns.scatterplot(x=0,y=1,data=dfs[df][0],ax=axs[i],color="r",s=10)
    i+=1
    fig.tight_layout()
    #plt.show()
```

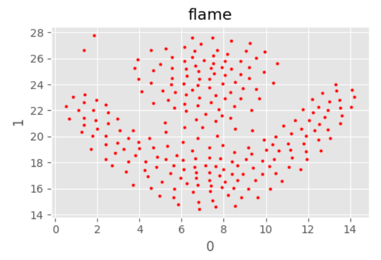

S1
1e6
1
0
1e6


S4
1e6
1
0


pathbased
1
0


spiral
1
0


jain
1
0


flame
1
0

```
flame
```

	0	1	true_cluster
0	1.85	27.80	0
1	1.35	26.65	0
2	1.40	23.25	1
3	0.85	23.05	1
4	0.50	22.35	1
…	…	…	…
235	7.50	26.20	0
236	7.50	25.65	0
237	7.05	25.85	0
238	6.90	27.15	0
239	6.15	26.90	0

```
S1.columns
```

```
Index([0, 1], dtype='int64')
```

Kmeans

Kmeans tries to minimize within cluster variability. Within cluster variability is defined as sum of sqaured distance of each pair of data in a cluster. The Distance is defined as Euclidean Distance. The Optimization of this objective is not trivial. Instead in the K-means algorithm a local optimum is obtained by the following operation.

Initialization:

Samples are randomly assigned to a cluster First Step:

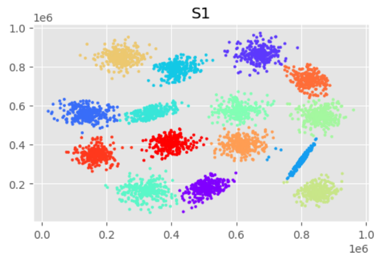
Cluster Centroid is calculated (a vector with k dimensions each feature with the mean of samples in the cluster)

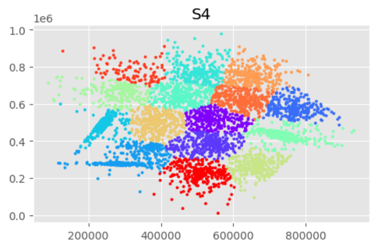
Second Step: The observations that have the minimum distance to a centroid are assigned to that cluster

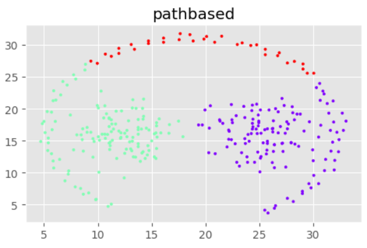
First and Second Steps Are iterated .

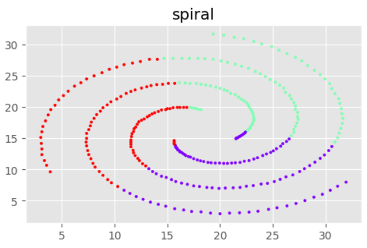
```
from sklearn.cluster import KMeans

fig,axs=plt.subplots(6,1,figsize=(5,20))
```

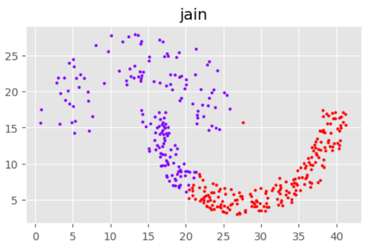
```
axs=axs.ravel()
i=0
for df_name in dfs.keys():
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]

    kmeans=KMeans(n_clusters=k,n_init='auto')
    kmeans.fit(dataset.loc[:,0:1])
    dataset["kmeans_cluster"]=kmeans.labels_
    axs[i].set_title(f'{df_name}')

    #sns.scatterplot(x=0,y=1,data=dataset,ax=axs[i],hue='kmeans_cluster',s=10)
    axs[i].scatter(x=dataset.loc[:,0],y=dataset.loc[:,1],c=dataset.loc[:,'kmeans_cluster']
    i+=1
    fig.tight_layout()
    #plt.show()
```

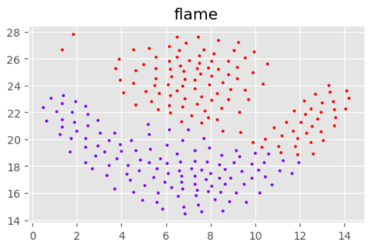

S1
1e6
1e6
0.0
0.2
0.4
0.6
0.8
1.0


S4
1e6
0.0
0.2
0.4
0.6
0.8
1.0
200000
400000
600000
800000


pathbased
5
10
15
20
25
30


spiral
5
10
15
20
25
30


jain
0
5
10
15
20
25
30
35
40


flame
0
2
4
6
8
10
12
14
16
18
20
22
24
26
28

Hierarchial Clustering

Two Dissimilarity measures need to be defined here: Metric : is a measure of distance of two observations. could be euclidean,l1,l2, correlation based and etc. Linkage: is about how we find the dissimilarity between two groups of observations. Ward: minimizes the variance of clusters Single: calculates pairwise distances of observations of two clusters and considers the smallest one Complete: calculates pairwise distances of observations of two clusters and considers the largest one Average: calculates pairwise distances of observations of two clusters and averages them Centroid: Dissimilarity between center of one cluster and the center of the other cluster. Center is a mean feature vector of dim p

Documentation of Scikit learn

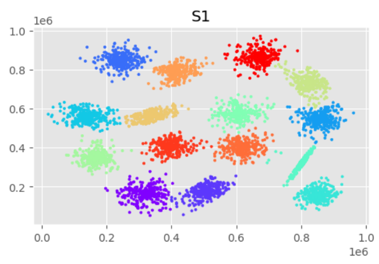
Metric : str or callable, default=None Metric used to compute the linkage. Can be "euclidean", "l1", "l2", "manhattan", "cosine", or "precomputed". If set to `None` then "euclidean" is used. If linkage is "ward", only "euclidean" is accepted. If "precomputed", a distance matrix is needed as input for the fit method.

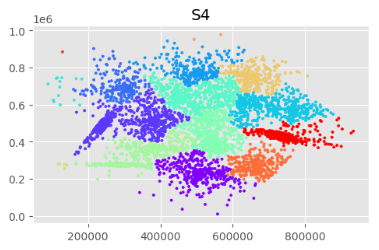
linkage : {'ward', 'complete', 'average', 'single'}, default='ward' Which linkage criterion to use. The linkage criterion determines which distance to use between sets of observation. The algorithm will merge the pairs of cluster that minimize this criterion.

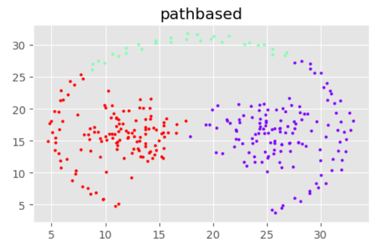
- ward minimizes the variance of the clusters being merged.
- average uses the average of the distances of each observation of the two sets.
- complete or maximum linkage uses the maximum distances between all observations of the two sets.
- single uses the minimum of the distances between all observations of the two sets

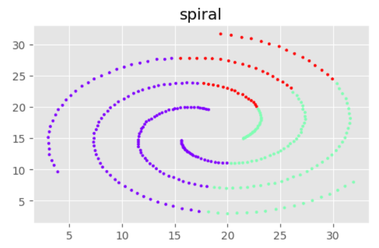
Average Linkage

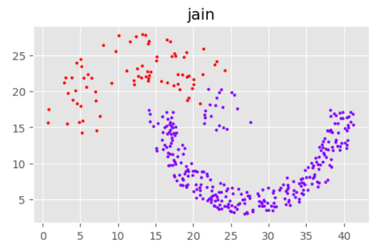
```
from sklearn.cluster import AgglomerativeClustering

fig,axs=plt.subplots(6,1,figsize=(5,20))
axs=axs.ravel()
i=0
for df_name in dfs.keys():
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]

    hierarchical_cluster = AgglomerativeClustering(n_clusters=k, metric='euclidean', linka
    labels = hierarchical_cluster.fit_predict(dataset.loc[:,0:1])
    dataset["avg_hcluster"]= labels
    axs[i].set_title(f'{df_name}')

    #sns.scatterplot(x=0,y=1,data=dataset,ax=axs[i],hue='kmeans_cluster',s=10)
    axs[i].scatter(x=dataset.loc[:,0],y=dataset.loc[:,1],c=labels,cmap='rainbow',s=5)
    i+=1
    fig.tight_layout()
    #plt.show()
```

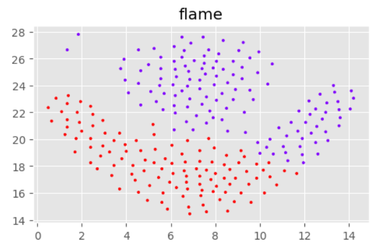

S1
1e6
1.0
0.8
0.6
0.4
0.2
0.0
0.2
0.4
0.6
0.8
1.0
1e6


S4
1e6
1.0
0.8
0.6
0.4
0.2
0.0
200000
400000
600000
800000


pathbased
30
25
20
15
10
5
5
10
15
20
25
30

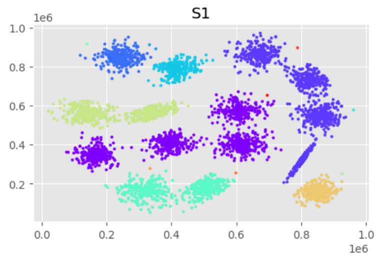

spiral
30
25
20
15
10
5
5
10
15
20
25
30

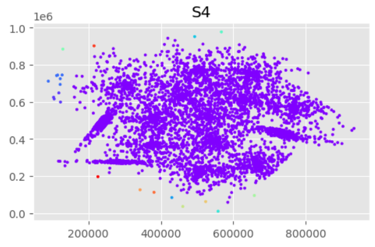

jain
25
20
15
10
5
0
5
10
15
20
25
30
35
40

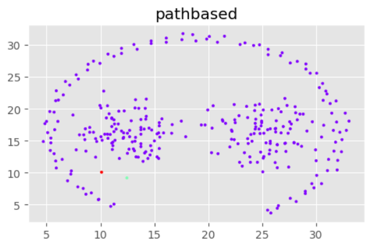

flame
28
26
24
22
20
18
16
14
0
2
4
6
8
10
12
14

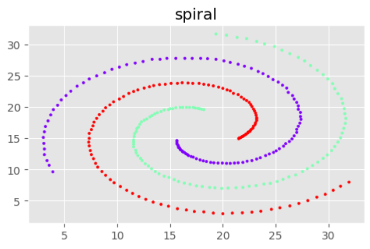
Single Linkage

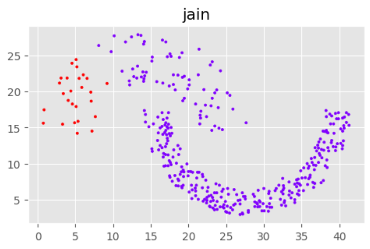
```
from sklearn.cluster import AgglomerativeClustering

fig,axs=plt.subplots(6,1,figsize=(5,20))
axs=axs.ravel()
i=0
for df_name in dfs.keys():
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]

    hierarchical_cluster = AgglomerativeClustering(n_clusters=k, metric='euclidean', linka
    labels = hierarchical_cluster.fit_predict(dataset.loc[:,0:1])
    dataset["single_hcluster"]= labels
    axs[i].set_title(f'{df_name}')

    #sns.scatterplot(x=0,y=1,data=dataset,ax=axs[i],hue='kmeans_cluster',s=10)
    axs[i].scatter(x=dataset.loc[:,0],y=dataset.loc[:,1],c=labels,cmap='rainbow',s=5)
    i+=1
    fig.tight_layou+t()
    #plt.show()
```

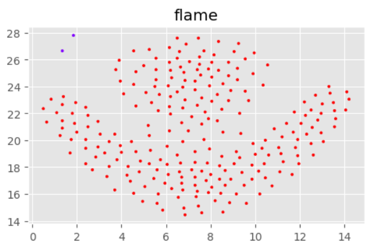

S1
1e6
1e6


S4
1e6


pathbased

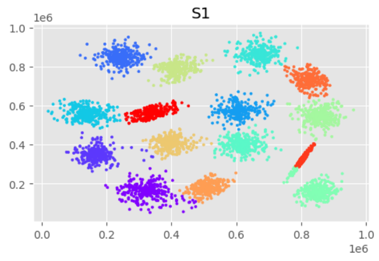

spiral

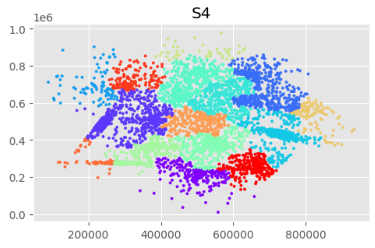

jain

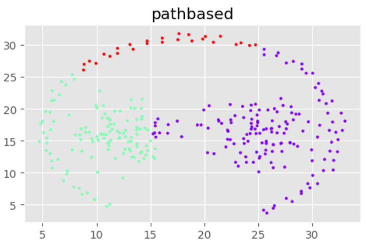

flame

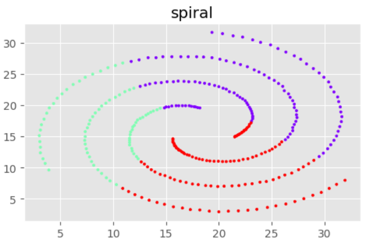
Complete Linkage

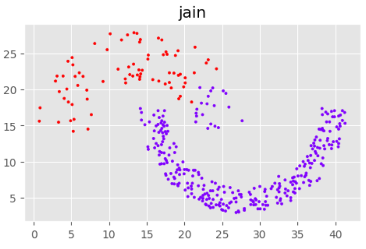
```
from sklearn.cluster import AgglomerativeClustering

fig,axs=plt.subplots(6,1,figsize=(5,20))
axs=axs.ravel()
i=0
for df_name in dfs.keys():
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]

    hierarchical_cluster = AgglomerativeClustering(n_clusters=k, metric='euclidean', linka
    labels = hierarchical_cluster.fit_predict(dataset.loc[:,0:1])
    dataset["complete_hcluster"]= labels
    axs[i].set_title(f'{df_name}')

    #sns.scatterplot(x=0,y=1,data=dataset,ax=axs[i],hue='kmeans_cluster',s=10)
    axs[i].scatter(x=dataset.loc[:,0],y=dataset.loc[:,1],c=labels,cmap='rainbow',s=5)
    i+=1
    fig.tight_layout()
    #plt.show()
```

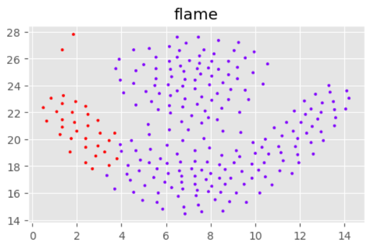

S1


S4


pathbased


spiral


jain


flame

Spectral Clustering

For this algorithm a similarity graph must be constructed. In this graph the edges represent the similarity between nodes (objects). Similar nodes are connected and the edge weight represents the similarity and if the similarity between two nodes is not above a certain threshold, they don't get connected. In this case the problem boils down to a graph partition problem, where we have to get the connected components of the graph such that edges in each component have high weight and edges between components have low weight. Two metrics should be defined here: 1-The measure of similarity between nodes: It's usually defined as $ s(xi, xj) = exp(-(xi-xj)^2/c)$

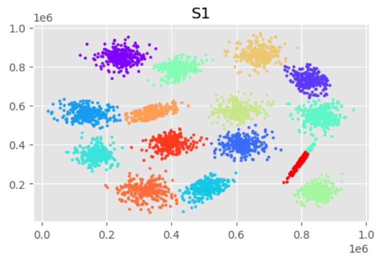
2- How we construct the graph similarity :- Mutual K-nearest-neighbor graph: If node v_i and v_j are both k-nearest neighbors of each other, they are connected and $w_{ij} = s_{ij}$ - Fully connected graph: connect all points and weight each edge with s_{ij} - eplison neighborhood graph

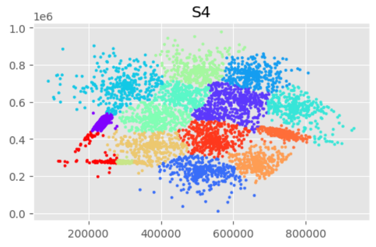
affinity : str or callable, default='rbf' How to construct the affinity matrix. - 'nearest_neighbors': construct the affinity matrix by computing a graph of nearest neighbors. - 'rbf': construct the affinity matrix using a radial basis function (RBF) kernel.

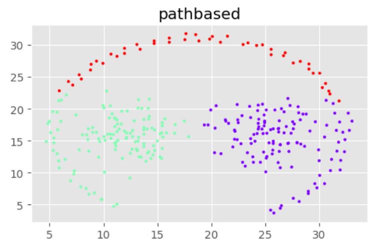
```
from sklearn.cluster import SpectralClustering
spectral_cluster = SpectralClustering(n_clusters=k, affinity="nearest_neighbors")
```

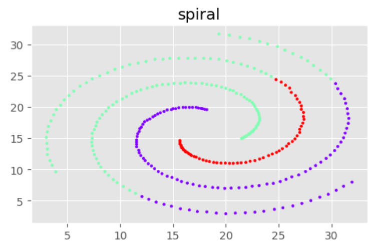
```
from sklearn.cluster import SpectralClustering

fig,axs=plt.subplots(6,1,figsize=(5,20))
axs=axs.ravel()
i=0
for df_name in dfs.keys():
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]

    spectral_cluster = SpectralClustering(n_clusters=k, affinity="nearest_neighbors")
    spectral_cluster.fit(dataset.loc[:,0:1])
    dataset["spectral_cluster"]= spectral_cluster.labels_
    axs[i].set_title(f'{df_name}')

    #sns.scatterplot(x=0,y=1,data=dataset,ax=axs[i],hue='kmeans_cluster',s=10)
    axs[i].scatter(x=dataset.loc[:,0],y=dataset.loc[:,1],c=dataset["spectral_cluster"],cma
    i+=1
    fig.tight_layout()
    #plt.show()
```

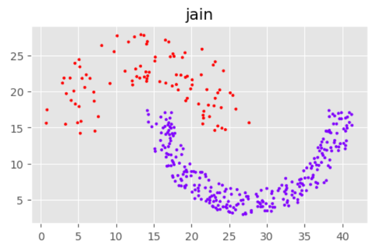
```
D:\Python3.11\Lib\site-packages\sklearn\manifold\_spectral_embedding.py:273: UserWarning: Gra
  warnings.warn(
```

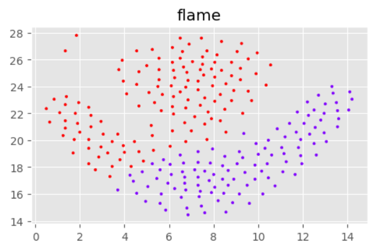

S1
1e6
1e6


S4
1e6

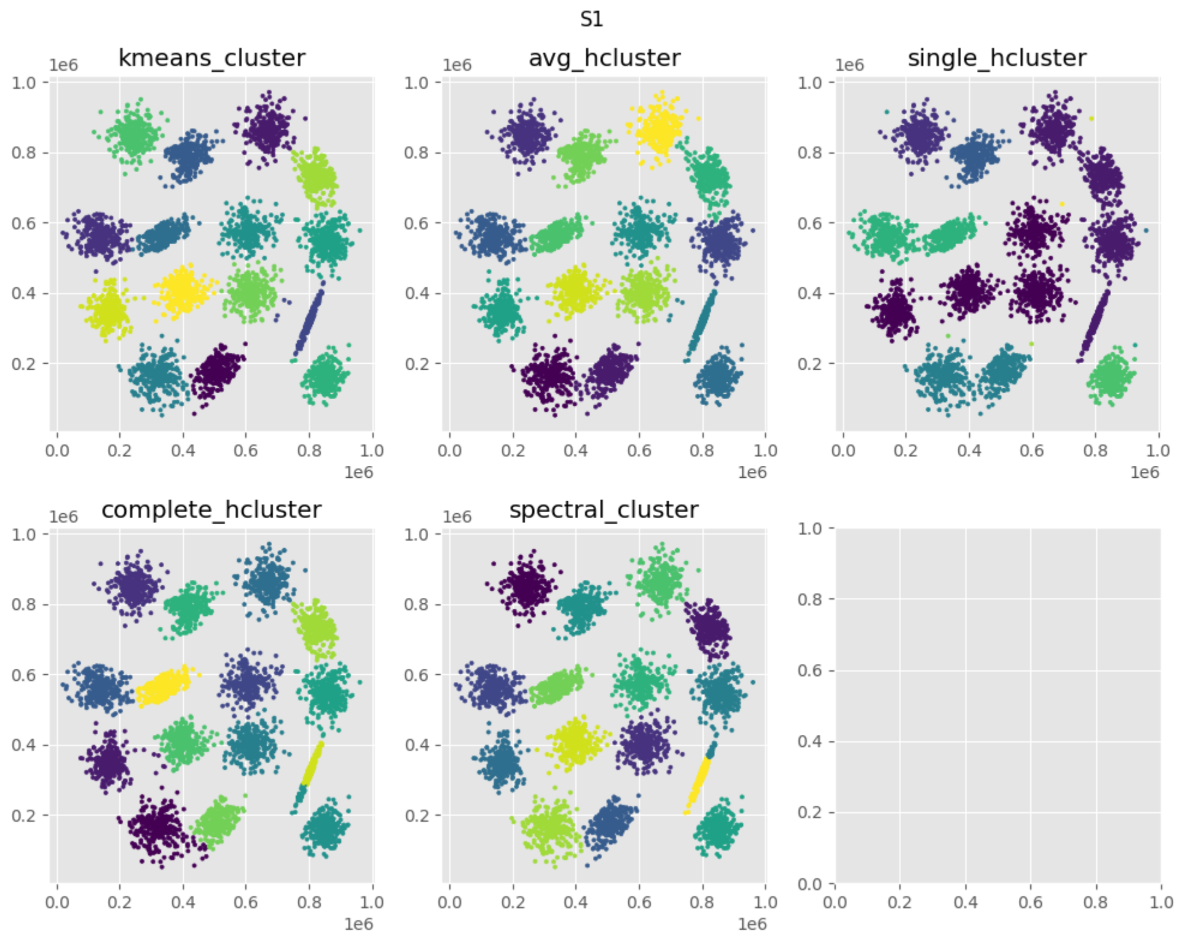

pathbased

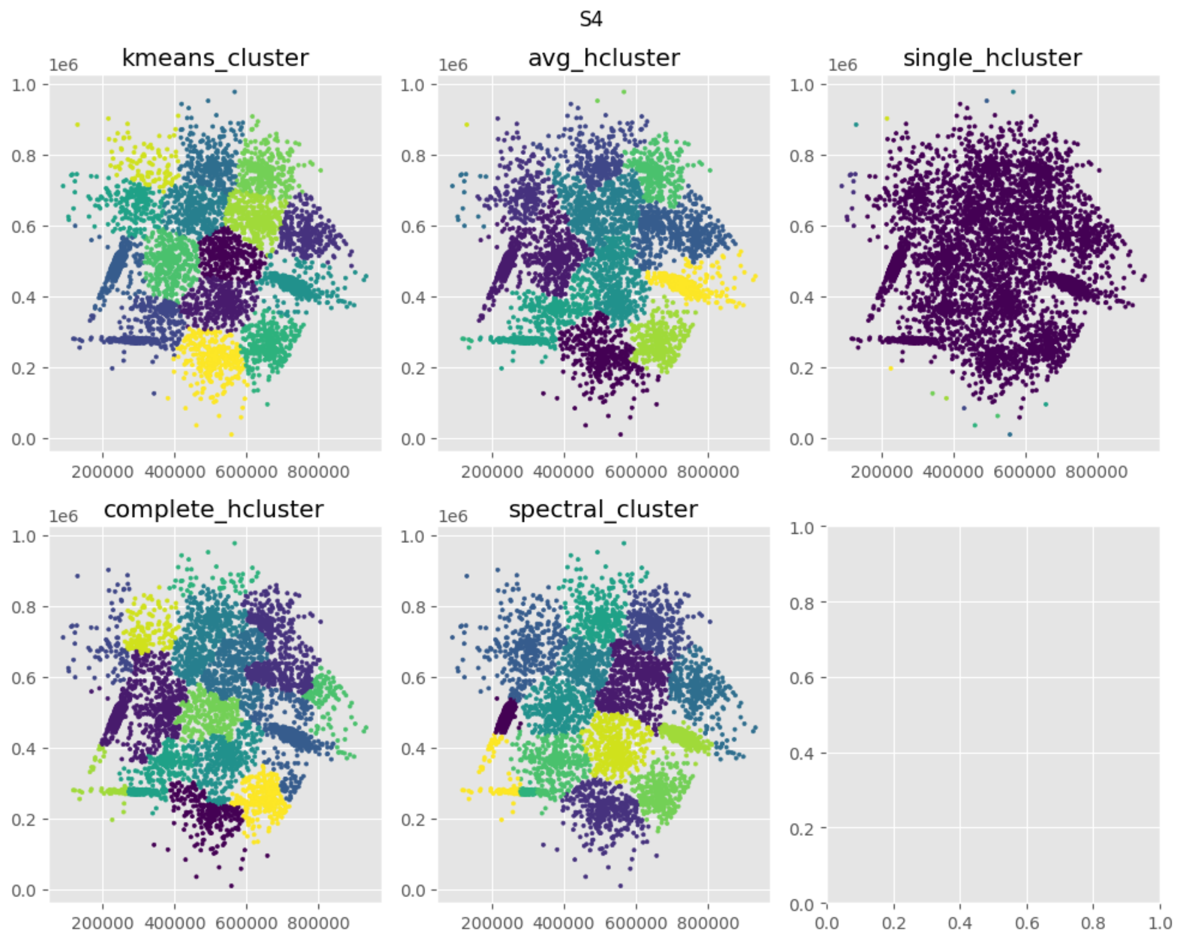

spiral

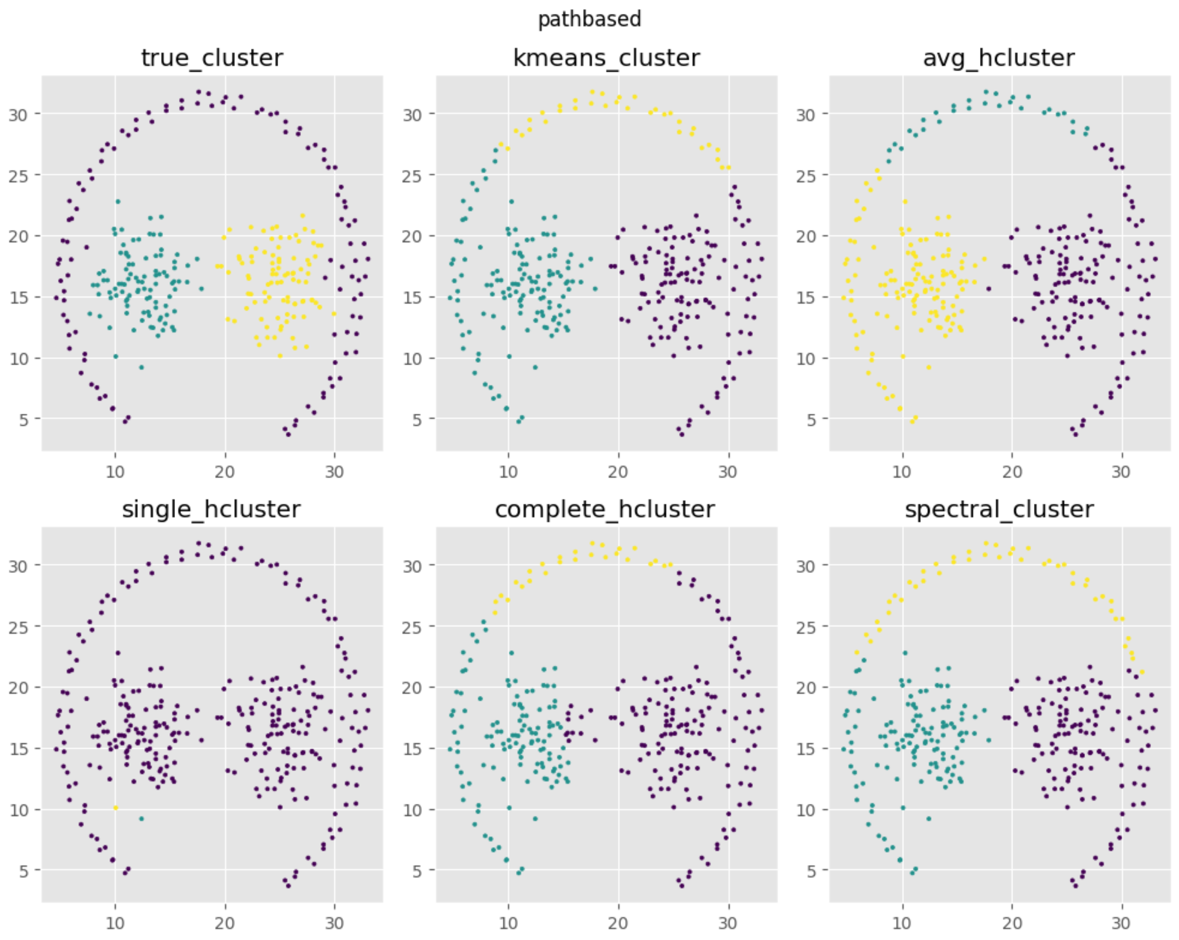

jain

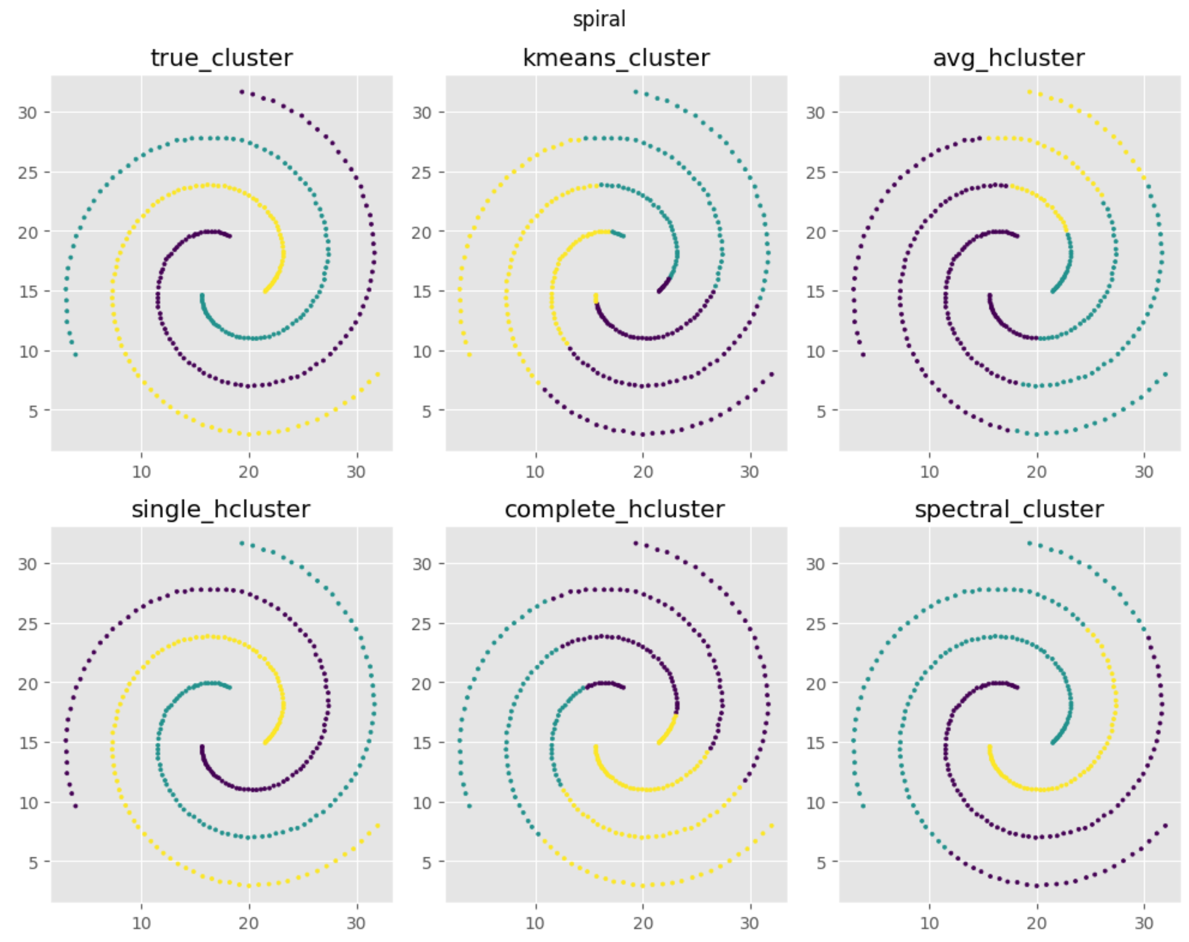

flame

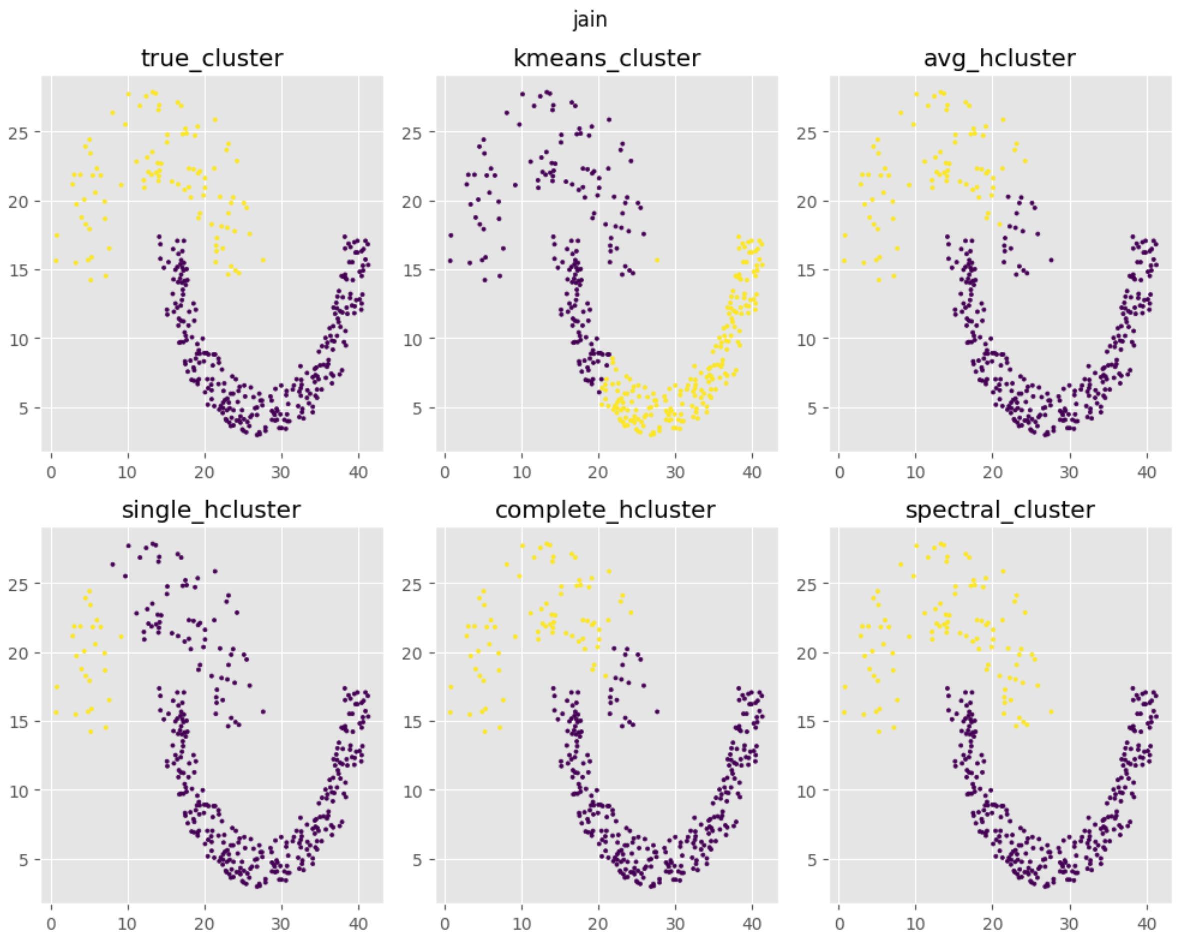
```
for df_name in dfs.keys():

    fig,axs=plt.subplots(2,3,figsize=(10,8))
    axs=axs.ravel()
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]
    fig.suptitle(f"{df_name}")
    for i in range(6):
        try:

            axs[i].set_title(f'{dataset.iloc[:,i+2].name}')

            #sns.scatterplot(x=0,y=1,data=dataset,ax=axs[i],hue='kmeans_cluster',s=10)
            #print(f"x:{x}\ny:{y}")
            axs[i].scatter(x=dataset.loc[:,0],y=dataset.loc[:,1],c=dataset.iloc[:,i+2],cma
        except:
            pass
        fig.tight_layout()

        #plt.show()
```

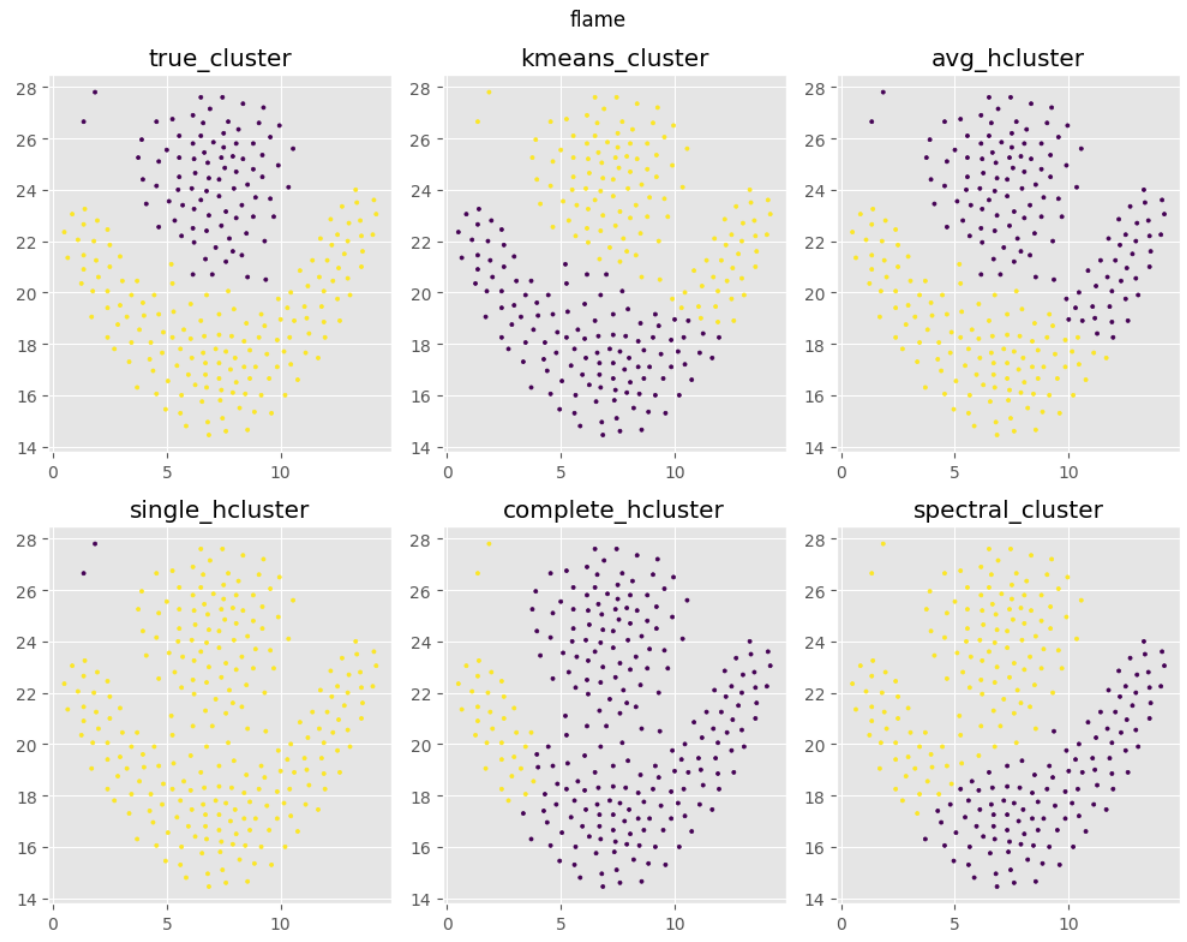

S1
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
1e6
1e6


S4
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
1e6
0.0
0.2
0.4
0.6
0.8
1.0
200000
400000
600000
800000


pathbased
true_cluster
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster

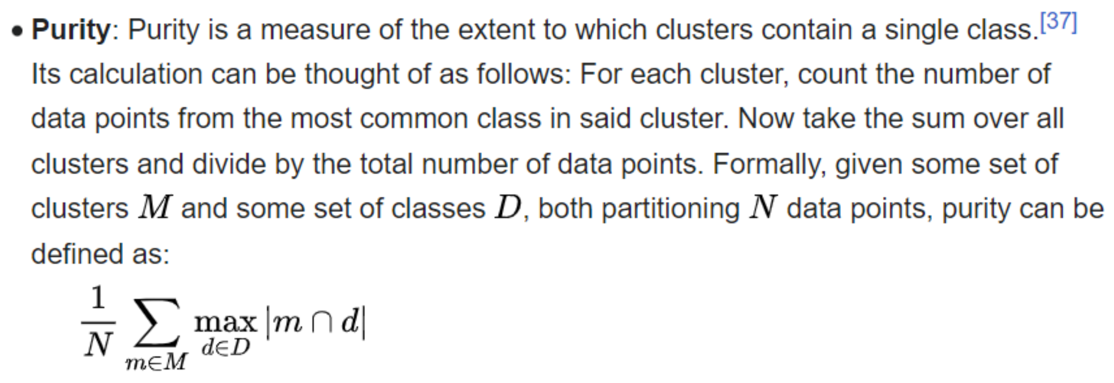

spiral
true_cluster
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
5
10
15
20
25
30


jain
true_cluster
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster



Purity index :

```
from sklearn.metrics import confusion_matrix,classification_report
for df_name in dfs.keys():
    if df_name=="S1" or df_name=="S4":
        continue
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]
    N= len(dataset)
    true= dataset.true_cluster
    #print()
    plt.suptitle(f"{df_name}")
    fig,axs=plt.subplots(2,3,figsize=(10,8))
```



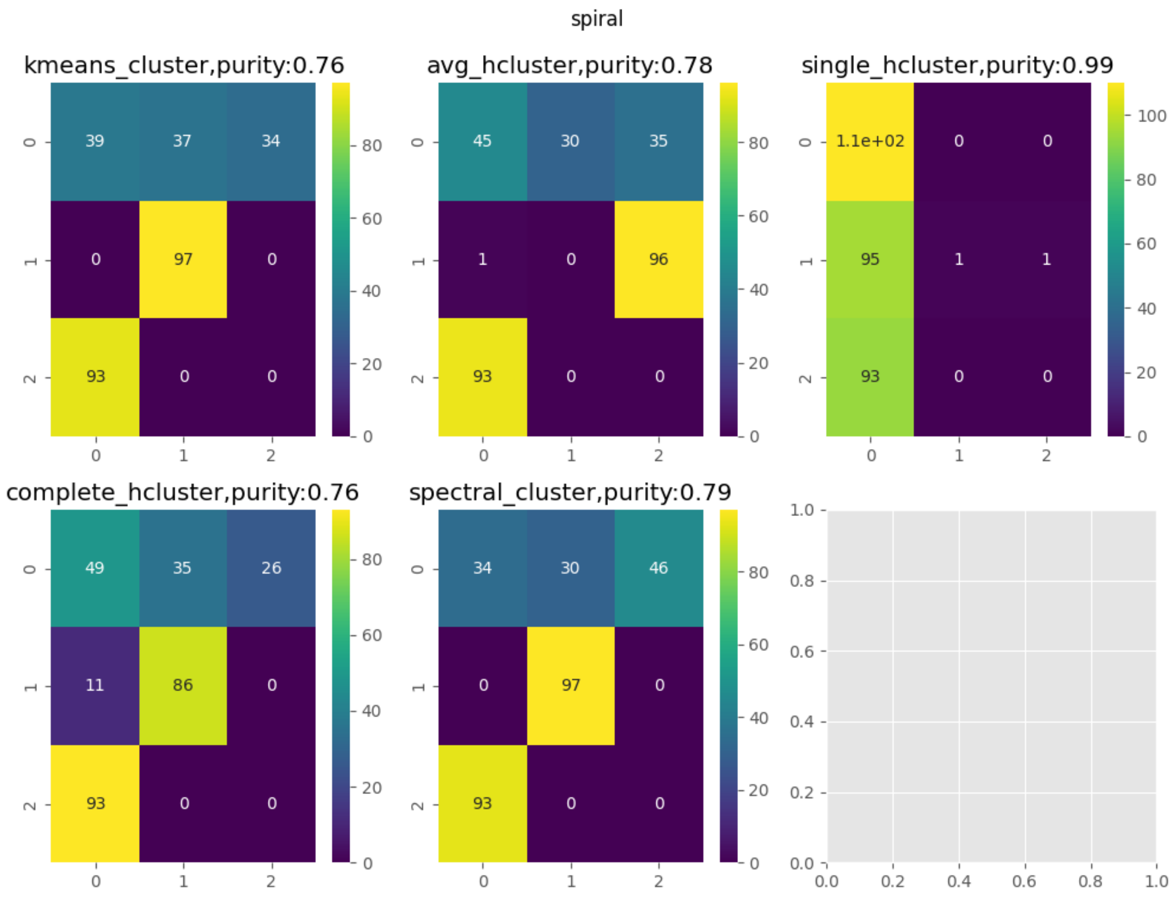
- **Purity**: Purity is a measure of the extent to which clusters contain a single class.[37] Its calculation can be thought of as follows: For each cluster, count the number of data points from the most common class in said cluster. Now take the sum over all clusters and divide by the total number of data points. Formally, given some set of clusters M and some set of classes D, both partitioning N data points, purity can be defined as:

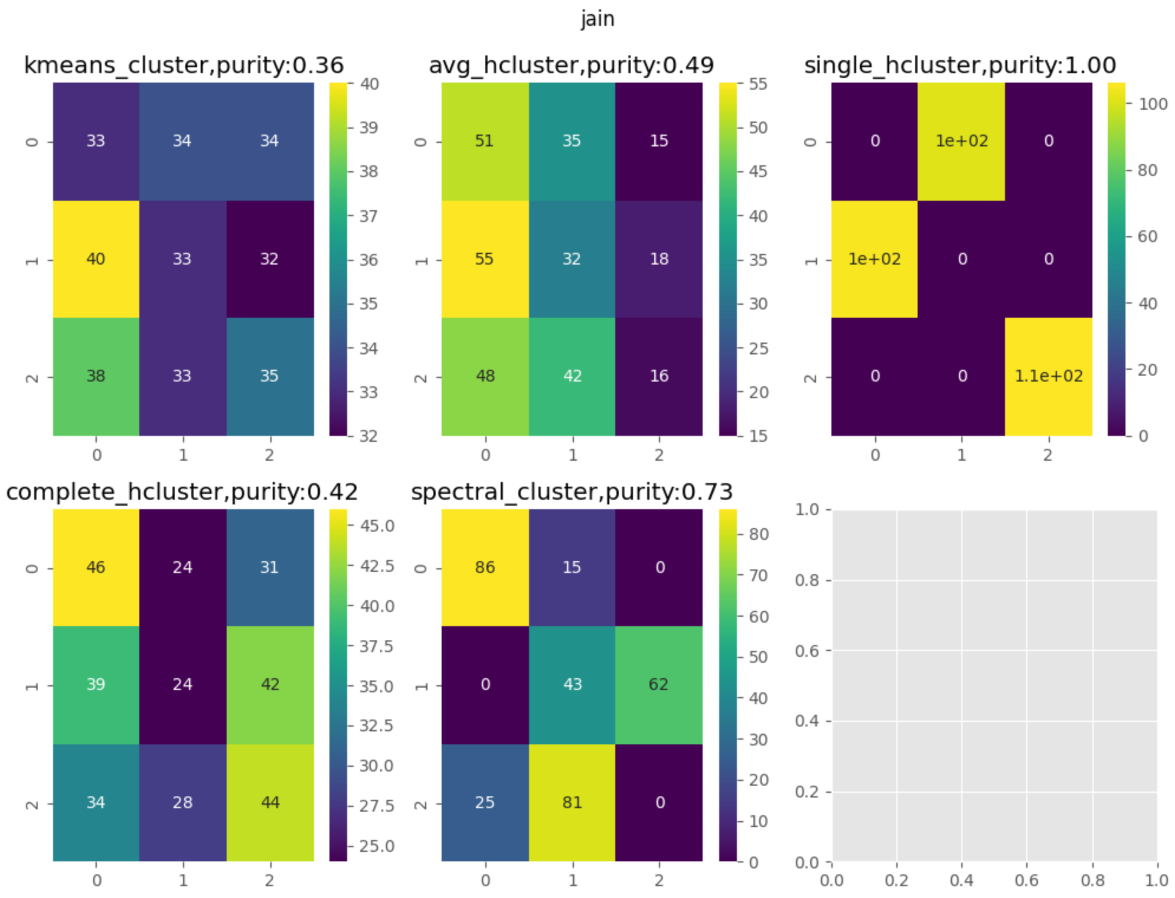
$$\frac{1}{N}\sum_{m\in M}\max_{d\in D}|m\cap d|$$

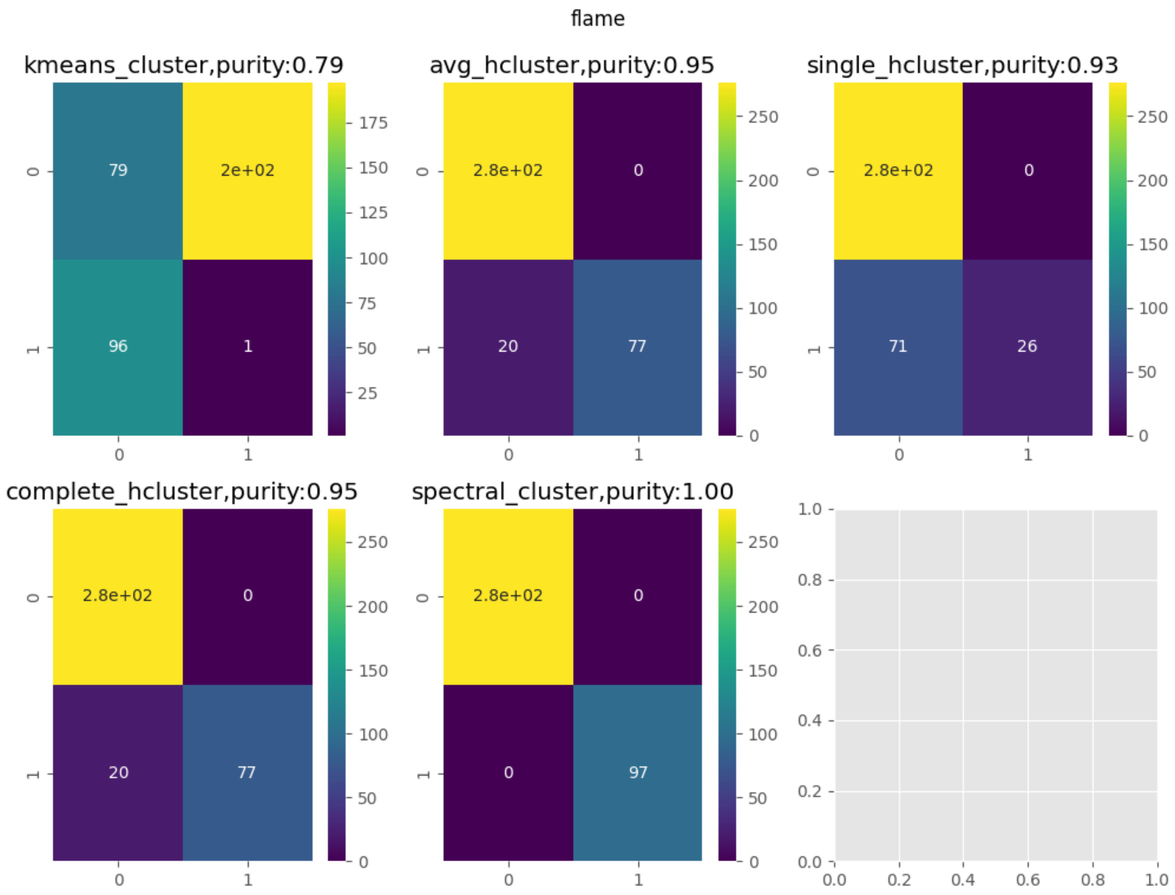
Figure 1: image.png

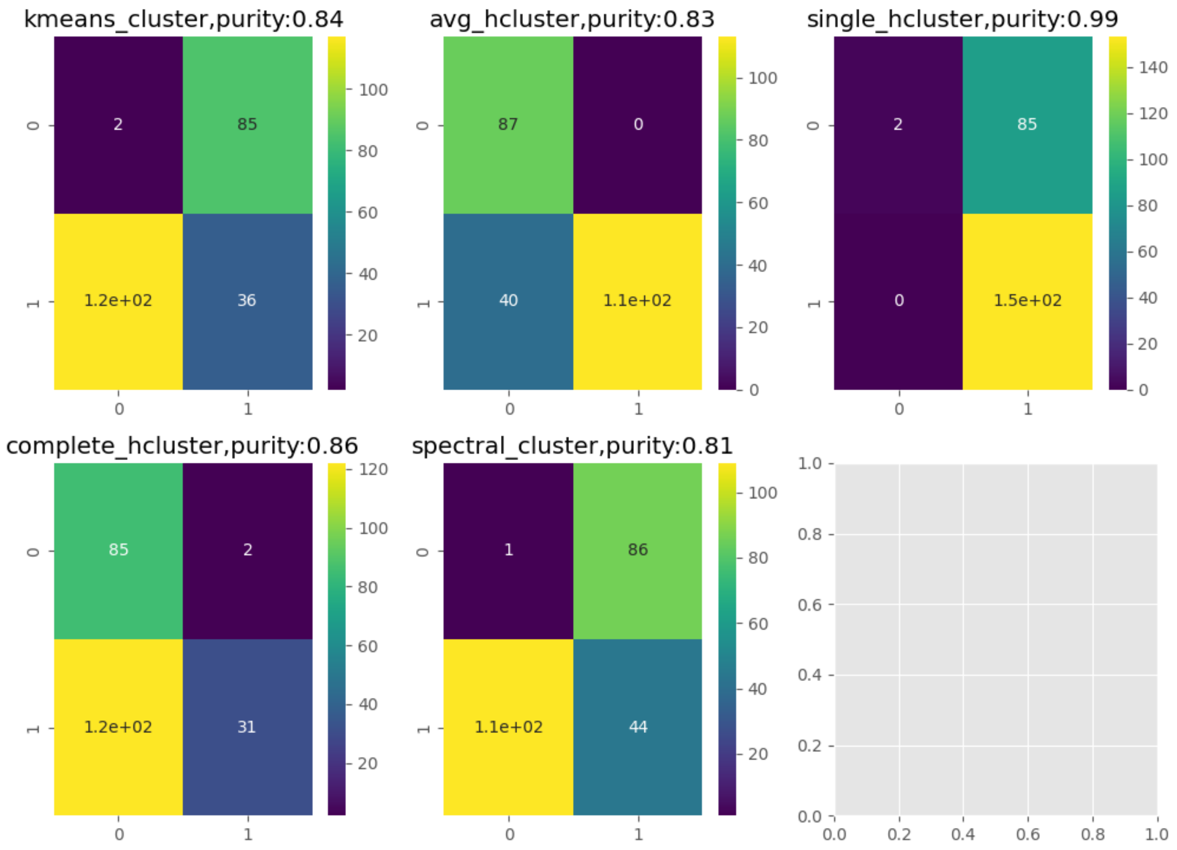
```
    axs=axs.ravel()
    for i in range(5):
        predicted=dataset.iloc[:,i+3]
        confusion_mat=confusion_matrix(true, predicted)
        #print(confusion_mat)
        purity= np.sum(np.amax(confusion_mat,axis=1))/len(dataset)
        #print(f"Purity Index of {dataset.iloc[:,i+3].name}:{purity}")
        axs[i].set_title(f"{dataset.iloc[:,i+3].name},purity:{purity:.2f}")

        sns.heatmap(confusion_mat,ax=axs[i],annot=True,cmap="viridis")
        fig.tight_layout(rect=[0, 0.03, 1, 0.95])
```

```
<Figure size 640x480 with 0 Axes>
```

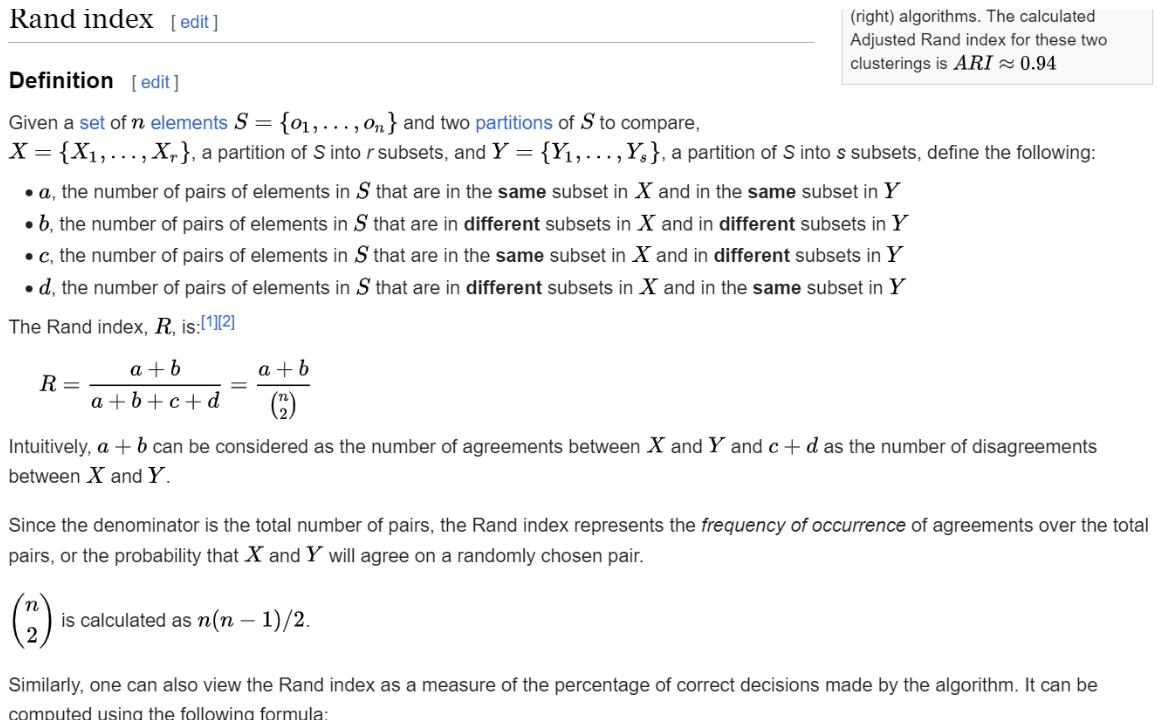

spiral
kmeans_cluster,purity:0.76
39
37
34
0
97
0
93
0
0
avg_hcluster,purity:0.78
45
30
35
1
0
96
93
0
0
single_hcluster,purity:0.99
1.1e+02
0
0
95
1
1
93
0
0
complete_hcluster,purity:0.76
49
35
26
11
86
0
93
0
0
spectral_cluster,purity:0.79
34
30
46
0
97
0
93
0
0


jain
kmeans_cluster,purity:0.36
avg_hcluster,purity:0.49
single_hcluster,purity:1.00
complete_hcluster,purity:0.42
spectral_cluster,purity:0.73


flame
kmeans_cluster,purity:0.79
79
2e+02
96
1
avg_hcluster,purity:0.95
2.8e+02
0
20
77
single_hcluster,purity:0.93
2.8e+02
0
71
26
complete_hcluster,purity:0.95
2.8e+02
0
20
77
spectral_cluster,purity:1.00
2.8e+02
0
0
97


kmeans_cluster,purity:0.84
2
85
1.2e+02
36
avg_hcluster,purity:0.83
87
0
40
1.1e+02
single_hcluster,purity:0.99
2
85
0
1.5e+02
complete_hcluster,purity:0.86
85
2
1.2e+02
31
spectral_cluster,purity:0.81
1
86
1.1e+02
44

Rand index :



(right) algorithms. The calculated Adjusted Rand index for these two clusterings is $ARI \approx 0.94$

Rand index [edit]

Definition [edit]

Given a set of n elements $S = \{o_1, \ldots, o_n\}$ and two partitions of S to compare, $X = \{X_1, \ldots, X_r\}$, a partition of *S* into *r* subsets, and $Y = \{Y_1, \ldots, Y_s\}$, a partition of *S* into *s* subsets, define the following:

- a, the number of pairs of elements in S that are in the **same** subset in X and in the **same** subset in Y
- b, the number of pairs of elements in S that are in **different** subsets in X and in **different** subsets in Y
- c, the number of pairs of elements in S that are in the **same** subset in X and in **different** subsets in Y
- d, the number of pairs of elements in S that are in **different** subsets in X and in the **same** subset in Y

The Rand index, R, is:[1][2]

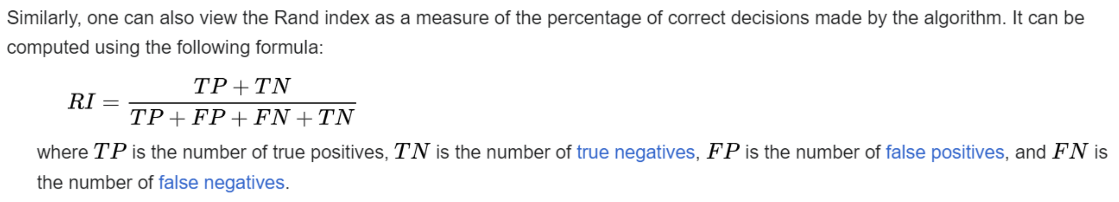
$$R = \frac{a+b}{a+b+c+d} = \frac{a+b}{\binom{n}{2}}$$

Intuitively, $a+b$ can be considered as the number of agreements between X and Y and $c+d$ as the number of disagreements between X and Y.

Since the denominator is the total number of pairs, the Rand index represents the *frequency of occurrence* of agreements over the total pairs, or the probability that X and Y will agree on a randomly chosen pair.

$\binom{n}{2}$ is calculated as $n(n-1)/2$.

Similarly, one can also view the Rand index as a measure of the percentage of correct decisions made by the algorithm. It can be computed using the following formula:

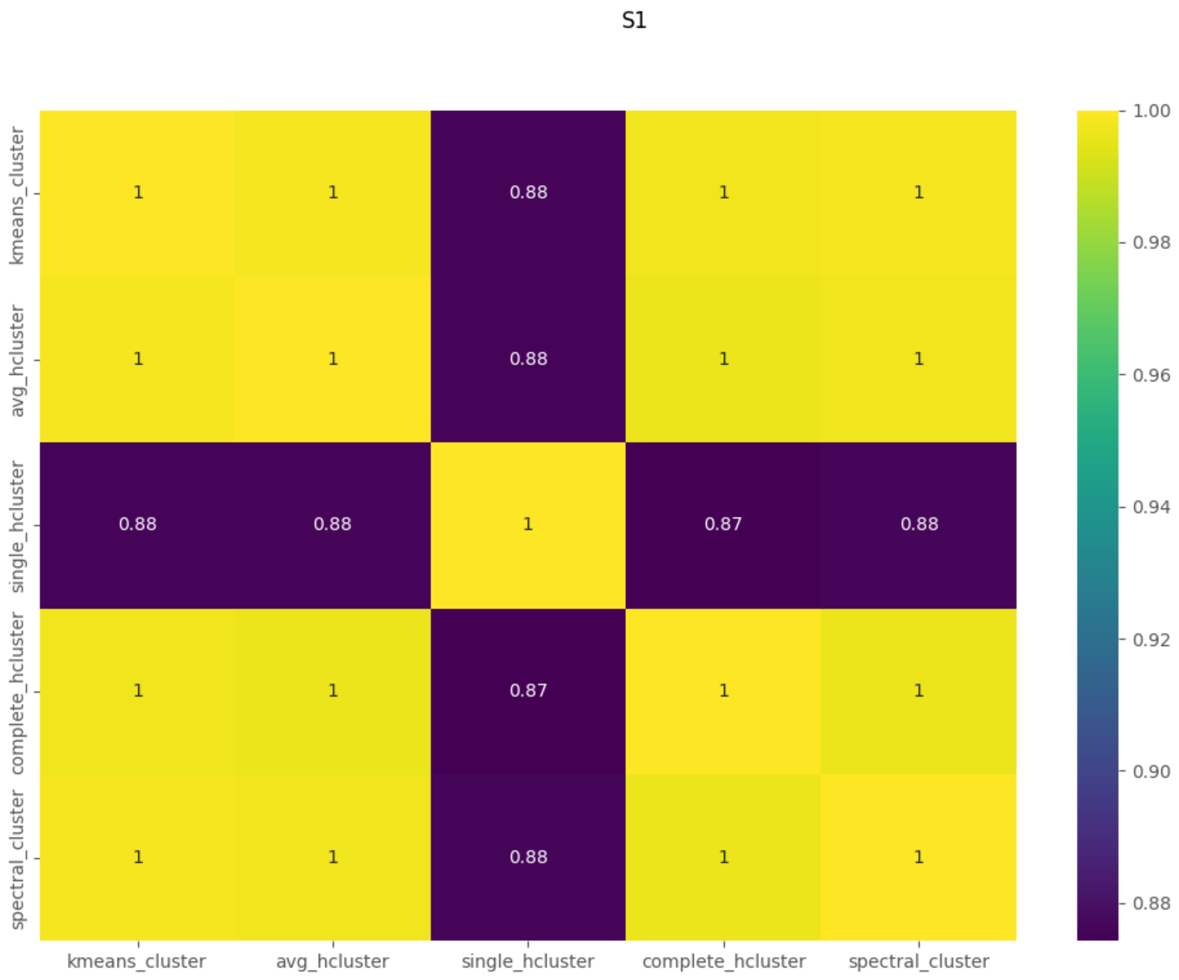


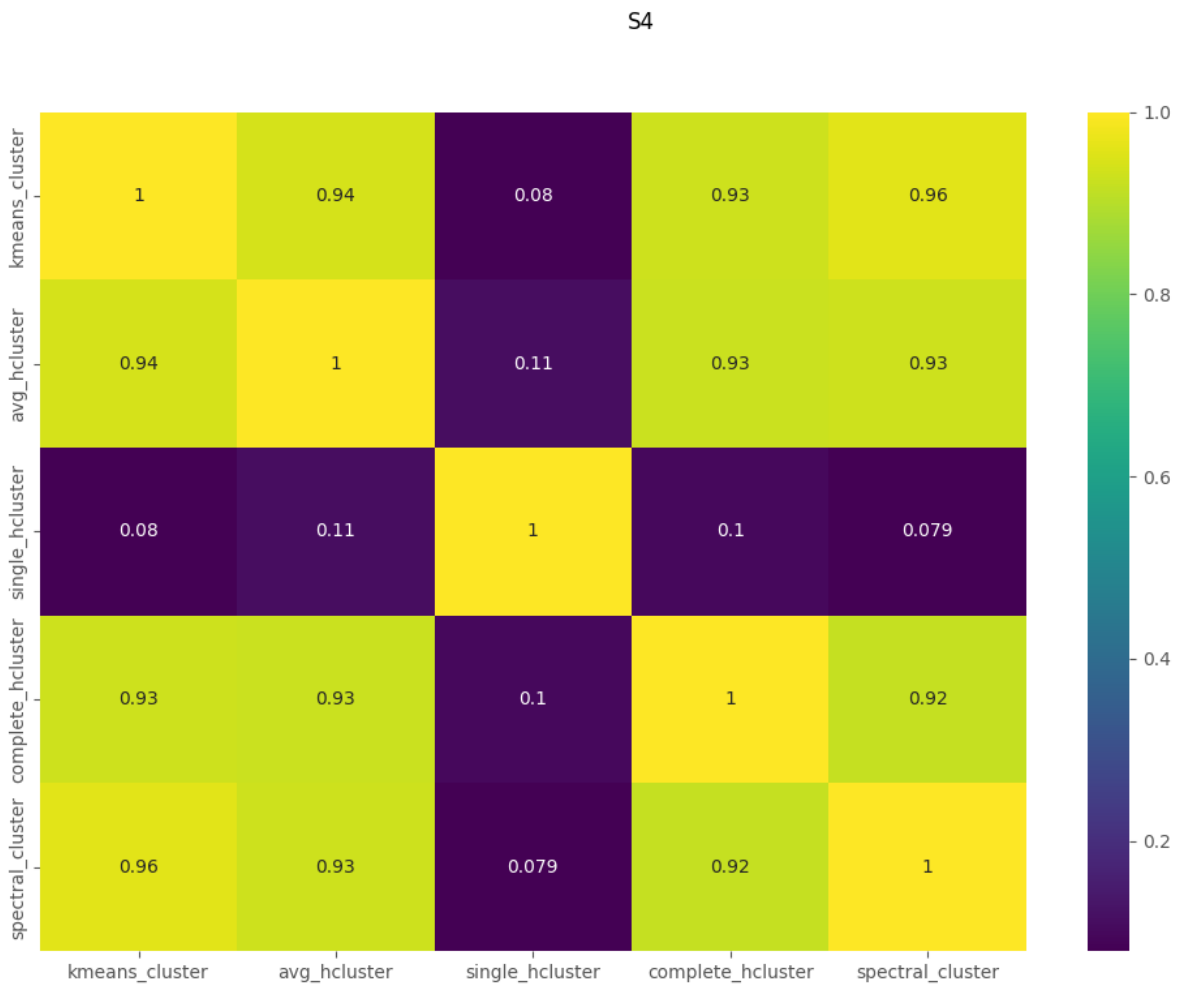
Similarly, one can also view the Rand index as a measure of the percentage of correct decisions made by the algorithm. It can be computed using the following formula:

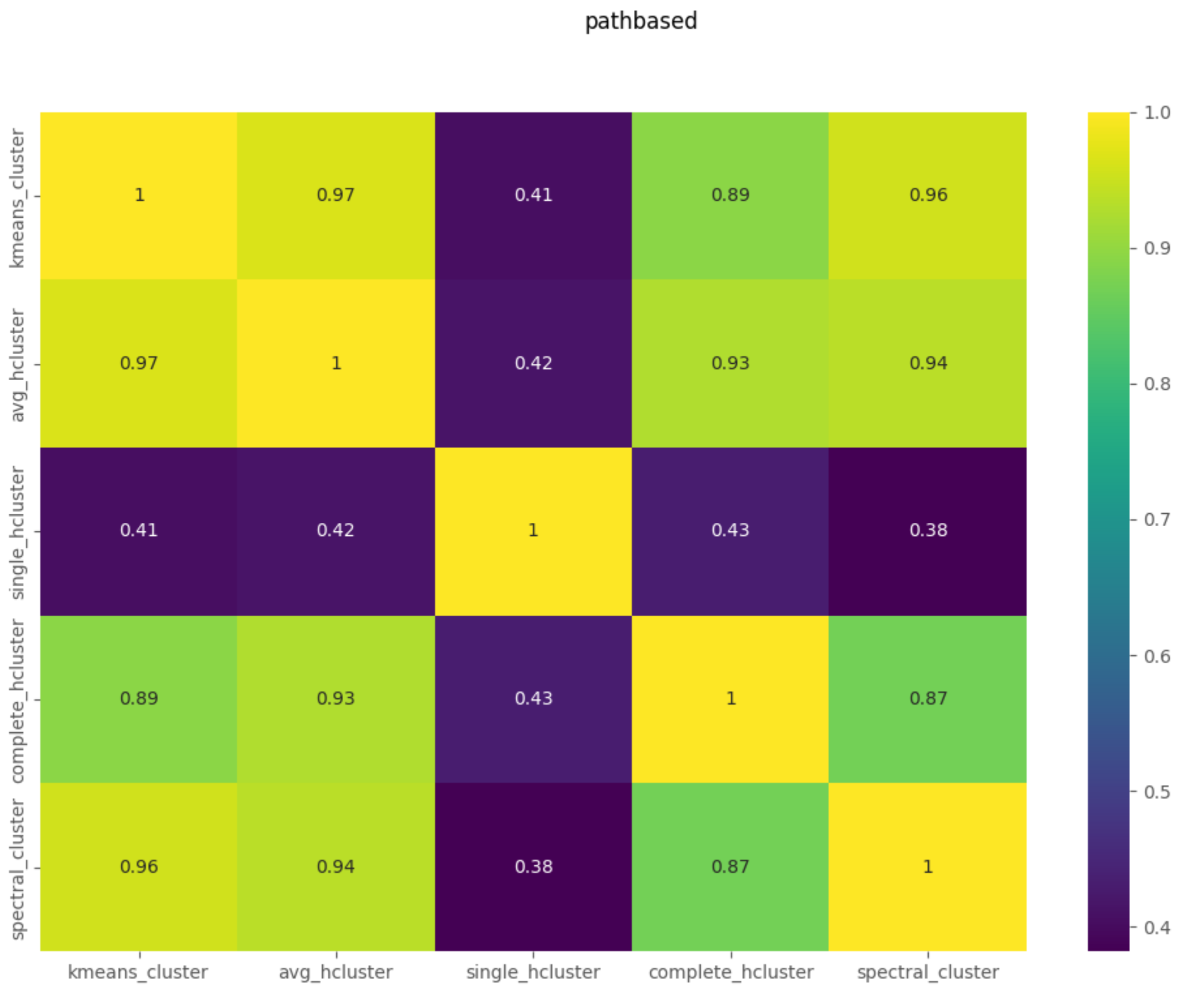
$$RI = \frac{TP+TN}{TP+FP+FN+TN}$$

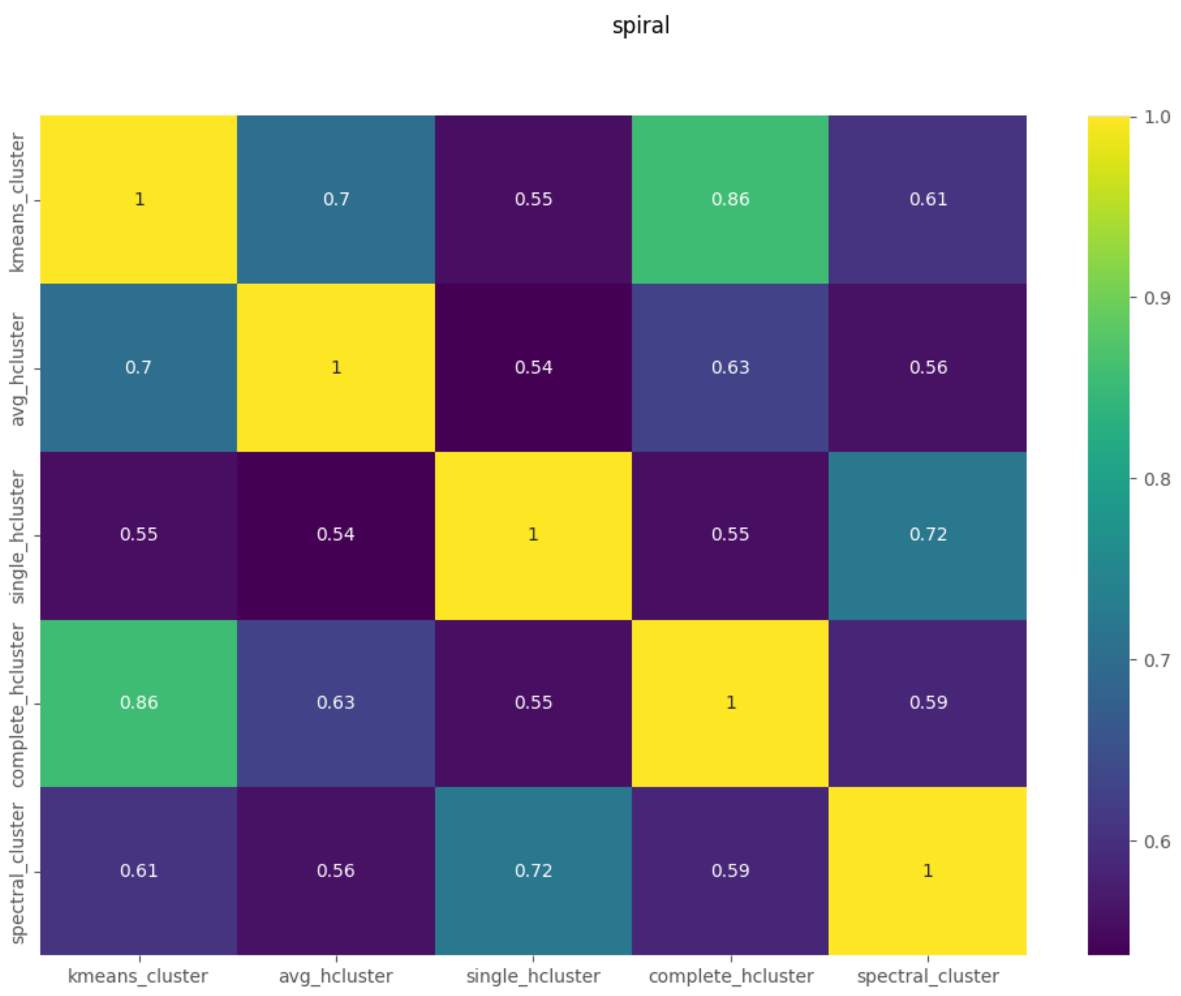
where TP is the number of true positives, TN is the number of true negatives, FP is the number of false positives, and FN is the number of false negatives.

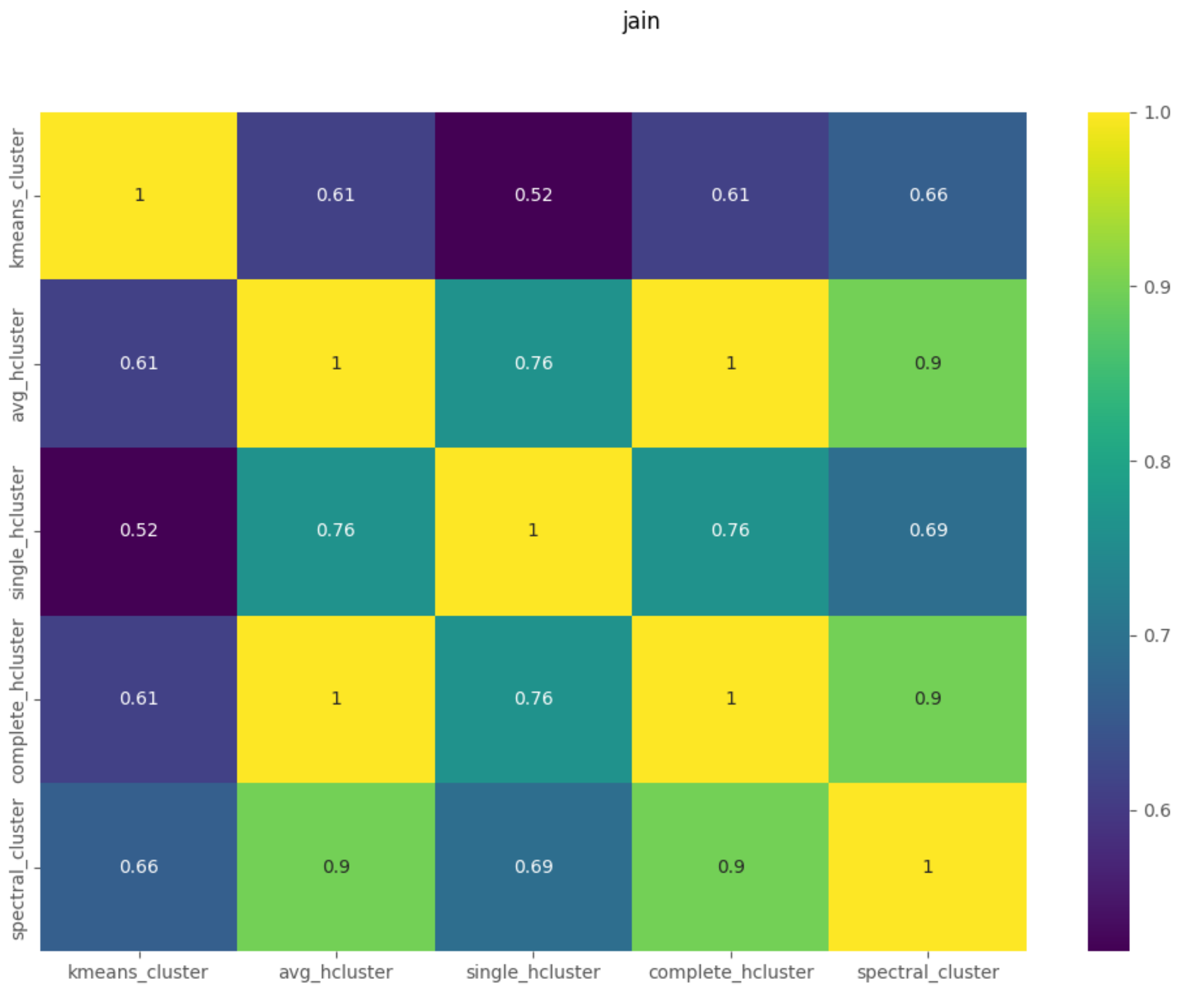
```python
from sklearn.metrics.cluster import rand_score
methods=S1.columns[2:]
for df_name in dfs.keys():
    dataset=dfs[df_name][0]
    k = dfs[df_name][1]
    N= len(dataset)
    fig,axs=plt.subplots(1,1,figsize=(10,8))
    randind_mat=np.zeros((5,5))
    for i in range(5):
        for j in range(5):
            randind_mat[i,j]= rand_score(dataset.loc[:,methods[i]],dataset.loc[:,methods[j
sns.heatmap(randind_mat,annot=True,cmap="viridis",xticklabels=methods,yticklabels=meth
fig.suptitle(f"{df_name}")

fig.tight_layout(rect=[0, 0.03, 1, 0.95])
```



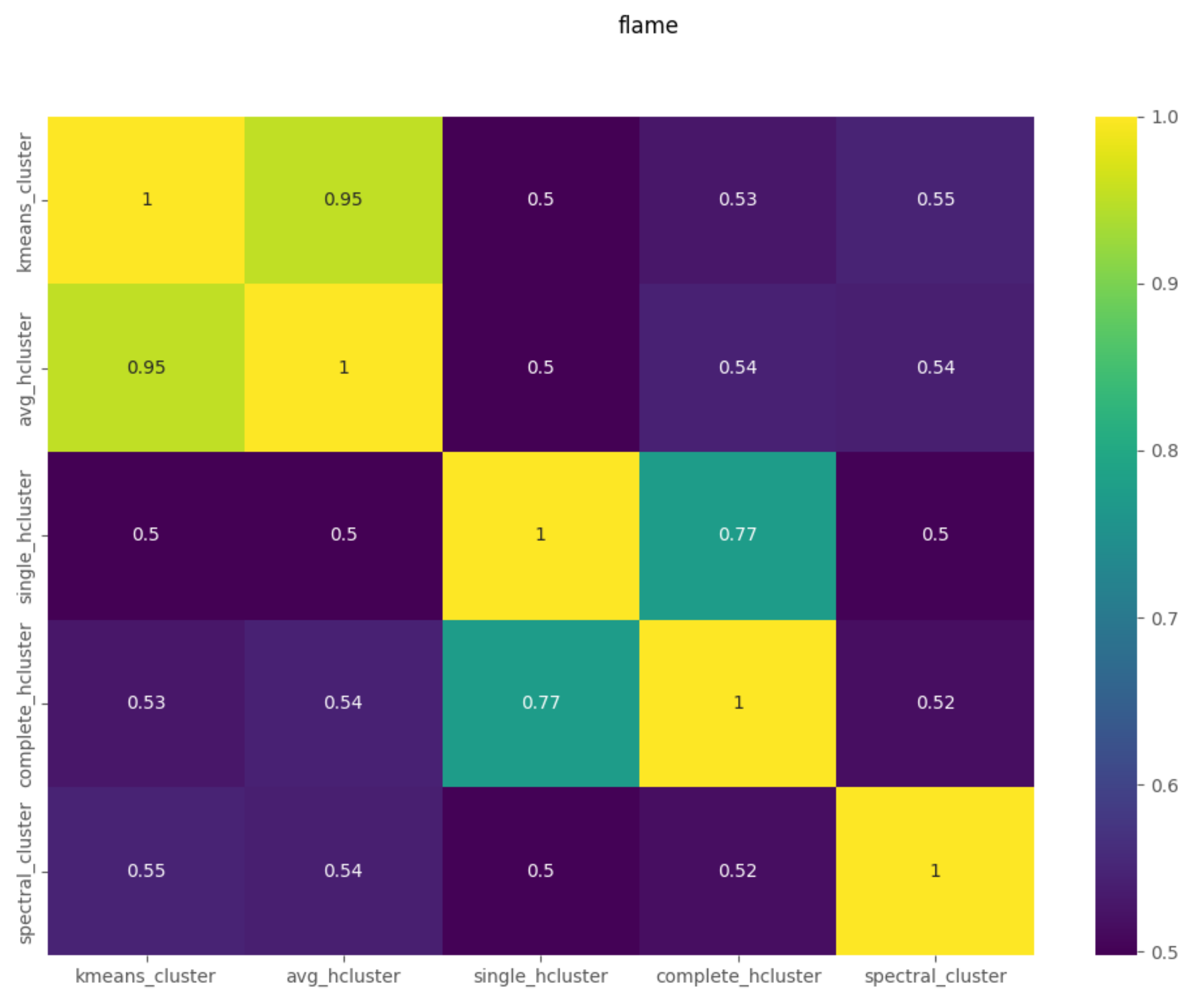

S4
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
1 0.94 0.08 0.93 0.96
0.94 1 0.11 0.93 0.93
0.08 0.11 1 0.1 0.079
0.93 0.93 0.1 1 0.92
0.96 0.93 0.079 0.92 1
1.0
0.8
0.6
0.4
0.2


pathbased
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
1
0.97
0.41
0.89
0.96
0.97
1
0.42
0.93
0.94
0.41
0.42
1
0.43
0.38
0.89
0.93
0.43
1
0.87
0.96
0.94
0.38
0.87
1
1.0
0.9
0.8
0.7
0.6
0.5
0.4


spiral
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
1 0.7 0.55 0.86 0.61
0.7 1 0.54 0.63 0.56
0.55 0.54 1 0.55 0.72
0.86 0.63 0.55 1 0.59
0.61 0.56 0.72 0.59 1
kmeans_cluster
avg_hcluster
single_hcluster
complete_hcluster
spectral_cluster
1.0
0.9
0.8
0.7
0.6



	kmeans_cluster	avg_hcluster	single_hcluster	complete_hcluster	spectral_cluster
kmeans_cluster	1	0.61	0.52	0.61	0.66
avg_hcluster	0.61	1	0.76	1	0.9
single_hcluster	0.52	0.76	1	0.76	0.69
complete_hcluster	0.61	1	0.76	1	0.9
spectral_cluster	0.66	0.9	0.69	0.9	1



References

Websites:

1- https://www.w3schools.com/python/python_ml_k-means.asp

2- https://www.w3schools.com/python/python_ml_hierarchial_clustering.asp

3- https://scikit-learn.org/stable/modules/generated/sklearn.cluster.SpectralClustering.html

4- https://scikit-learn.org/stable/modules/generated/sklearn.metrics.confusion_matrix.html

5- https://stats.stackexchange.com/questions/95731/how-to-calculate-purity