Dataset Analysis
K-Means & Other Clustering Algorithms:

Unsupervised learning via clustering algorithms. Let's work with the Karate Club dataset to perform several types of clustering algorithms.

Clustering is the grouping of objects together so that objects belonging to the same group (cluster) are more similar to each other than those in other groups (clusters).

Article Resources

- **Dataset:** available see paper: *An Information Flow Model for Conflict and Fission in Small Groups(Have shared the paper for you own perusal)*

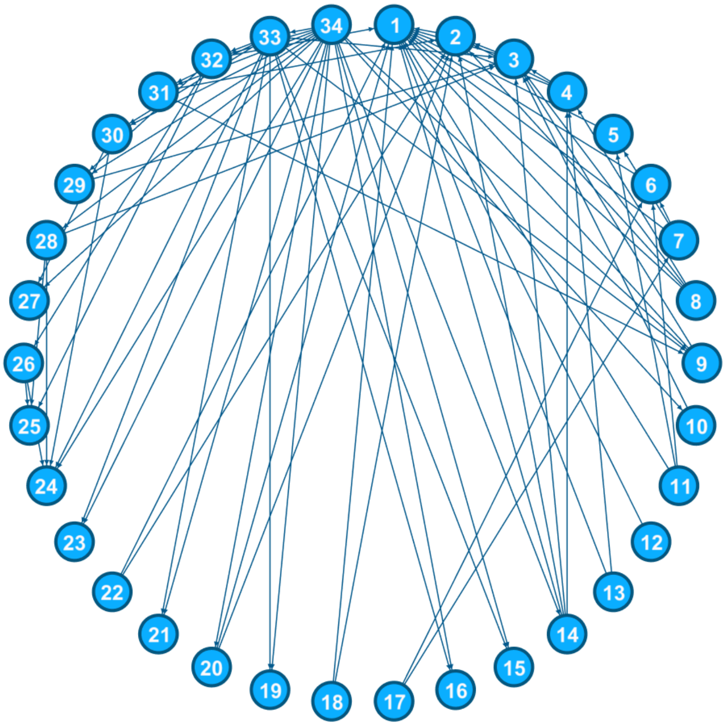
The Dataset

For the clustering problem, we will use the famous *Zachary's Karate Club* dataset. For more detailed information on the study see the linked paper.

Essentially there was a karate club that had an administrator "John A" and an instructor "Mr. Hi", and a conflict arose between them which caused the students to split into two groups; one that followed John and one that followed Mr. Hi.

The **students are the nodes** in our graph, and the edges, or links, between the nodes are the result of social interactions outside of the club between students.

Since there was an eventual split into two groups (clusters) by the end of the karate club dispute, and we know which group each student ended up in, we can use the results as truth values for our clustering to gauge performance between different algorithms.



Social relationships (edges) of each student (node) outside of the Karate Club

Getting Started with Clustering

Imports

```
from sklearn import cluster
import networkx as nx
from collections import defaultdict
import matplotlib.pyplot as plt
from matplotlib import cm, colors
import seaborn as sns
import pandas as pd
import numpy as np
from sklearn.metrics.cluster import normalized_mutual_info_score
from sklearn.metrics.cluster import adjusted_rand_score
```

We'll be using the scikit-learn, pandas , and numpy stack with the addition
of matplotlib, seaborn and networkx for graph visualization. A simple pip/conda install should work with each of these.

Let's go ahead and import the dataset directly from networkx and also set up the spring layout positioning for the graph visuals:

```python
G = nx.karate_club_graph()

pos = nx.spring_layout(G)
```

Let's go ahead a create a function to let us visualize the dataset:

```python
def draw_communities(G, membership, pos):
    """Draws the nodes to a plot with assigned colors for each individual cluster
    Parameters
    ----------
    G : networkx graph
    membership : list
        A list where the position is the student and the value at the position is the student club membership.
        E.g. `print(membership[8]) --> 1` means that student #8 is a member of club 1.
    pos : positioning as a networkx spring layout
        E.g. nx.spring_layout(G)
    """
    fig, ax = plt.subplots(figsize=(16,9))

    # Convert membership list to a dict where key=club, value=list of students in club
    club_dict = defaultdict(list)
    for student, club in enumerate(membership):
        club_dict[club].append(student)

    # Normalize number of clubs for choosing a color
    norm = colors.Normalize(vmin=0, vmax=len(club_dict.keys()))

    for club, members in club_dict.items():
        nx.draw_networkx_nodes(G, pos,
                               nodelist=members,
                               node_color=cm.jet(norm(club)),
                               node_size=500,
                               alpha=0.8,
                               ax=ax)

    # Draw edges (social connections) and show the final plot
    plt.title("Zachary's Karate Club")
    nx.draw_networkx_edges(G, pos, alpha=0.5, ax=ax)
    plt.show()
```

In order to color the student nodes according to their club membership, we're using matplotlib's Normalize class to fit the number of clubs into the (0, 1) interval. You might be wondering why we need to do this when there's only two clubs that resulted from the study, but we'll find out later that some clustering algorithms didn't get it right and we need to be able to colorize more than two clubs.

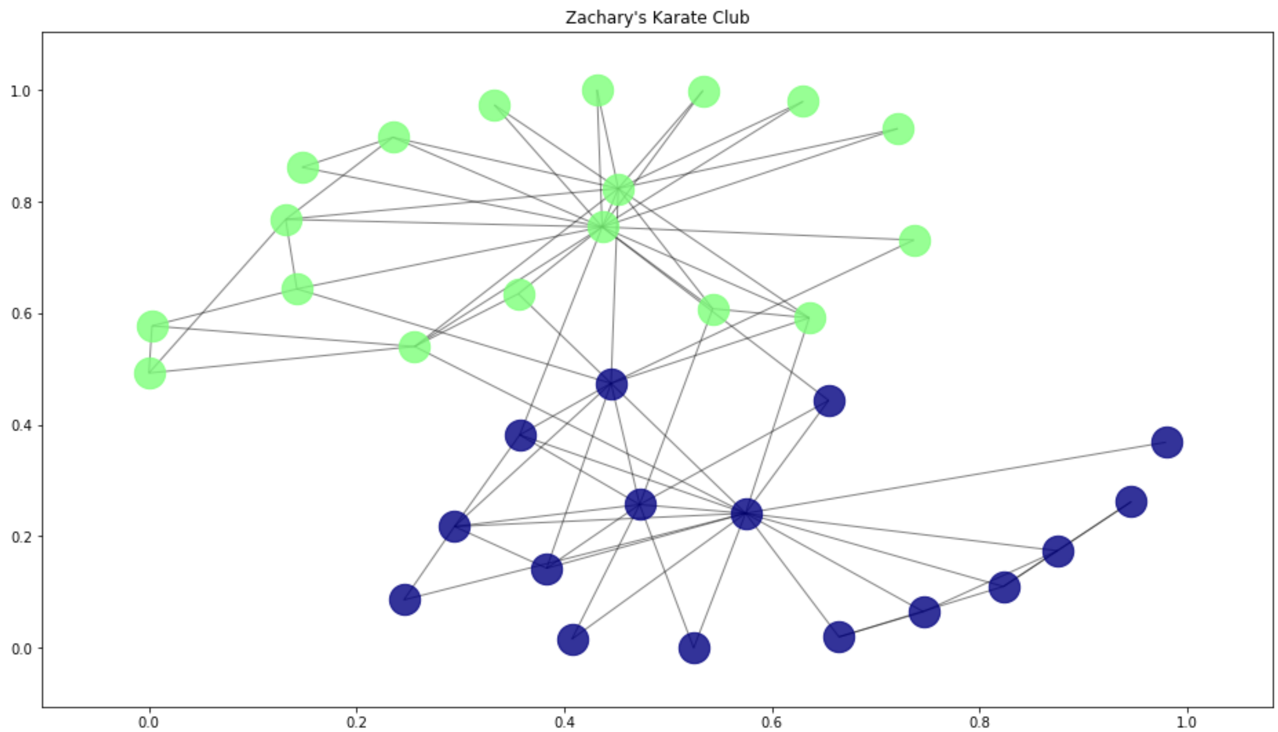
To compare our algorithm's, performance we want the true labels, i.e. where each student ended up after the club fission. Unfortunately, the true labels are not provided in the networkx dataset, but we can retrieve them from the study itself and hardcode them here:

```python
# True labels of the group each student (node) unded up in. Found via the original paper
y_true = [0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 0, 1, 1, 0, 0, 1, 0, 1, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
```

Now, let's use our draw function to visualize the true student club membership and their social connections:

```
draw_communities(G, y_true, pos)
```

RESULT:



This is the true division of the Karate Club. We'll see how our algorithms do when trying to cluster on their own below.

Before that, we need to preprocess the data by transforming the graph into a matrix since that is the format required for the clusterers. Remember this edge_mat variable below, we'll be using this for input to our clustering models in the next few sections:

```python
def graph_to_edge_matrix(G):
    """Convert a networkx graph into an edge matrix.
    See https://www.wikiwand.com/en/Incidence_matrix for a good explaination on edge matrices

    Parameters
    ----------
    G : networkx graph
    """
    # Initialize edge matrix with zeros
    edge_mat = np.zeros((len(G), len(G)), dtype=int)

    # Loop to set 0 or 1 (diagonal elements are set to 1)
    for node in G:
        for neighbor in G.neighbors(node):
            edge_mat[node][neighbor] = 1
        edge_mat[node][node] = 1

    return edge_mat
```

```python
edge_mat = graph_to_edge_matrix(G)
edge_mat
```

```
array([[1, 1, 1, ..., 1, 0, 0],
       [1, 1, 1, ..., 0, 0, 0],
       [1, 1, 1, ..., 0, 1, 0],
       ...,
       [1, 0, 0, ..., 1, 1, 1],
       [0, 0, 1, ..., 1, 1, 1],
       [0, 0, 0, ..., 1, 1, 1]])
```

That transform our graph into a matrix and print the result to see what it contains:

Clustering Algorithms

Unsupervised learning via clustering can work quite well in a lot of cases, but it can also perform terribly. We'll go through a few algorithms that are known to perform very well and see how they do on the same dataset. Fortunately, we can use the true cluster labels from the paper to calculate metrics and determine which is the best clustering option.

K-Means Clustering

```python
k_clusters = 2
results = []
algorithms = {}

algorithms['kmeans'] = cluster.KMeans(n_clusters=k_clusters, n_init=200)

algorithms['agglom'] = cluster.AgglomerativeClustering(n_clusters=k_clusters, linkage="ward")

algorithms['spectral'] = cluster.SpectralClustering(n_clusters=k_clusters, affinity="precomputed", n_init=200)

algorithms['affinity'] = cluster.AffinityPropagation(damping=0.6)

for model in algorithms.values():
    model.fit(edge_mat)
    results.append(list(model.labels_))
```

K-means is considered by many to be the gold standard when it comes to clustering due to its simplicity and performance, so it's the first one we'll try out.

When you have no idea at all what algorithm to use, K-means is usually the first choice.

K-means works by defining spherical clusters that are separable in a way so that the mean value converges towards the cluster center. Because of this, K-Means may underperform sometimes.

To simply construct and train a K-means model, we can use sklearn's package. Before we do, we are going to define the number of clusters we know to be true (two), a list to hold results (labels), and a dictionary containing each algorithm we end up trying:

```
k_clusters = 2
results = []
algorithms = {}

algorithms['kmeans'] = cluster.KMeans(n_clusters=k_clusters, n_init=200)

algorithms['agglom'] = cluster.AgglomerativeClustering(n_clusters=k_clusters, linkage="ward")

algorithms['spectral'] = cluster.SpectralClustering(n_clusters=k_clusters, affinity="precomputed", n_init=200)

algorithms['affinity'] = cluster.AffinityPropagation(damping=0.6)

for model in algorithms.values():
    model.fit(edge_mat)
    results.append(list(model.labels_))
```

To fit this model, we could simply call algorithms['kmeans'].fit(edge_mat).

Since we'll be testing a bunch of clustering packages, we can loop over each and fit them at the same time. See below.

Agglomerative Clustering

The main idea behind Agglomerative clustering is that each node first starts in its own cluster, and then pairs of clusters recursively merge together in a way that minimally increases a given linkage distance.

The main advantage of Agglomerative clustering (and hierarchical clustering in general) is that you don't need to specify the number of clusters. That of course, comes with a price: performance. But, in sklearn's implementation, you can specify the number of clusters to assist the algorithm's performance.

Let's create and train an agglomerative model and add it to our dictionary:

algorithms['agglom'] = cluster.AgglomerativeClustering(n_clusters=k_clusters, linkage="ward")

Spectral Clustering

The Spectral clustering technique applies clustering to a projection of the normalized Laplacian. When it comes to image clustering, Spectral clustering works quite well.

algorithms['spectral'] = cluster.SpectralClustering(n_clusters=k_clusters, affinity="precomputed", n_init=200)

Affinity Propagation

Affinity propagation is a bit different. Unlike the previous algorithms, this one does not require the number of clusters to be determined before running the algorithm.

Affinity propagation performs really well on several computer vision and biology problems, such as clustering pictures of human faces and identifying regulated transcripts, but we'll soon find out it doesn't work well for our dataset.

Let's add this final algorithm to our dictionary and wrap it all up by fitting each model:

algorithms['affinity'] = cluster.AffinityPropagation(damping=0.6)

```
k_clusters = 2
results = []
algorithms = {}

algorithms['kmeans'] = cluster.KMeans(n_clusters=k_clusters, n_init=200)

algorithms['agglom'] = cluster.AgglomerativeClustering(n_clusters=k_clusters, linkage="ward")

algorithms['spectral'] = cluster.SpectralClustering(n_clusters=k_clusters, affinity="precomputed", n_init=200)

algorithms['affinity'] = cluster.AffinityPropagation(damping=0.6)

for model in algorithms.values():
    model.fit(edge_mat)
    results.append(list(model.labels_))
```

Metrics & Plotting

Well, it is time to choose which algorithm is more suitable for our data. A simple visualization of the result might work on small datasets, but imagine a graph with one thousand, or even ten thousand, nodes. That would be slightly chaotic for the human eye. So, let calculate the Adjusted Rand Score (ARS) and the Normalized Mutual Information (NMI) metrics for easier interpretation.

Normalized Mutual Information (NMI)

Mutual Information of two random variables is a measure of the mutual dependence between the two variables. *Normalized Mutual Information* is a normalization of the *Mutual Information (MI)* score to scale the results between 0 (no mutual information) and 1 (perfect correlation). In other words, 0 means dissimilar and 1 means
a perfect match.

Subscribe

Adjusted Rand Score (ARS)

Adjusted Rand Score on the other hand, computes a similarity measure between two clusters. ARS considers all pairs of samples and counts pairs that are assigned in the same or different clusters in the predicted and true clusters.

If that's a little weird to think about, have in mind that, for now, 0 is the lowest similarity and 1 is the highest.

In order to plot our scores, let's first calculate them. Remember that y_true is still a dictionary where the key is a student and the value is the club they ended up in. We need to get y_true's values first in order to compare them to y_pred:

```
nmi_results = []
ars_results = []

y_true_val = np.array(y_true)

# Append the results into lists
for y_pred in results:
    nmi_results.append(normalized_mutual_info_score(y_true_val, y_pred))
    ars_results.append(adjusted_rand_score(y_true_val, y_pred))
```

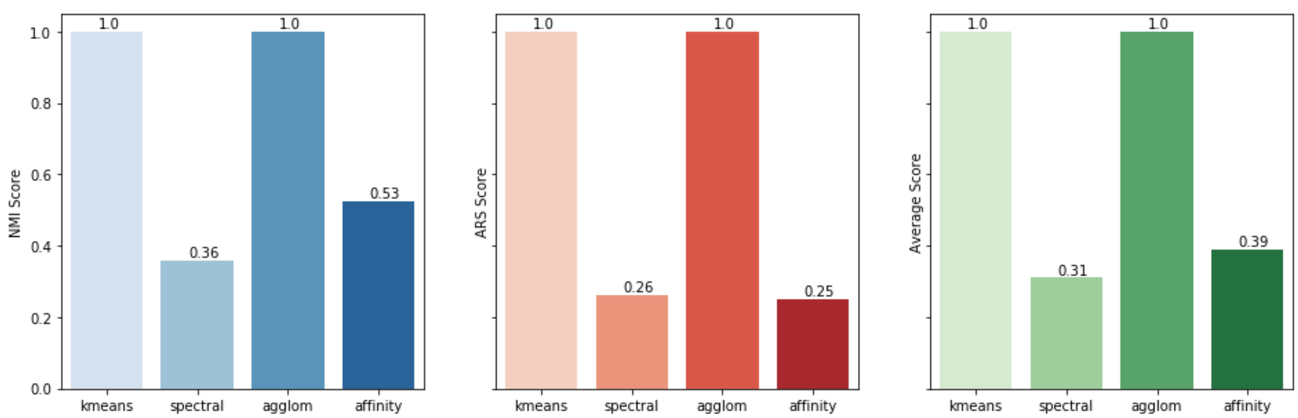
Let's now plot both scores side-by-side along with their averages for a better comparison.

We're using Seaborn's barplot along with matplotlib just for simpler coloring syntax. Most of the following is pretty simple.

The only thing fancy we added was the text on top of the bars. This is achieved on each subplot by referencing each axes (subplot), then using the index (*i*) as the x-coordinate, the score (*v*) as the y-coordinate, followed by the rounded value of *v* as the actual text to show on top.

```python
fig, (ax1, ax2, ax3) = plt.subplots(1, 3, sharey=True, figsize=(16, 5))

x = np.arange(len(xlabels))
avg = [sum(x) / 2 for x in zip(nmi_results, ars_results)]

xlabels = list(algorithms.keys())

sns.barplot(x, nmi_results, palette='Blues', ax=ax1)
sns.barplot(x, ars_results, palette='Reds', ax=ax2)
sns.barplot(x, avg, palette='Greens', ax=ax3)

ax1.set_ylabel('NMI Score')
ax2.set_ylabel('ARS Score')
ax3.set_ylabel('Average Score')

# # Add the xlabels to the chart
ax1.set_xticklabels(xlabels)
ax2.set_xticklabels(xlabels)
ax3.set_xticklabels(xlabels)

# Add the actual value on top of each bar
for i, v in enumerate(zip(nmi_results, ars_results, avg)):
    ax1.text(i - 0.1, v[0] + 0.01, str(round(v[0], 2)))
    ax2.text(i - 0.1, v[1] + 0.01, str(round(v[1], 2)))
    ax3.text(i - 0.1, v[2] + 0.01, str(round(v[2], 2)))

# Show the final plot
plt.show()
```

RESULT:



As you can see in the resulting chart, K-means and Agglomerative clustering have the best possible outcome for our dataset. That, of course, does not mean that Spectral and Agglomerative are low-performing algorithms, just that the did not fit in our particular dataset.

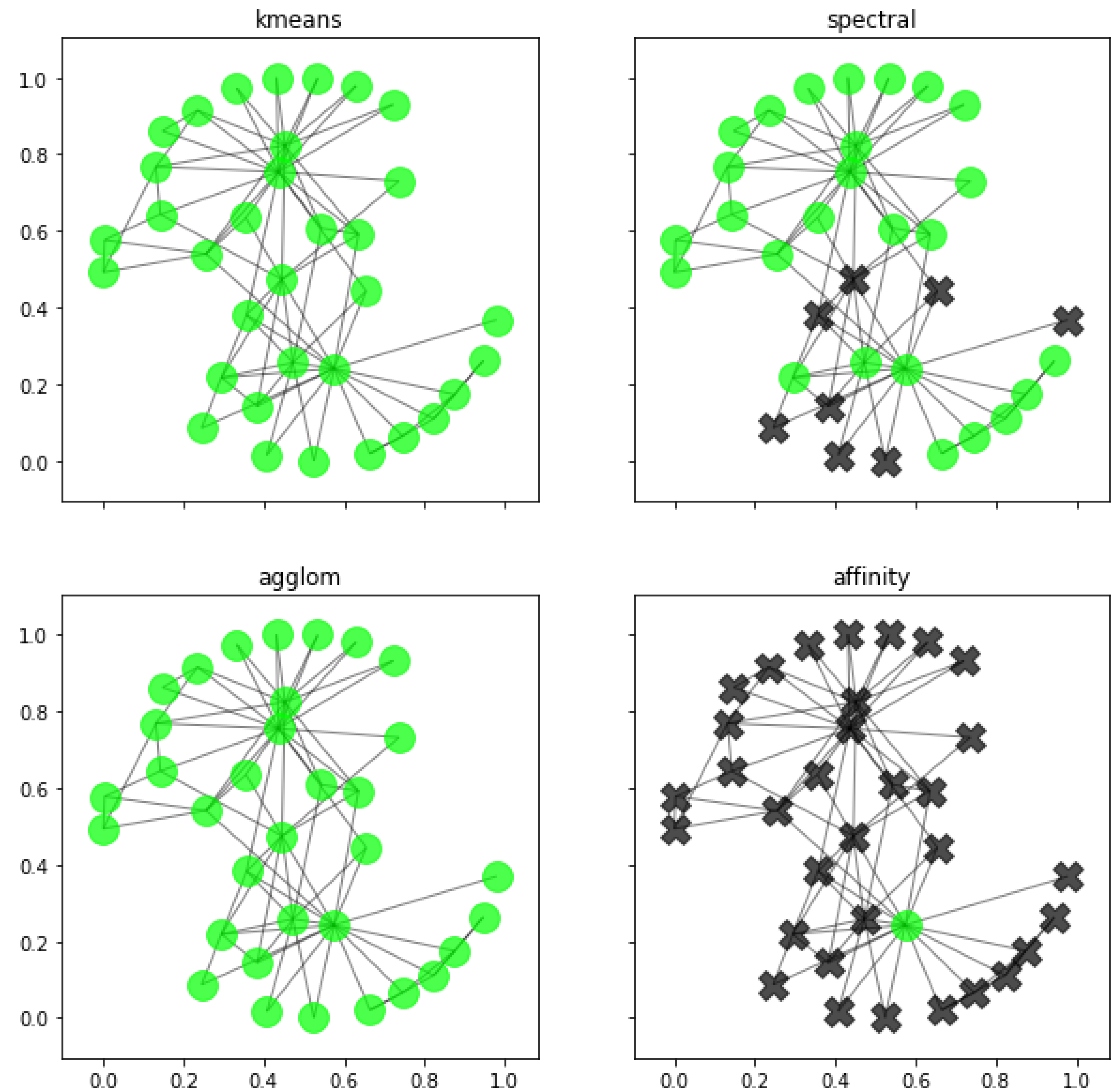
Out of curiosity, let's create a new function to plot where each algorithm went wrong by comparing the predicted student clusters with the true student clusters:

```python
def draw_true_vs_pred(G, y_true, y_pred, pos, algo_name, ax):

    for student, club in y_true.items():
        if y_pred is not None:
            if club == y_pred[student]:
                node_color = [0, 1, 0]
                node_shape = 'o'
            else:
                node_color = [0, 0, 0]
                node_shape = 'X'

        nx.draw_networkx_nodes(G, pos,
                               nodelist=[student],
                               node_color=node_color,
                               node_size=250,
                               alpha=0.7,
                               ax=ax,
                               node_shape=node_shape)

    # Draw edges and show final plot
    ax.set_title(algo_name)
    nx.draw_networkx_edges(G, pos, alpha=0.5, ax=ax)
```

```python
fig, ((ax1, ax2), (ax3, ax4)) = plt.subplots(2, 2, sharex=True, sharey=True, figsize=(10, 10))

for algo_name, ax in zip(algorithms.keys(), [ax1, ax2, ax3, ax4]):
    draw_true_vs_pred(G, y_true, algorithms[algo_name].labels_, pos, algo_name, ax)
```

This graph depicts each algorithm's correct (green circle) and incorrect (black X) cluster assignments.

RESULT:



This graph depicts each algorithm's correct (green circle) and incorrect (black X) cluster assignments.

Interestingly, we see that although the Affinity algorithm had a higher average score, it only put one node in the correct cluster.

To see the reason why, we can look at the cluster information from that algorithm:

```
cluster_centers_indices = algorithms['affinity'].cluster_centers_indices_

n_clusters_ = len(cluster_centers_indices)

print(n_clusters_)

# 8
```

Since we were not able to define the number of clusters for Affinity Propagation, it determined that there were eight clusters. Our metrics didn't hint at this problem since our scoring wasn't based off of clustering accuracy.

Let's wrap it up but taking a look at what our Affinity algorithm actually clustered:

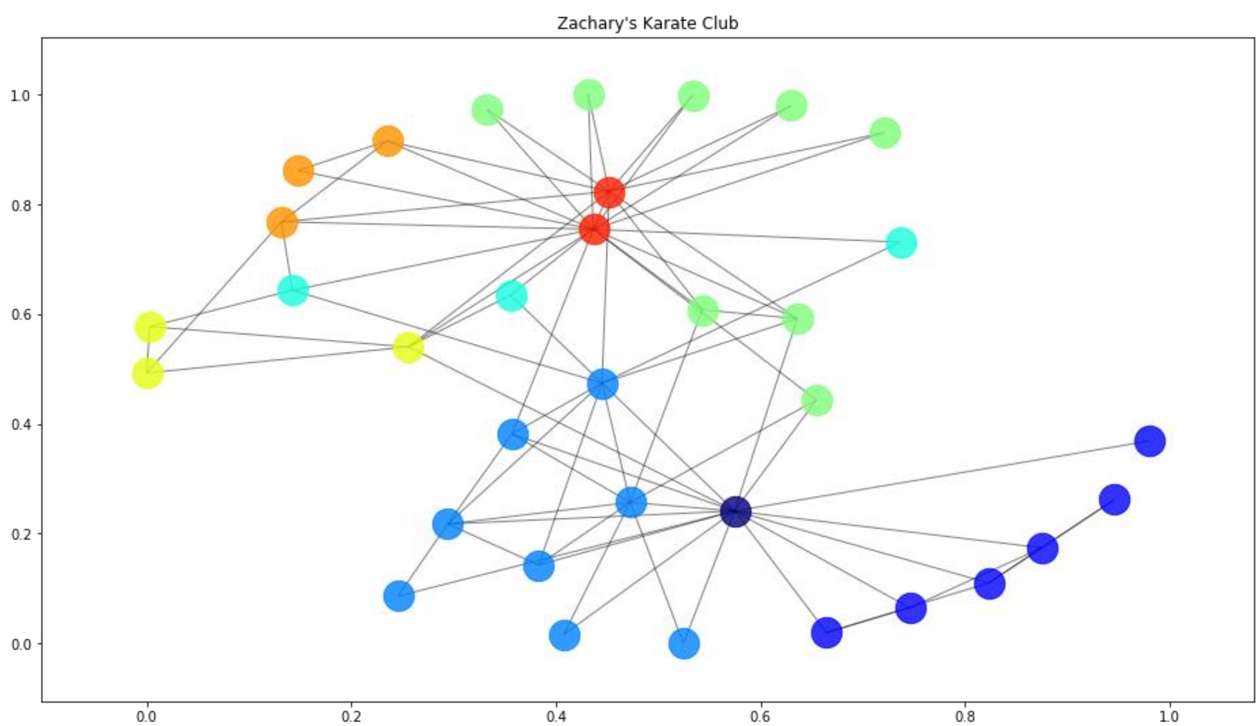
The resulting clubs

algorithms['affinity'].labels_

array([0, 2, 2, 2, 1, 1, 1, 2, 4, 3, 1, 1, 2, 2, 4, 4, 1, 2, 4, 4, 4, 2, 4, 5, 5, 6, 3, 3, 6, 4, 5, 7, 7], dtype=int64)

draw_communities(G, algorithms['affinity'].labels_, pos)

RESULT:



American Football Dataset

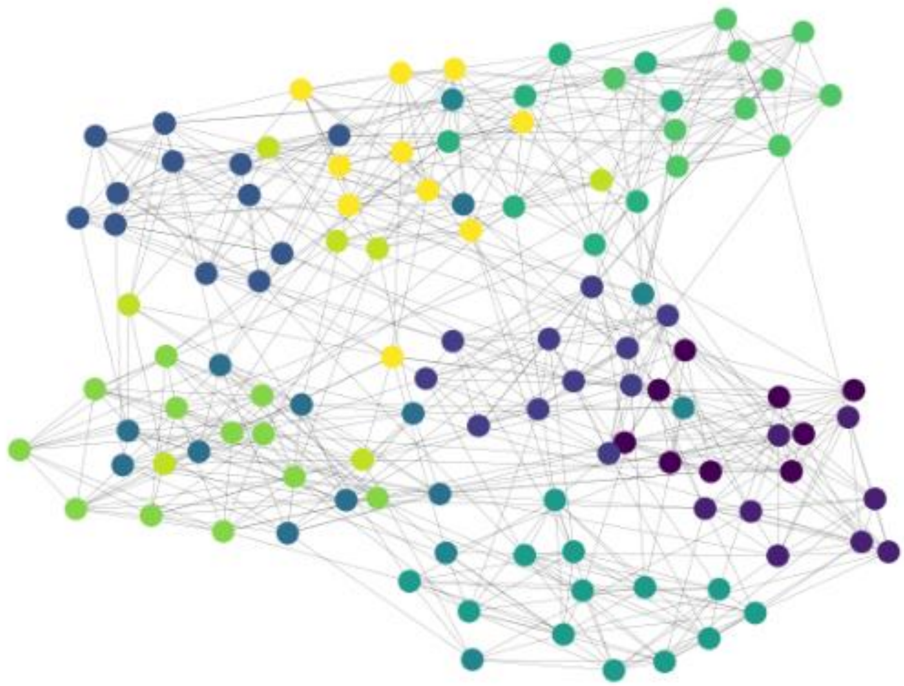
The American college football network contains the network of all Division IA college football games during the regular season in Fall 2000 with vertex property "Conference" indicating a team's respective conference and the edge weight indicating the number of games between teams.

The above approach is the same approach we have used to analyses the American football network dataset.

It has the following output

```
The file football.gml contains the network of American football games
between Division IA colleges during regular season Fall 2000, as compiled
by M. Girvan and M. Newman.  The nodes have values that indicate to which
conferences they belong.  The values are as follows:

   0 = Atlantic Coast
   1 = Big East
   2 = Big Ten
   3 = Big Twelve
   4 = Conference USA
   5 = Independents
   6 = Mid-American
   7 = Mountain West
   8 = Pacific Ten
   9 = Southeastern
  10 = Sun Belt
  11 = Western Athletic
```

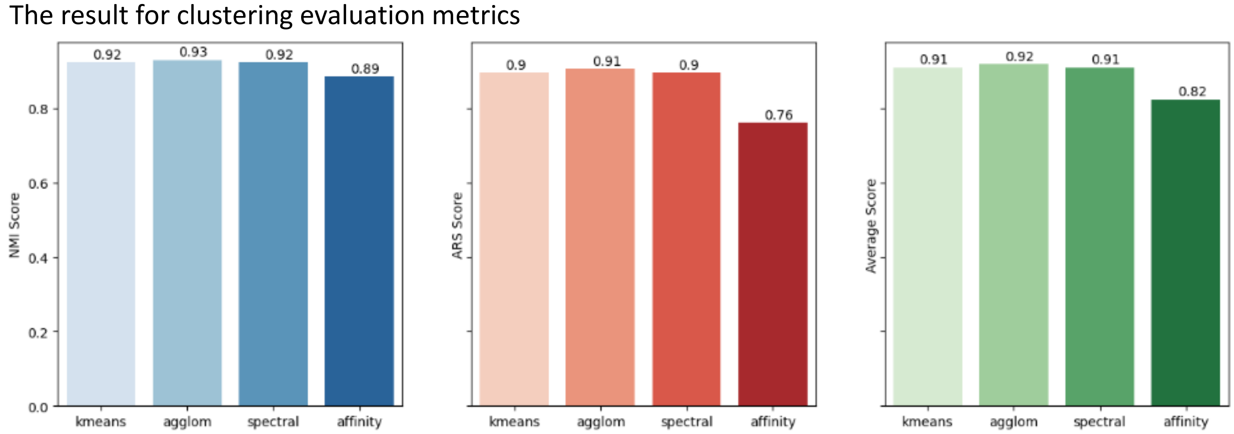
The network graph



We have hard coded the true values as they were not given in the dataset and got the following list of values

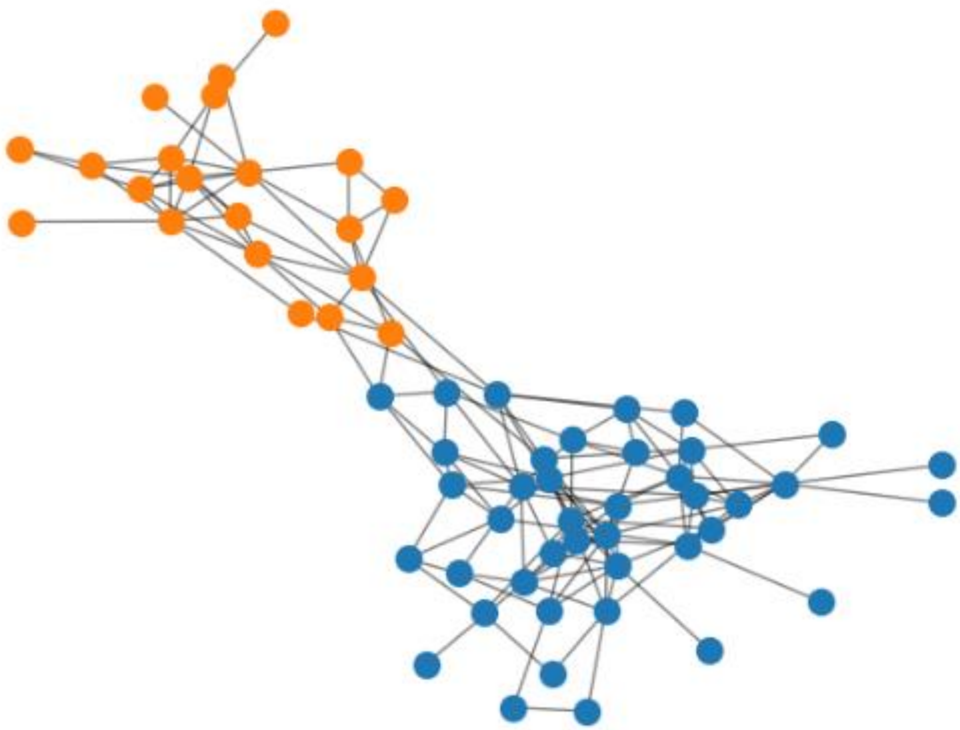
```
# True labels of the group each node ended up in.
y_true = [7, 0, 2, 3, 7, 3, 2, 8, 8, 7, 3, 10, 6, 2, 6, 2, 7, 9, 6, 1, 9, 8, 8, 7, 10, 0, 6, 9, 11, 1, 1, 6, 2, 0, 6, 1, 5, 0,
          6, 2, 3, 7, 5, 6, 4, 0, 11, 2, 4, 11, 10, 8, 3, 11, 6, 1, 9, 4, 11, 10, 2, 6, 9, 10, 2, 9, 4, 11, 8, 10, 9, 6, 3,
          11, 3, 4, 9, 8, 8, 1, 5, 3, 5, 11, 3, 6, 4, 9, 11, 0, 5, 4, 4, 7, 1, 9, 9, 10, 3, 6, 2, 1, 3, 0, 7, 0, 2, 3, 8, 0,
          4, 8, 4, 9, 11]
```

The result for clustering evaluation metrics



The Bottlenose Dolphins network dataset
A social network of bottlenose dolphins. The dataset contains a list of all of links, where a link represents frequent associations between dolphins.

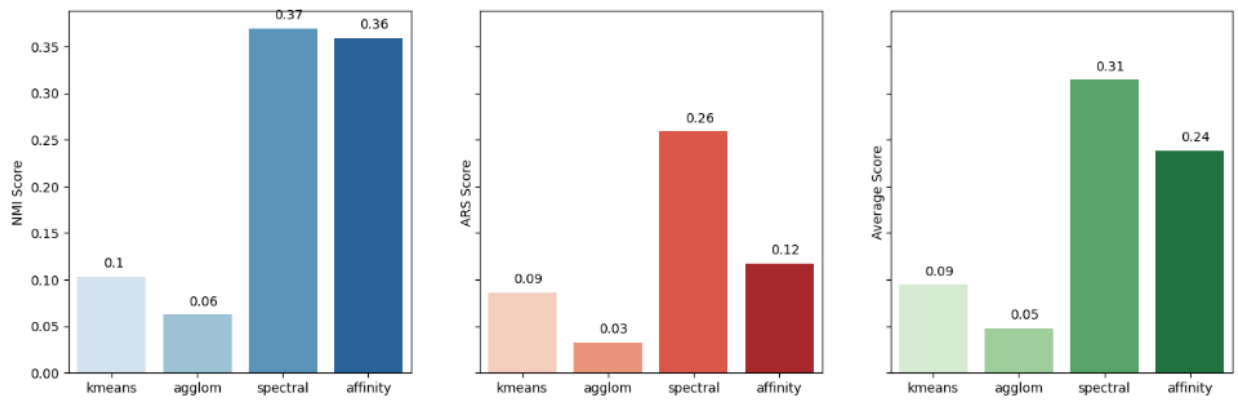
It have the following output
2 communities and it graph is:



True labels

```
# True labels of the group each node ended up in
y_true = [0, 1, 0, 4, 2, 1, 1, 1, 4, 1, 0, 2, 3, 1, 3, 2, 3, 1, 2, 1, 3,
          2, 1, 2, 2, 1, 1, 1, 0, 2, 0, 1, 1, 3, 3, 2, 4, 3, 3, 4, 3, 1,
          0, 3, 3, 2, 3, 0, 1, 3, 3, 2, 3, 3, 1, 2, 1, 1, 3, 4, 1, 3]
```

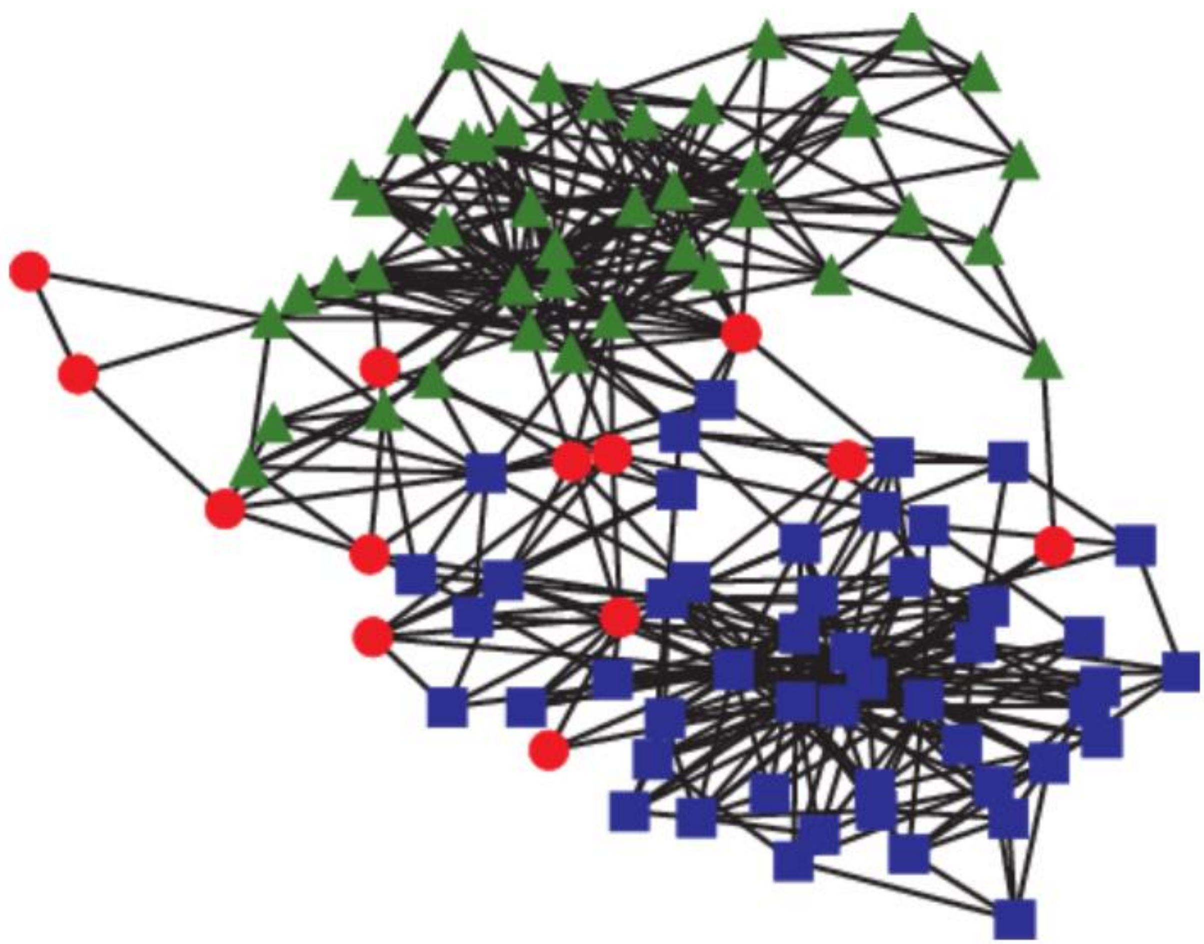
The result for clustering evaluation metrics

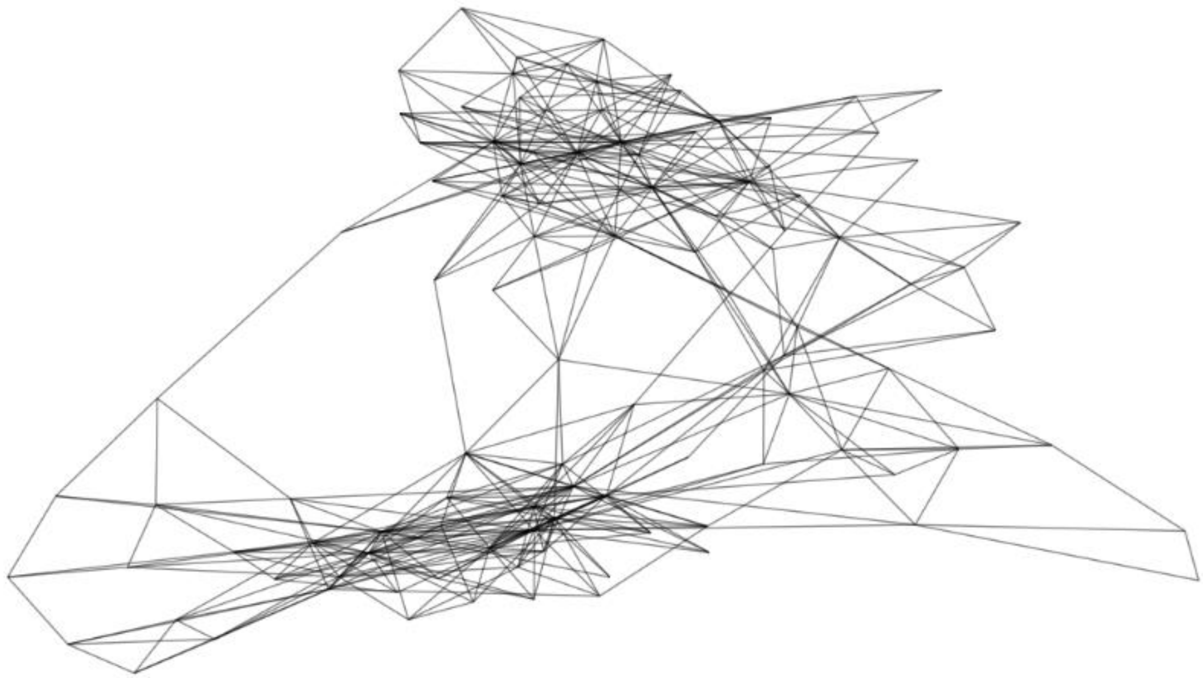


The Books about US politics networks dataset

Network of the books about US politics created by Krebs with 105 vertices, 441 edges, and 3 communities. This network represents the co-purchasing relationship of the books sold by the online bookseller Amazon.com. Each community in this network expresses the principles of each book .

The graph:

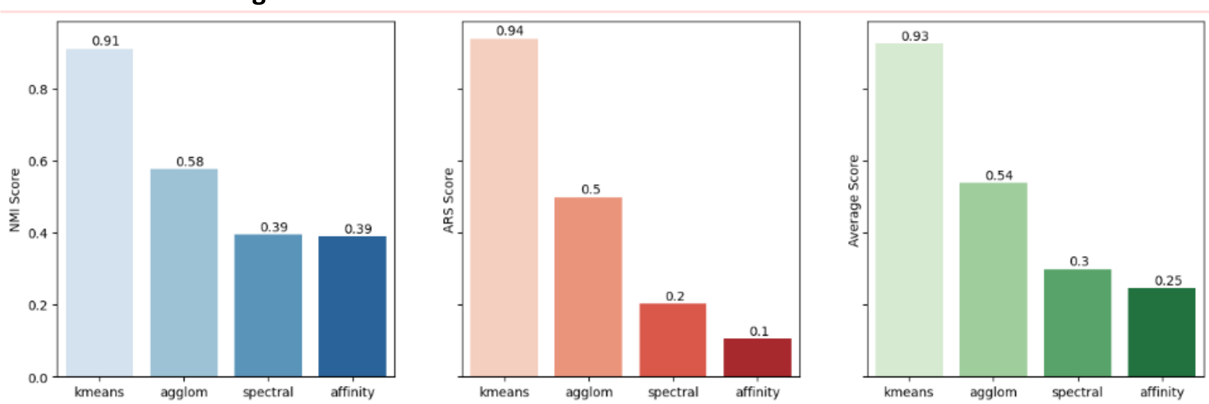




The true values

```
# True labels of the group each node ended up in.
y_true = [0, 0, 0, 1, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 0, 0, 1, 0,
          0, 1, 1, 1, 1, 1, 0, 1, 1, 0, 0, 2, 2, 1, 1, 0, 1, 1, 1,
          1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 1, 0, 0,
          0, 0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 2, 2, 2, 2, 2,
          2, 0, 0, 2, 0, 0, 2, 2, 2, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0,
          0, 0, 0, 0, 2, 2, 0, 0, 0, 0]
```

The result for clustering evaluation metrics

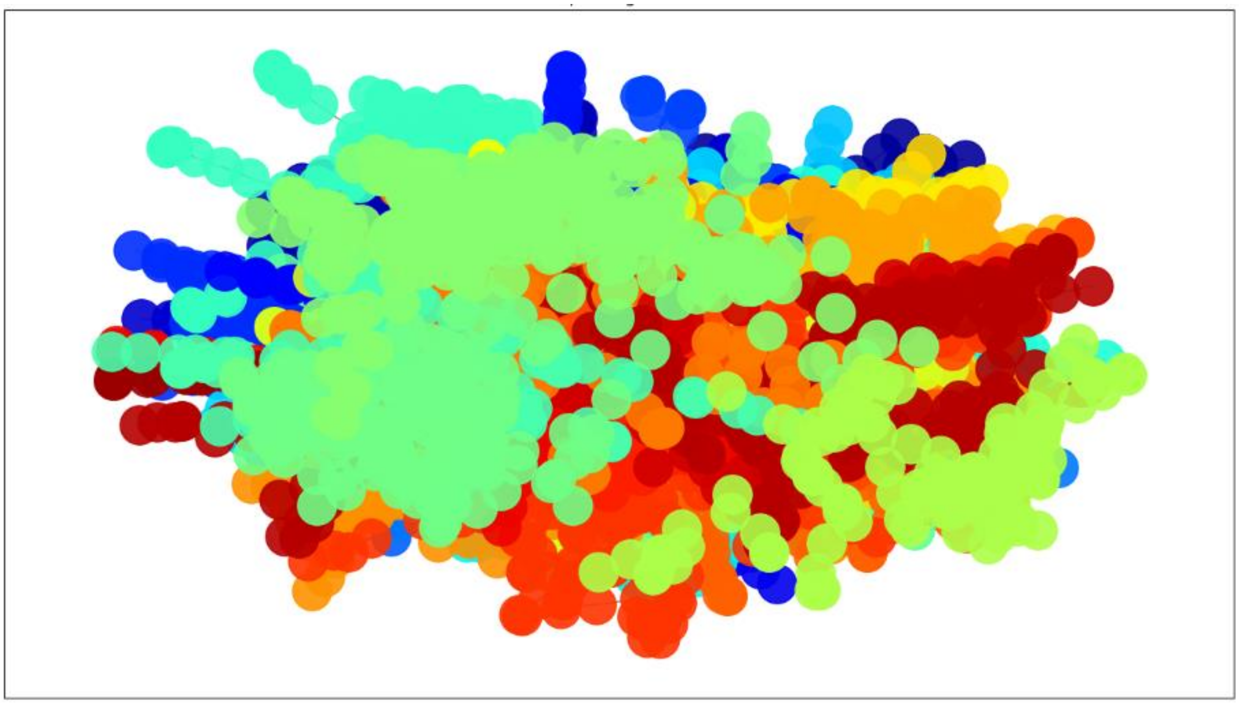


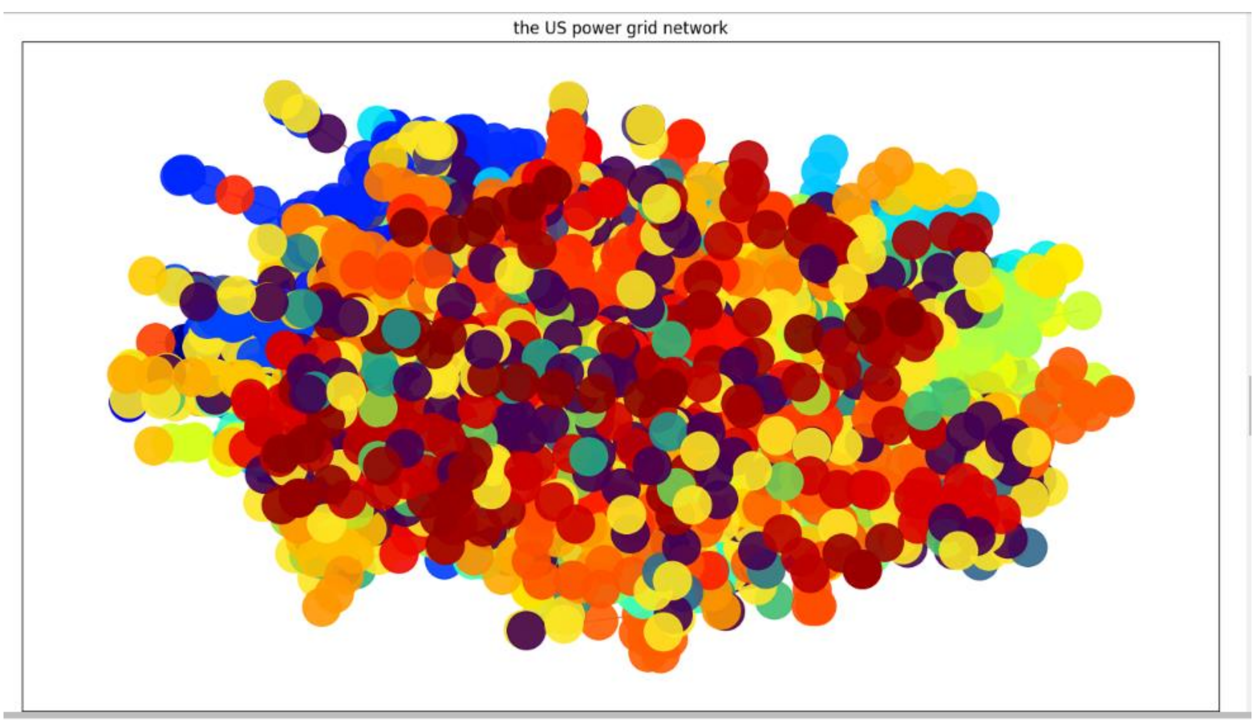
The US power grid network

This undirected network contains information about the power grid of the Western States of the United States of America. An edge represents a power supply line. A node is either a generator, a transformator or a substation.

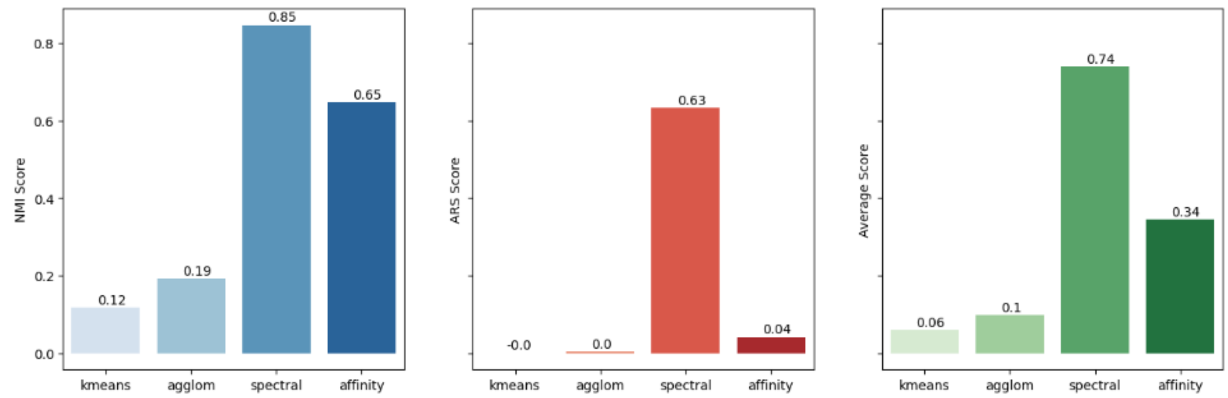
it has the following output

36 communities and its graph is





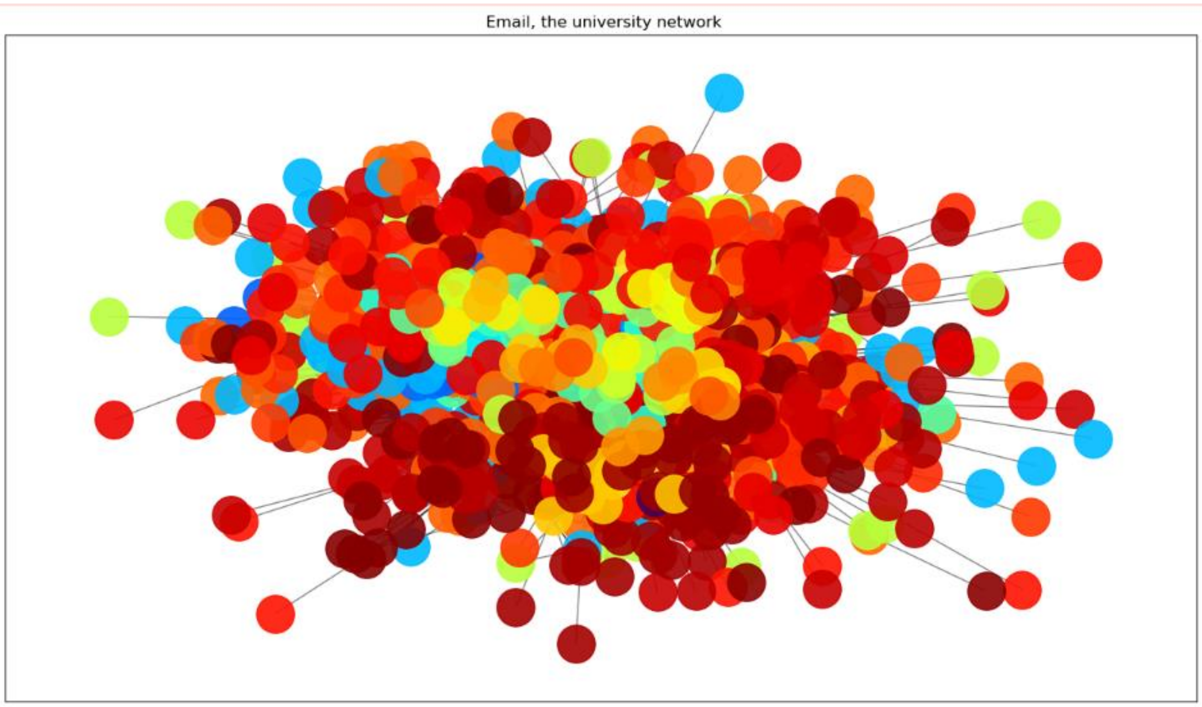
The result for clustering evaluation metrics



Email, the university network

This is the email communication network at the University Rovira i Virgili in Tarragona in the south of Catalonia in Spain. Nodes are users and each edge represents that at least one email was sent. The direction of emails and the number of emails between two persons are not stored.

It has 9 communities and its graph is



The result for clustering evaluation metrics