CSE 601 - Project 2: Clustering Algorithms

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K-means:

Algorithm Description:

- K-means is a clustering algorithm which partitions ‘n’ data points into ‘k’ clusters.
- The cluster for each data point is chosen in such a way that the data point is closer to the center of a cluster, than to the center of any other cluster. This center is called the centroid.
- The number of clusters or ‘k’ is usually specified.
- The initial centroids are also specified or can be random values.

Cluster Initialization

- The number of clusters or ‘k’ is predefined(input) so that the ‘n’ data points can be partitioned.
- The initial cluster centers or centroids are also defined(input) or can be random values.
- The function get_initial_clusters() generates random clusters if the clusters are not specified in the input.
- The number of iterations is also given as an input parameter.

Cluster Assignment

- Now, for each data point, we compute the euclidean distance from the data point to the different centroids.
- We assign the cluster whose centroid is closest to the data point.
- The function kmeans() computes this euclidean distance for all the data points from the cluster centers and also assigns the data points to the corresponding clusters. This function also calls new_centroids() to compute the new centroids until convergence.

Centroid Updation

- Once all the data points have been assigned to a particular cluster, we compute the mean of the data points from each cluster.
- This serves as the new centroid or cluster center.
- Now, we have to repeat Cluster assignment until the old and new centroids are the same. This is when we achieve convergence.
- The function new_centroids() computes the mean of the data points in a particular cluster and calls kmeans() if there is no convergence.

Result Visualization:

cho.txt

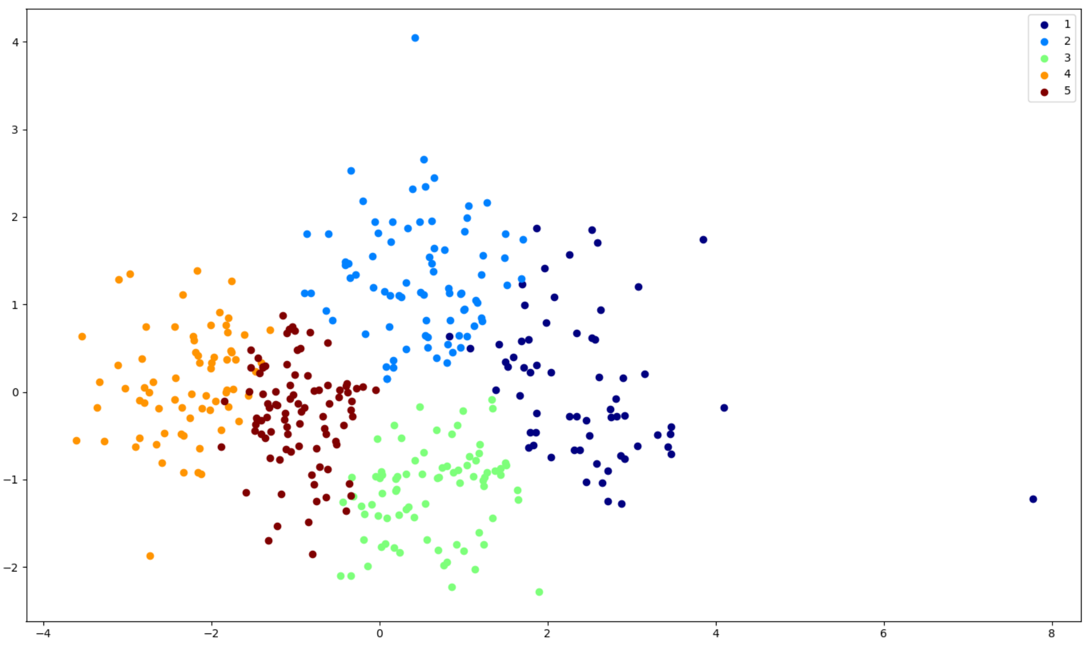
Number of clusters: 5

Maximum iterations: 20

Cluster Centers: [27, 362, 131, 66, 36]

Jaccard Value: 0.40784657011

Rand Index Value: 0.800236247953



iyer.txt

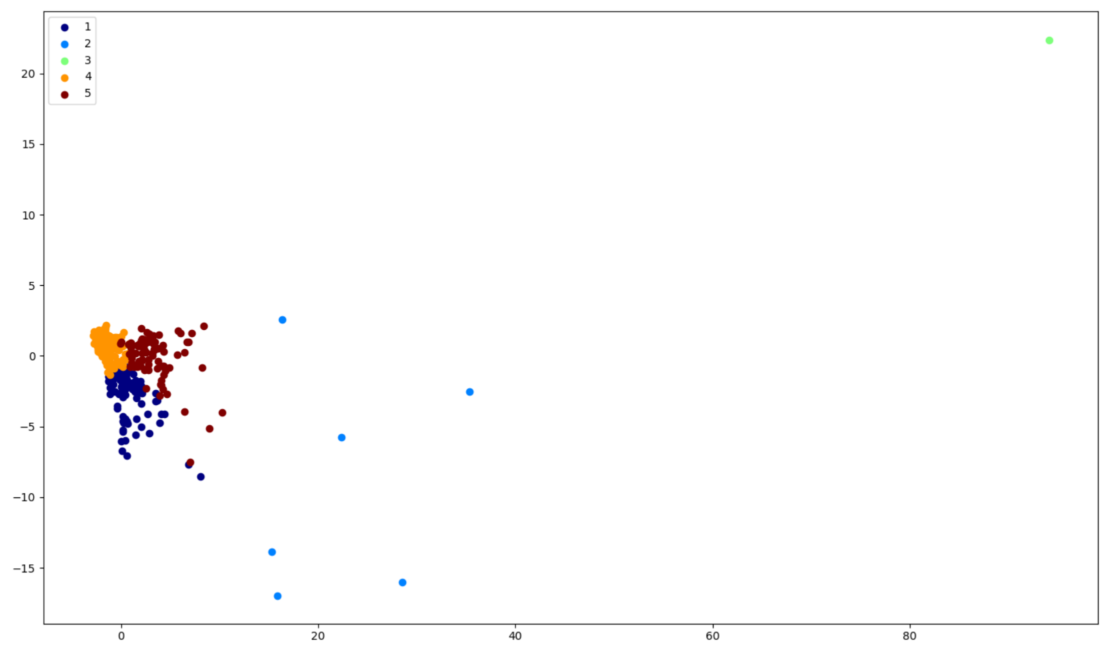
Number of clusters: 5

Maximum iterations: 20

Cluster Centers: [319, 498, 49, 166, 362]

Jaccard Value: 0.276806304995

Rand Index Value: 0.637471051933



Result Evaluation:

Advantages:

- Easy to implement
- Guarantees convergence
- Scales well to large datasets as well

Disadvantages:

- Need to specify the number of clusters(k)
- Empty clusters may appear
- Kmeans does not work well with differing sizes, densities and irregular shapes

Hierarchical Agglomerative clustering with Min approach:

- In the Agglomerative approach, we start from the bottom where the objects are merged at each step and propagated upwards as clusters.
- The algorithm begins with each individual object and merges the two closest objects. The distance between two clusters is calculated using the Euclidean distance.
- The process is iterated until all objects are aggregated into a single group.

Algorithm Description:

1. Convert the features of the object into a distance matrix.
2. Set each object as a cluster.

3. Iterate until the number of clusters become one.
4. Merge two closest clusters.
5. Update the distance matrix then go to step 3.

Implementation:

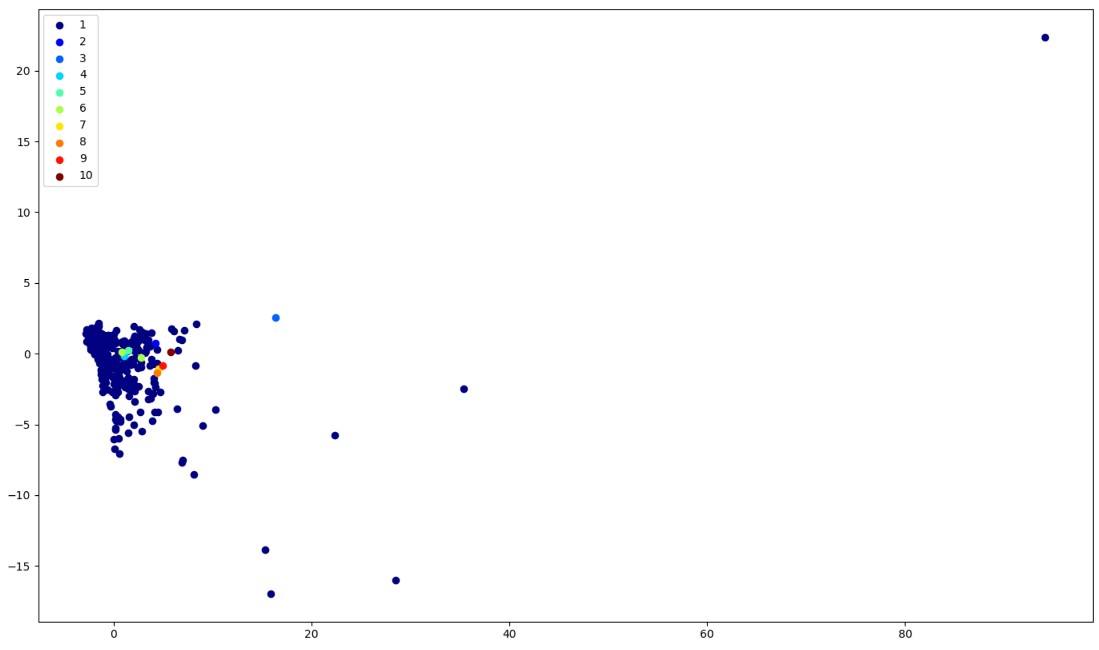
1. The first step involves feeding the dataset to getDistMatrix() function which calculates the distance matrix required for hierarchical clustering.
2. Initially the Distance matrix will be of size n*n where n denotes the total number of objects in the dataset.
3. Then at each iteration till we reach the number of clusters desired we run the algorithm merging two of the closest clusters at each iteration and then updating the Distance matrix accordingly.
4. Calculate the Jaccard and Rand Coefficients to identify the performance of the algorithm using the predicted and ground-truth values

Result Visualization:

iyer.txt:

Rand Index: 0.1882868355974245

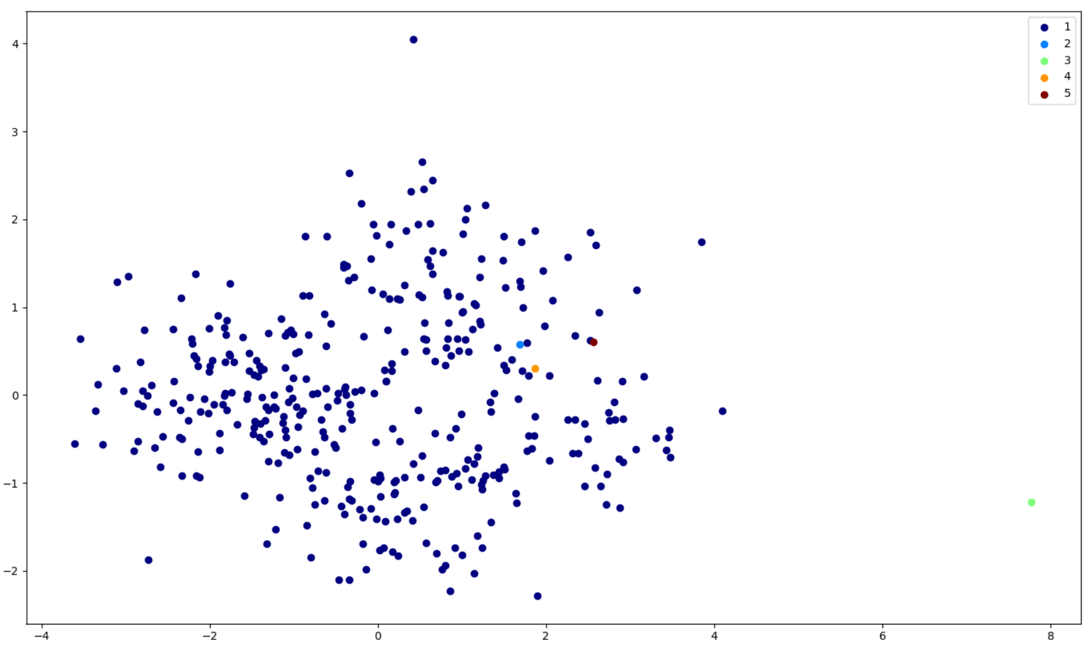
Jaccard index is: 0.15824309696642858



cho.txt:

Rand: 0.24027490670890495

Jaccard: 0.22839497757358454



Result Evaluation:

- Its space Complexity is O(N^2) since we are using a distance matrix. Its time complexity is O(N^3) in most cases since we need delete certain rows and columns for N iterations and we search the matrix for the minimum distance which takes O(N^2). It can be optimized to O(N^2LogN) for some cases.

- From the results observed performance seems to be poor when compared to other algorithms such as K-means or GMM since there is no objective function that is minimized.

Advantages:

- Can handle non-elliptical shapes
- Any number of desired clusters can be obtained

Disadvantages:

- No objective function to directly minimize
- Once a cluster is formed it cannot be undone
- Sensitive to noise and outliers

DBSCAN:

- Density Based Spacial Clustering of Applications with Noise or DBSCAN is a clustering algorithm that seperates data points based on the density of the region they belong to.
- Clusters are defined as dense regions in the data space, separated from regions of lower density.
- The size of the region is defined by the ε-Neighborhood which gives the region within a radius of ε from a data point.
- Before jumping into the algorithm, some of the key concepts are described below:

- **Core point** - A point is a core point if it has more than a specified number of points (MinPts) within Eps —These are points that are at the interior of a cluster.
- **Border point** - A border point has fewer than MinPts within Eps, but is in the neighborhood of a core point.
- **Noise point** - A noise point is any point that is not a core point nor a border point.
- **Directly density-reachable** - An object q is directly density-reachable from object p if p is a core object and q is in p’s ε-neighborhood.

Algorithm:

For each point in the dataset that is not yet classified do the following steps:

- Check if the point is a core point or not.
- If the point is not a core point label it as a noise point
- If the point is indeed a core point, collect all the points that are density reachable from the current point and label them as a new cluster
- Repeat the above steps until all the points are visited and labeled into a cluser or as noise.

Implementation:

1. The parameters ε and MinPts are specified when running the program. We choose a small epsilon value typically between 0.5 to 1.5 and MinPts value as 3 for optimal results.

2. Using the 'regionQuery' function find the neighbors of the point using ε and MinPts and euclidean distance, for each unvisited point in the matrix.

3. If the number of neighbors is more than the minimum number of points, classify the point to the corresponding cluster id.

4. If the number of neighbors is less than the minimum number of points, classify the label of that point to be -1.

5. The 'expandCluster' function is used to assign every unvisited point in the neighborhood of point to the same cluster id. The point's neighbors are calculated by 'regionQuery' and then added on to the existing neighboring points.

Result Visualization:

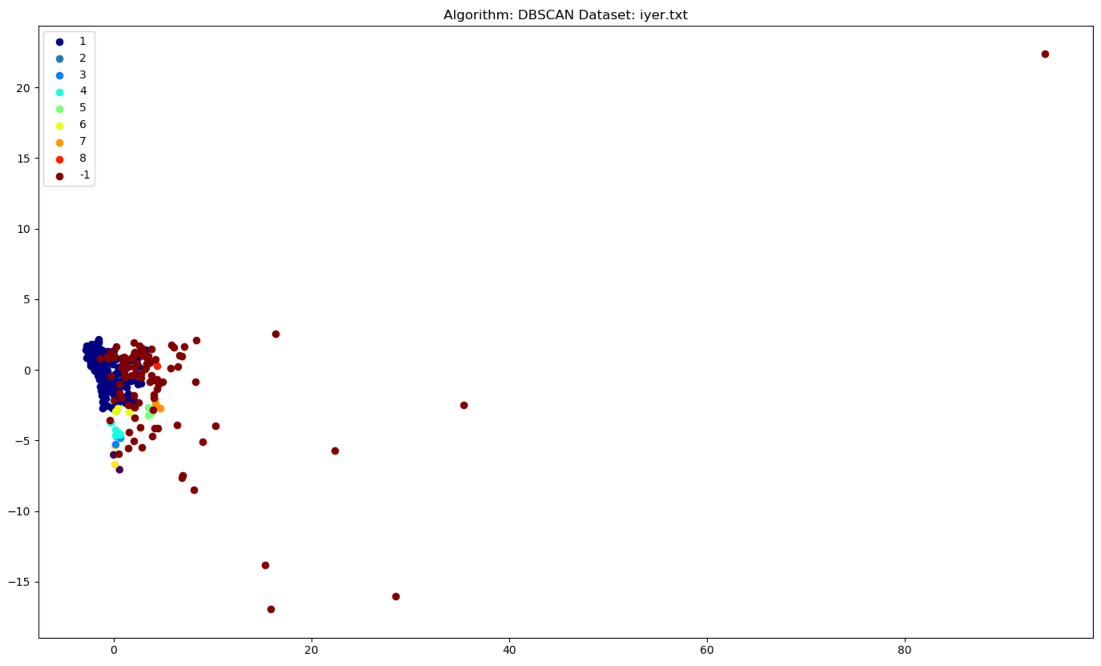
iyer.txt:

Epsilon: 1.3

MinPts: 3

Rand index: 0.6526755683922646

Jaccard index: 0.2835567491646023



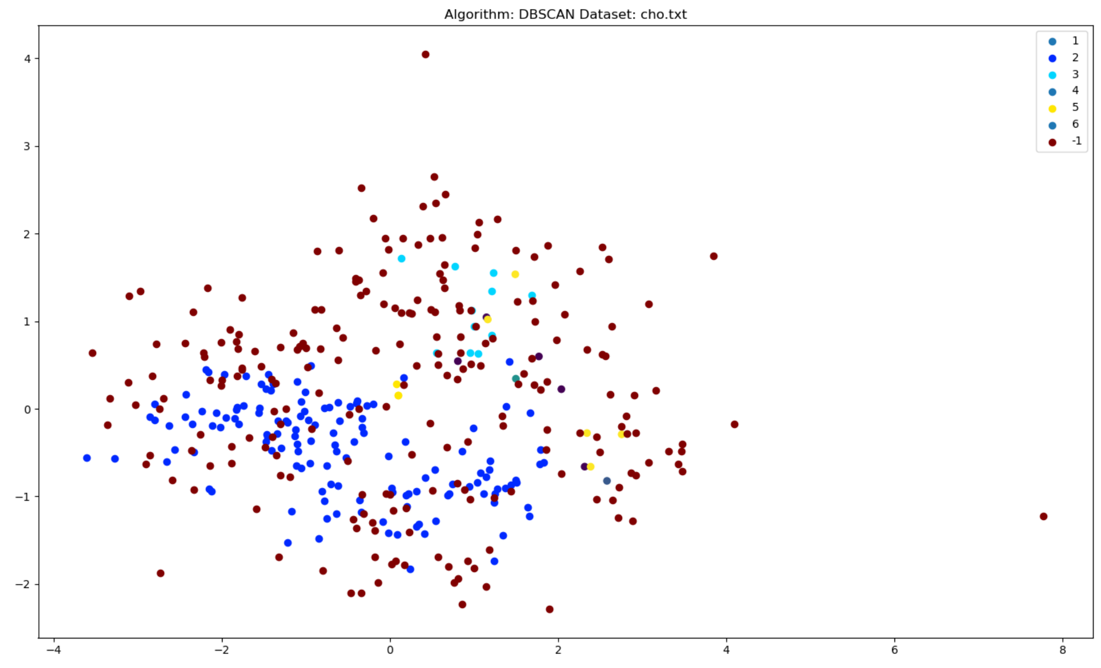
cho.txt:

Epsilon: 1

MinPts: 3

Rand index: 0.5664715831297484

Jaccard index: 0.2037425112793077



Result Evaluation:

- The time complexity of this algorithm is O(n^2), so it is reasonably fast when compared to algorithms like HAC and Spectral Clustering.
- If dataset is too large small clusters are likely to be labeled as noise
- If dataset is too small, even a small number of closely spaced that are noise or outliers will be incorrectly labeled as clusters.
- DBSCAN performs exceptionally well on datasets having well seperated dense regions of arbitrary shapes and sizes as demonstrated by the high jaccard value for the demo dataset while it performed poorly with iyer and cho datasets as a fixed epsilon value cannot account for the sparseness and disparity in distribution of the former two datasets.

Advantages:

- DBSCAN can find arbitrarily sized and shaped clusters.
- We don’t need to specify the number of clusters, as opposed to k-means.
- DBSCAN is resistant to outliers, as opposed to k-means.

Disadvantages:

- DBSCAN cannot perform well with data spread across varying densities since ε and MinPts are provided as constants for the entire dataset.
- DBSCAN is not completely deterministic. Depending on the order of processing the data, border points reachable from more than one cluster can be part of different clusters across multiple runs of the same algorithm.

Guassian Mixture Model:

- A mixture model is an probabilistic unsupervised model for clustering applications.
- In a Guassian Mixture model we use multiple Probability Density Functions to model the data into clusters.
- Unlike other clustering algorithms which do hard clustering where every point belongs to exactly one cluster, GMM performs soft clustering where every point belongs to several clusters with certain degrees.
- We use Expectation Maximization framework to train the model using GMM.

Implementation:

1. While running the program we specify number of clusters which is a required parameter and optional parameters like the initial mean, covariance, pi, convergenece threshold, maximum iterations and smoothing value as input to the program.

2. **Expectation:** For the given parameter values we predict the values of the latent variables. We use sklearn's multivariate_normal.logpdf function to calculate the probability distribution function to be multiplied with the probability parameter pi to obtain a prediction for each cluster. Below code snippet shows the impementation:

```
    for j in range(N):
        for k in range(self.num_clusters):
            pdf = multivariate_normal.pdf(
                self.X[j], mean=mu[:, k], cov=sigma[k])
            self.predicted[j, k] = pi[k] * pdf
        self.predicted[j] /= np.sum(self.predicted[j])
```

3. **Maximization:** The objective is to maximize the log likelihood function. We use the smoothing value to avoid singular matrix errors and use the multivariate_normal.logpdf function available in sklearn package to determine the log likelihood value. We then update the mean and covariance with the newly obtained values. Below snippet shows the steps involved in maximization:

```
def log_likelihood(self, mu, sigma, pi):
   ...
    for n in range(N):
        for k in range(self.num_clusters):
            np.fill_diagonal(
                sigma[k], sigma[k].diagonal()+self.smoothing_value)
            loss += self.predicted[n, k]*math.log(pi[k])
            loss += self.predicted[n, k] * \
                multivariate_normal.logpdf(
                    self.X[n], mean=mu[:, k], cov=sigma[k])
    return loss
...
curr_likelihood = self.log_likelihood(mu, sigma, pi)

pred_sum = np.sum(self.predicted, axis=0)
pi = pred_sum / N
mu = np.dot(self.X.T, self.predicted) / pred_sum
sigma = np.zeros((self.num_clusters, M, M))
...
```

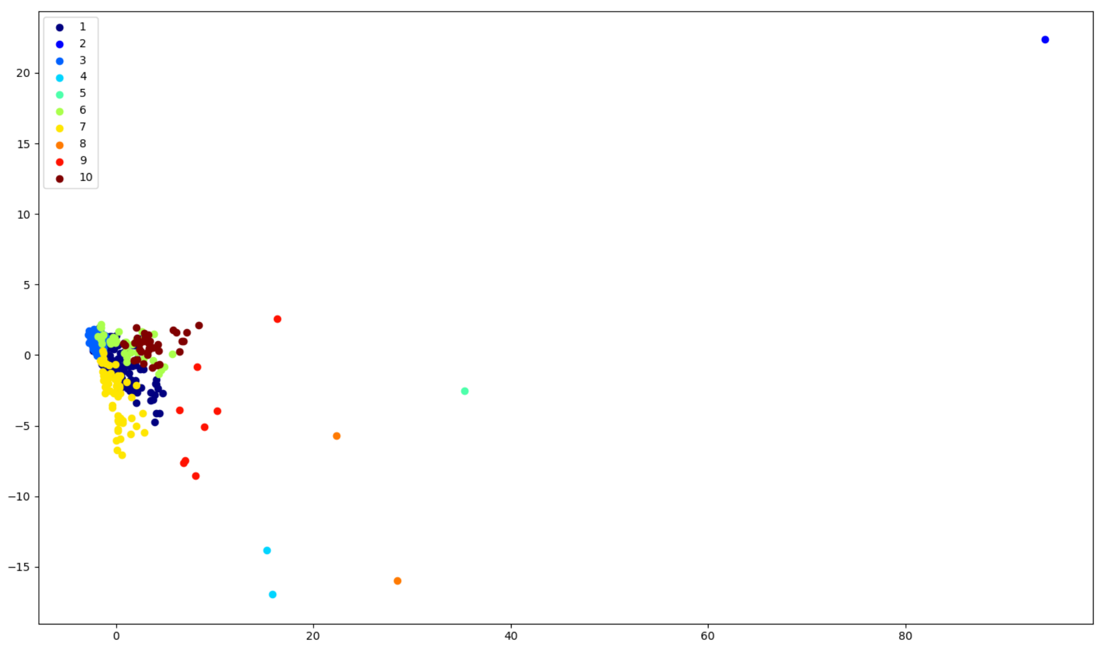
Result Visualization:

iyer.txt

Mean, covariance: Initialized using labels from K-means Number of clusters: 10 Smoothing threshold: $5*10^{-8}$

Rand index: 0.7618083796938894

Jaccard index: 0.3529943801384132

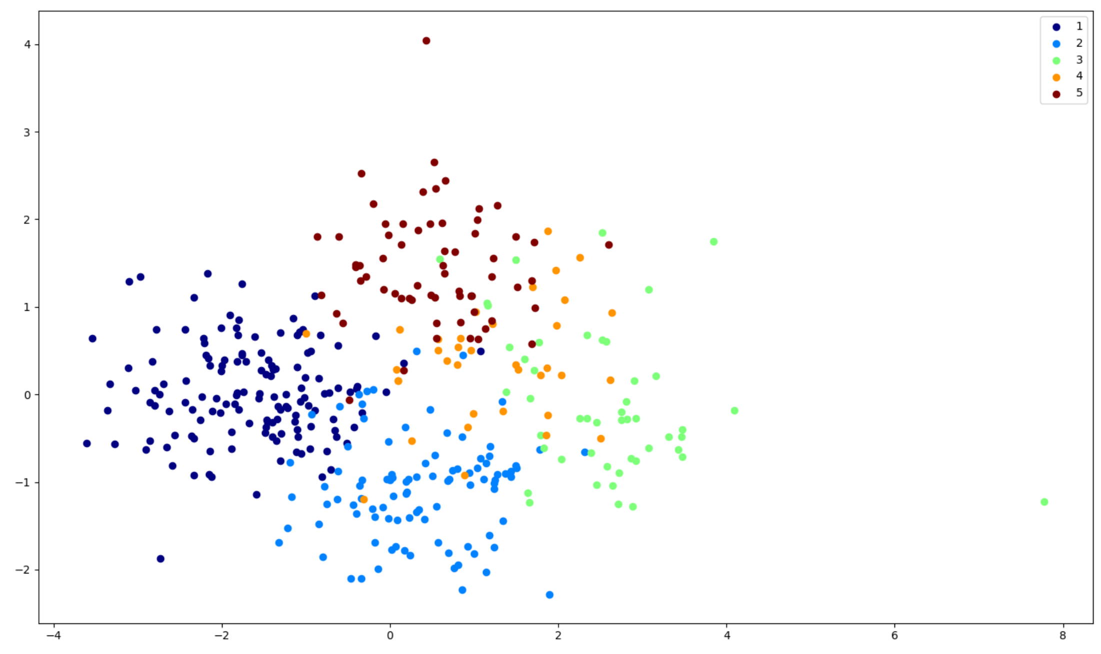


cho.txt

Mean, covariance: Initialized using labels from K-means Number of clusters: 5 Smoothing threshold: 10^{-15}

Rand index: 0.7959005610888883

Jaccard index: 0.4018254061922184



Result Evaluation:

- GMM has provided more accurate results than density based given that it is initialized by K-means and the fact that it uses probabilistic assignments instead of hard assignments based on near neighbor density.
- Though density based clustering is not accurate for sparsely seperated cho dataset and disparity in distribution of points in iyer dataset, GMM is able to provide more accuracy leveraging multiple Guassians and probabilistic assignments.

Advantages:

- GMM can handle clusters with varying sizes and variance
- GMM gives probabilistic cluster assignments so that soft clustering can be performed for more accurate decision making. In contrast, density based clustering can wrongly assign border points.

Disadvantages:

- Initialization is crucial for generating accurate clusters using GMM. Other clustering algorithms like K-means are used to initialize the mean and covariance before running GMM.
- GMM has overfitting problems where the algorithm tries to fit the data points perfectly and ends up performing poorly on new data.

Spectral Clustering:

- Spectral clustering is a clustering technique which makes use of the Eigenvalues of the similarity matrix of the given dataset to perform dimensionality reduction before clustering into fewer dimensions.
- Spectral clustering treats clustering as a graph partitioning problem without making any assumptions about the clusters, unlike K-means.

Algorithm Description:

1. Construct the similarity matrix (W) which represents the graph where the weights of the edges are given by the gaussian kernel.
2. Then construct the degree matrix (D) which is the same size as that of the similarity matrix, except that it is a diagonal matrix where each entry in the diagonal corresponds to the sum of the values of that particular row in the similarity matrix.
3. Build the Laplacian matrix given by L = W - D
4. Find the eigen vectors and eigen values for L.
5. Find the k minimum eigen values and their corresponding eigen vectors.
6. Use the minimum eigen vectors to build the n*k reduced space data where n is the total number of objects.
7. Run K-means on the reduced space data to obtain the clusters.

Implementation:

1. Construct the similarity matrix from getSimilarityMatrix() function by passing the dataset along with sigma value.
2. Using the similarity matrix construct the degree matrix and compute the laplacian matrix using getLaplacianMatrix() function.

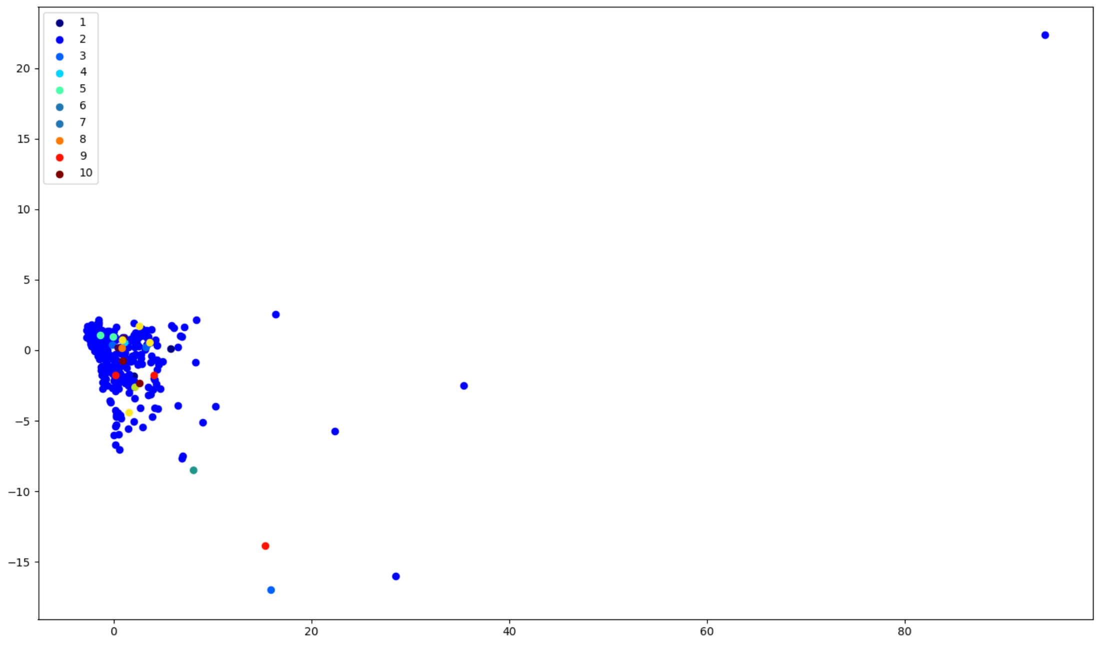
3. Find the eigen vectors and eigen values using linalg.eig() funtion from numpy.
4. Find the minimum eigen vectors and eigen values by constructing a dictionary and sorting the dictionary keys based on the key which is the eigen value.
5. Construct the reduced space n*k space data and run Kmeans using kmeans() funtion by passing the initial centroids and the number of clusters.
6. Find the predicted clusters and find the Jaccard and Rand coefficients using predicted and ground-truth values.

Result Visualization:

iyer.txt:

Jaccard index: 0.16369894314733768

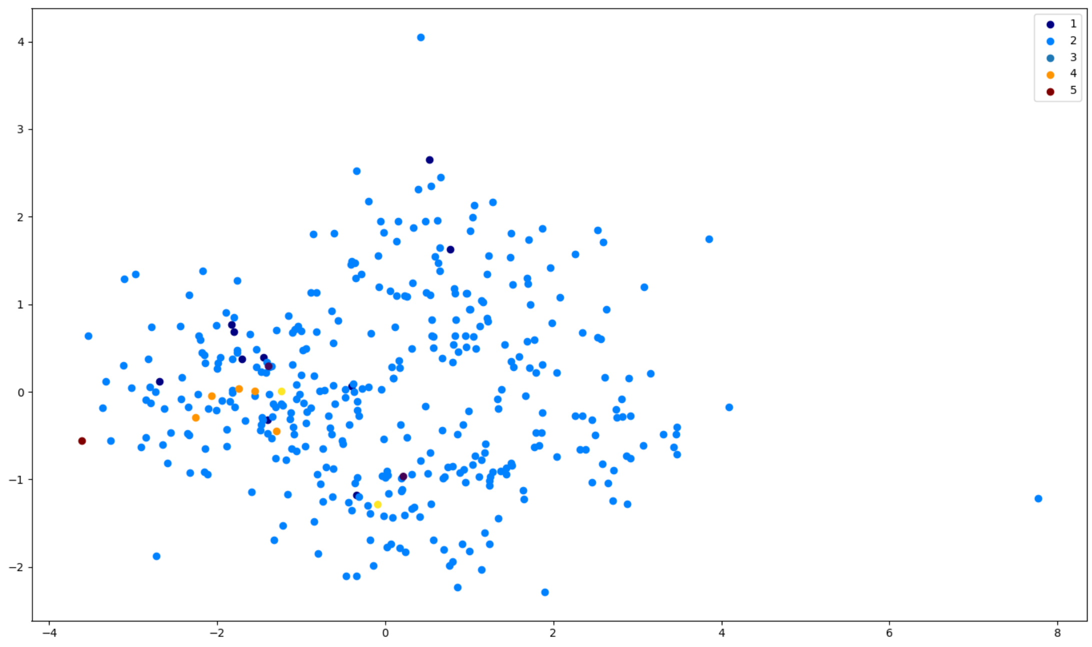
Rand index: 0.24003606583136605



cho.txt:

Jaccard: 0.21558520315342633

Rand index: 0.27075894654890065



Result Evaluation:

Spectral clustering generally performs well with datasets with outliers that cannot be easily determined by algorithms like K-means. In case of these datasets, algorithms like K-means performed well and the upside of using Spectral clustering cannot be seen here. In fact, in this case, spectral clustering performed worse than most of the other clustering algorithms.

Advantages:

1. Spectral clustering does not make any strong assumptions about the shape and size of the clusters unlike K-means.
2. Relatively easy to implement and reasonably fast for sparse datasets.

Disadvantages:

1. Since we use K-means to compute the clusters after dimensionality reduction, the cluster assignment is not always deterministic. Depends on the choice of centroids.
2. Computationally expensive since we've to calculate the Eigenvalues and Eigenvectors. Doing this for a very large dataset would increase the overall time complexity.