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OPTIMAL NUMBER OF CLUSTERS

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ABSTRACT

Clustering is an important analysis methods in Data Analytics and Pattern Recognition. The process divides the data into groups without any supervision or external labels and it is a subjective analysis as the definition of a cluster is context dependent. Because of this reason many algorithms, like k-nearest neighbors, require the number of clusters to be fixed a priori. Each clustering algorithm depends on a distance metric to identify different groups in the data. Once the number of centers are fixed, each algorithm tries to find the best separation according of its distance measure by using an optimization algorithm. The distance metric determines the shape of the clusters generated. There are algorithms, like Ward, to determine how many clusters we have in a data set and these algorithms also depend on the same distance metrics where many metrics, like Euclidean and its derivatives, generate hyper ellipsoidal clusters and fail in nonlinearly clustered data. Another computationally expensive approach is to run a specific algorithm for different number of cluster centers and try to choose the best number. In this paper, we attempt to analyze the number of clusters using a previously developed Information Theoretical metric called CEF which; in its original use; can separate nonlinear clusters. Data points that are more similar to each other are incrementally joined together using a distance measure to create subclusters like joined data points against the rest of the data. The operation continues until all data elements are consumed. The CEF metric is used to measure the distance between obtained clusters where peaks in the measure indicates strong cluster separation. The method is tested in several artificial and real data sets and its advantages and disadvantages are discussed.

Keywords: Clustering, Distance Metric, Information Theory

1. INTRODUCTION

In pattern classification there are several unsupervised and supervised methods to analyze the data. One of the unsupervised methods is clustering where the input data is divided into dissimilar groups. The partitions are created such that points in one partition are closer to other points compared to any other group. The aim can be described as to find natural groups in the dataset [1-5]. The idea is used in many fields like image processing [7], computer security [8], biology [4], pattern recognition [3] and psychology [6].

In many clustering algorithms the expected number of cluster groups should be given as a parameter to the algorithm as the method cannot calculate the number of natural clusters in the dataset. If the estimation is less than the natural clusters, in this case the analysis may combine several clusters and will miss important structures in the data. On the other hand supplying a large number will end up having clusters without any relevant structure. To overcome this difficulty, it is possible to obtain results using different parameters and try to measure the compactness or quality of the obtained clusters. The process is called cluster validation [1].

The process is as follows. The number of cluster parameter is divided into N values and the resulted clusters are obtained for each value. Only one result may describe correctly the naturally occurring clusters in the dataset. Each result should be validated using a criteria.

Clusters can be validated using different methods. The methods mostly based on external, internal or relative criteria. Compactness of each cluster is one criteria. On the other hand how well the clusters are separated is another criteria that can be used [10-13]. It is also possible to use information theory or entropy in that sense. One approach is to have the proportion of objects in the group [14, 20, 21]. Yu and Cheng [15] study in their paper an optimal number using FCM clustering. Cluster validation indices can be used with other methods together like fuzzy C-means algorithms [16-18]. Chen et al. [19] work depends on a hierarchical calculation using two different passes.

Typically the steps to check cluster validity can be given as follows. The clustering algorithms are executed using different parameters. One of the parameters is the number of clusters. When the validity index fits in certain limits, the optimal clusters are obtained.

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2. INFORMATION THEORY AND CLUSTERING

Clustering is an unsupervised method to separate data into groups by using a certain metric or distance function so that that the groups or clusters are arranged closer within, compared to other grouping choices. Similar to edge detection, clustering is also a subjective division depending on the distance measure. Some distance measures can only divide the data using a linear boundary where others can perform a nonlinear separation. Even the human eye will cluster the same data differently depending on other conditions and context.

Information theory has been used as a distance measure successfully in one of the author's previous paper [5]. Using an information theoretic measure, nonlinear regions can be separated without any supervision. The derivation of the distance measure or CEF (Cluster Evaluation Function) was given elsewhere [5] and it will not be repeated here. Only the final formulation will be used. In (1), p and q are clusters of size Np and Nq, respectively where xi ∈ p and xj ∈ q. The Gaussian kernel needs a parameter σ for the kernel size. The proper value of this parameter is important in clustering which needs to be determined.

$$CEF(p,q,\sigma) = \frac{1}{N_p N_q}\sum_{i=1}^{N_p}\sum_{j=1}^{N_q} G\left(x_i - x_j, 2\sigma^2\right) \qquad (1)$$

A feature vector needs to be extracted from the data to be clustered. The feature set can be any original and/or transformed subset of the data which provides a good description of data. Using the feature set as an input to the distance measure, each cluster is labeled such that the distance between clusters is maximum. Searching the optimal labeling may need an exhaustive search and some heuristic algorithms are applied to limit the search space. As explained in [5], the final result is very promising and a nonlinear separation of clusters is possible with this method without any supervision as shown in Fig 1. It should be noted that the distance measured by CEF is inversely proportional to the distance between clusters.

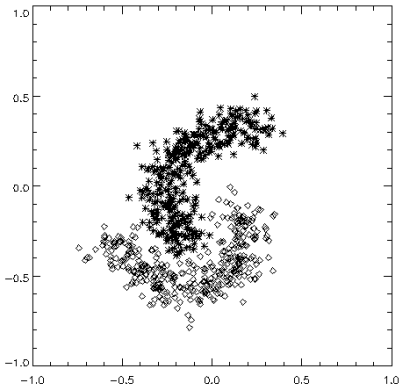

Figure 1: Dataset labels after an unsupervised clustering using CEF function [5]

3. PROPOSED CLUSTER SEPARATION INDEX

In this section, the proposed information theoretic cluster separation method is presented. The motivation of the proposed method is to process the data once and obtain information about possible cluster groups in the data. The distance function (CEF), described earlier, will be used in the calculation.

3.1. Subclusters and Grouping

The calculations start by forming two cluster sets, i.e. p and q. One cluster is formed initially by finding two closest point to each other in the dataset using a Euclidean distance measure. Since we are not measuring any cluster separation during this procedure, any distance metric can be used. The second cluster is formed by the rest of the data except the ones in the first cluster. At any time, the points belong either to the first cluster or to the second cluster. After the initialization of two clusters, the procedure continues by finding the closest point x in cluster q to any point in cluster p one at a time as shown in Fig. 2. The points x1 and x2 are the closest two points in the set. The first group is formed by putting these points together as cluster p. The rest of the data belongs to cluster q. During the next step, the closest point is found in cluster q to any member of cluster p. The point x3 is the closest point to the group formed by x1 and x2. The next stage is to move the point x3 from cluster q to the group (i.e. to cluster p). The cluster p grows one at a time by finding the closest point in cluster q.

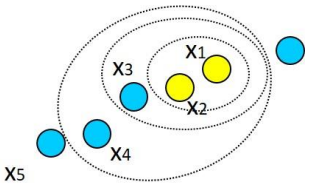

Figure 2: Group forming by finding the closest point to any group members

3.2. Cluster separation

During the iteration, cluster p will increase and cluster q will decrease one point at a time. After a new point is removed from cluster q and added to cluster p, the distance between these two clusters are measured using CEF distance function. One instance is shown in Fig. 3.

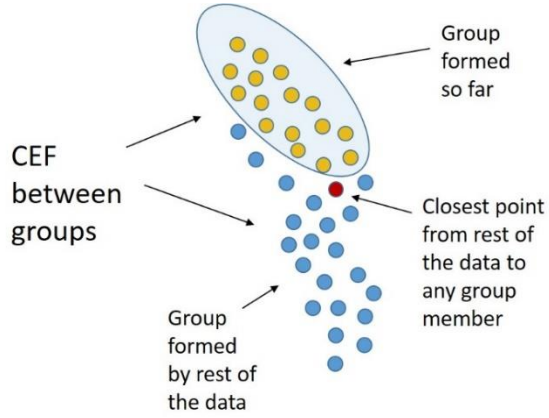

Figure 3: Two cluster groups are formed and CEF between these groups is calculated

Once each point is processed, the array obtained by calculating CEF distance between clusters at every step is analyzed to determine the possible clusters in the dataset. Low peaks in the plot indicate a strong indication of cluster separation. The algorithm is given in Fig. 4.

Number_of_Clusters Algorithm

INPUT:dataset
OUTPUT:CEFarray

1. $Cluster_p$ = []
2. $Cluster_q$ = [dataset]
3. [x1,x2] = find_closest_2_points(dataset)
4. $Cluster_p$ = $Cluster_p$ + [x1,x2]
5. $Cluster_q$ = $Cluster_q$ – [x1,x2]
6. CEFarray = size(dataset)
7. CEFarr(1) = = CEF ($Cluster_p$, $Cluster_q$)
8. for n=2 to size(dataset)
9. x = find_closest_point($Cluster_p$, $Cluster_q$)
10. $Cluster_p$ = $Cluster_p$ + x
11. $Cluster_q$ = $Cluster_q$ – x
12. CEFarray(n) = CEF ($Cluster_p$, $Cluster_q$)
13. endfor
14. plot CEFarray
15. find peaks(CEFarray)

Figure 4: Number of Clusters Algorithm

4. EXPERIMENTAL RESULTS

The algorithm is tested using several artificial and real datasets and the results are discussed.

4.1. Artificial datasets

An example dataset is shown in Fig. 5.

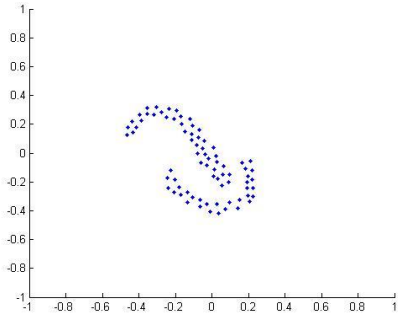

Figure 5: 2-dimensional dataset with 2 main clusters

The plot of CEF distance function is shown in Fig. 6. The horizontal axis consists of all points in the dataset and vertical axis is the $\log(CEF)$ value between clusters formed at every step during the iteration. The logarithm is displayed to enhance the small values in the calculation.

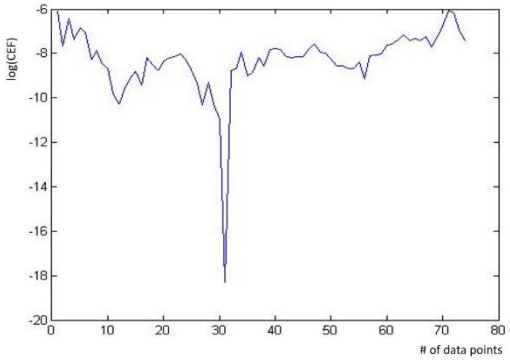

Figure 6: $\mathbf{log}(\boldsymbol{CEF})$ plot of the dataset

The plot indicates a very strong low value at point 31 which indicates that the data has 2 main clusters in it. The other less small peaks indicate other sub clusters and the importance of these clusters is context dependent. The cluster p and cluster q at point 31 is shown in Fig. 7.

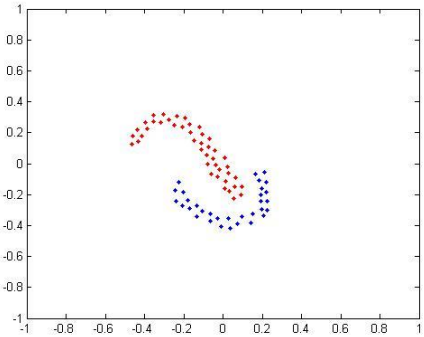

Figure 7: Cluster separation at lowest peak of CEF plot

When a different distance metric is used, the separation point is wrong unlike the point in CEF calculation. When we use a Euclidean distance the plot is given in Fig 8.

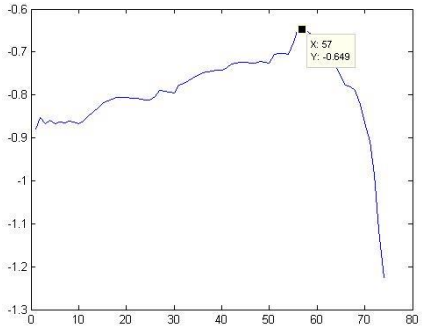

Figure 8: Euclidean Distance plot

The results for other artificial datasets are shown in Fig. 9. to Fig. 12.

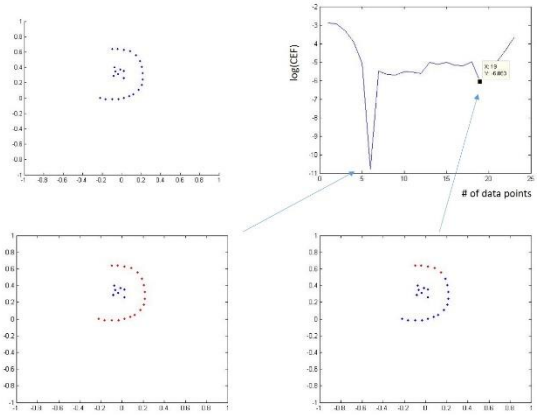

Figure 9: Results using a dataset with 2 clusters

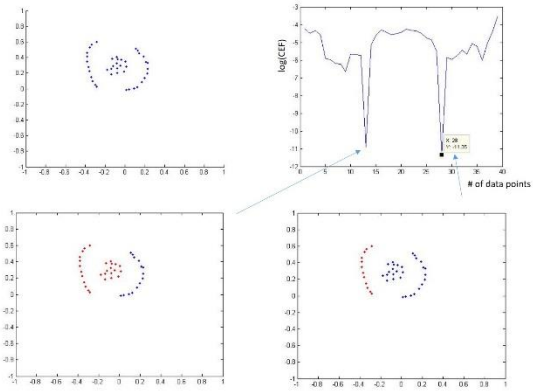

Figure 10: A dataset with 3 different main clusters

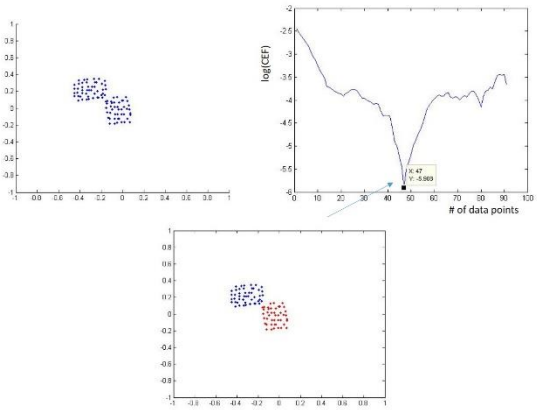

Figure 11: A different dataset with 2 main clusters

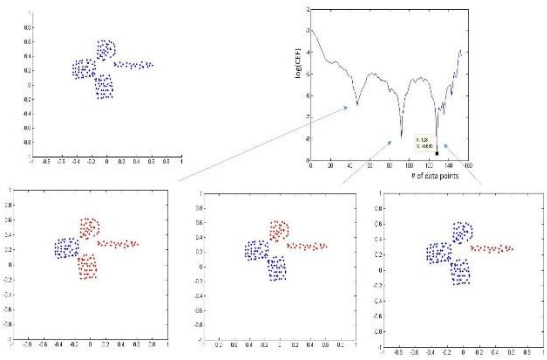

Figure 12: A dataset with 4 different main clusters

4.2. Real datasets

The algorithm is tested using Fisher's Iris data set. The Iris data set is 4 dimensional and it is not possible to plot all dimensions together. It is known that two species have overlapping features. Features 1 and 2 and the CEF plot are shown in Fig. 13 using different color and shapes for different species where the overlap can be seen very clearly. The CEF plot shows the first cluster but fails to show the second one.

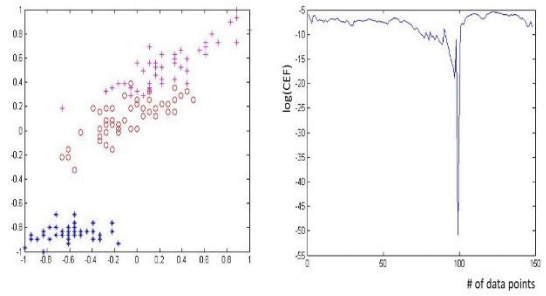

Figure 13: Iris data set and CEF plot

The second dataset is from UCI Machine Learning Repository [22]. The Banknote Authentication dataset has 4 dimensional feature set with two classes. When we plot different combinations of features, we can see that the classes overlap heavily. Also sub clusters are visible in the dataset as in Fig. 14.

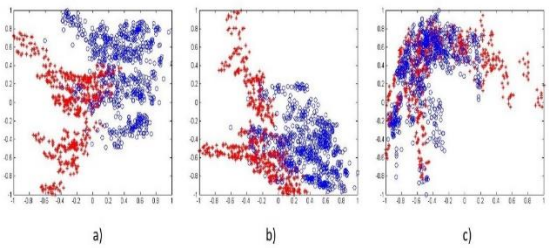

Figure 14: Banknote dataset a) 1st and 2nd features b) 1st and 3rd features c) 3th and 4th features

The CEF plot shows noisy output at borders where one cluster has most of the points and the other cluster is almost empty. Ignoring the end points, the plot shows a strong indication for 2 clusters as shown in Fig 15. But it also shows other major cluster separations as well which can be seen in Fig. 14.

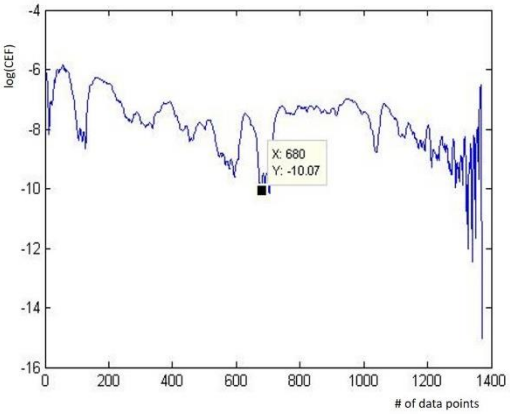

Figure 15: Banknote CEF plot showing 2 main clusters and smaller sub clusters

5. DISCUSSION

When the clusters are well separated even highly nonlinearly (nonconvex), the CEF Index has not trouble identifying strong cluster separation points. The calculation requires only one pass through the data points and it is possible to calculate a good measure about the cluster groups. On the other hand, overlapping features are reducing the separation since no assumptions are done about any model or distribution. Another concern is that the initial and ending conditions of the plot shows noisy output because of the reduction of points in one cluster. It is wise to assume that outliers will create a similar problem. Extra calculations are needed to compensate the reduction.

6. CONCLUSION

In this paper an algorithm is developed to find information about the cluster groups in a dataset. The present algorithms are trying to find the number of clusters by running a given clustering algorithm by changing the cluster value from a predefined minimum number up to a maximum number. During the calculation different metrics are used to measure the validity of the clusters generated. Running the algorithms repeatedly by changing the assumed number of clusters is a time consuming task. The proposed algorithm is going through the dataset only

once without assuming any number of clusters. The nonlinearly weighted CEF distance functions shows a strong separation at cluster boundaries and by counting the minimum peaks, it is possible to get a very reliable information about the possible number of clusters in any dataset.

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