A New Method to Enhance the Clustering Algorithm

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Abstract—In this paper we have presented a new method to enhance the clustering algorithm. Clustering is a method to label points in a two or more dimensional scatter plot. Some algorithms such as FCM, KNN or K-means implement this, but the problem occurs in the case that the clusters are close to each other or even they have overlaps (like neural data which we first encountered). In this state the human observer can detect some clusters on the scatter plot but the algorithms fail or they offer different clusters. To solve this problem we propose that the TPS transform on the primary data (clusters) can improve the clustering solution which is more likely to human perception of the clusters. To show the validity of our method we have used the SPSS analyses.

Index Terms—FCM, TPS, subtractive clustering, image registration.

I. INTRODUCTION

In many cases we extract features from a signal, image. These features may be amplitude, frequency, special Fourier coefficients, PCA components, or etc. Instead of processing the source signal or raw data we can process these features. For example to cluster neural spikes, we can first calculate the principle components (PCA) of signal. These features are points in a scatter plot. Clustering of these features is easier than the neural spikes [1], [2].

As we were working on neural data, we found that when our signal is transformed on a feature vector (scatter plot) usually features were close to each other and even they had overlaps. In other words in the scatter plot we saw some clusters which have overlaps. Figure 1 shows an example of these overlaps of clusters. However, in figure 2 three different clusters without any overlaps can be detected.

Fig. 1. Overlapping clusters

Fig. 2. Three different clusters

Applying any clustering algorithm on figure 2 usually will have unique answer. However, in figure 1 it is hard for the clustering algorithm to detect the clusters exactly or even with a very small error.

The data points on figure 1 should be transformed such that the clustering result resembles the human perception of the clusters. To achieve this, first some centers in the data points should be determined. These centers show the probable locations of clusters. It can be shown that subtractive clustering can do this job.

II. SUBSTRUCTIVE CLUSTERING

If there is not a clear idea how many clusters are present in a given set of data, subtractive clustering, is a fast, one-pass algorithm for estimating the number of clusters and the cluster centers in a set of data points. The subtractive clustering method assumes each data point is a potential cluster center and calculates a measure of the likelihood that each data point would define the cluster center, based on the density of the surrounding data points. The algorithm selects the data point with the highest potential to be the first cluster center, then removes all the data points in the vicinity of the first cluster center (as it is determined by radius), in order to determine the next data cluster and its center location, this process is iterated until all of the data points are within the radius of a cluster center [3]. The subtractive clustering provides a powerful comparison of clusters and is a first step for finding non-obvious (hidden) differences and minimizing the human prejudice during the analysis [4].

In this paper first we have a global estimation of probable clusters using this method. After finding the initial guess of centers all the data should be transformed by applying the TPS transform.

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III. TPS TRANSFORM

Thin Plate Spline (TPS) is a method to warp an image in accordance with input and base control points. In other words it is a method for image registration. Given a set of data points, a weighted combination of thin plate spline centered about each data point gives the interpolation function that exactly passes through the points while minimizing the so-called bending energy. The name "Thin Plate Spline" refers to a physical analogy involving the bending of a thin sheet of metal. There are many references for this transformation [3]-[7].

Generally speaking the TPS acts as a function that transforms all the points of a grid to another warped grid as shown in equation (1).

$$T(x, y, z) = \begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} a_{00} & a_{01} & \dots & \dots & a_{0n} \\ a_{10} & \dots & \dots & \dots & a_{1n} \\ a_{20} & \dots & \dots & \dots & a_{2n} \\ 0 & 0 & \dots & \dots & 1 \end{pmatrix} \begin{pmatrix} \theta_1(x, y, z) \\ \theta_2(x, y, z) \\ \dots \\ \theta_n(x, y, z) \\ 1 \end{pmatrix} \quad (1)$$

In the equation (1) x, y, z are the input points and x', y', z' are warped points. a_{ij} s are the coefficients that are determined by the control points. Equation (2) shows a general form for a TPS transfer function.

$$T(x) = P(x) + \sum_{i=1}^n A_i g(r_i) \quad (2)$$

In this equation $P(x)$ is a polynomial that determines the rigid or affine function and $g(r_i)$ is a Radial Basis Function and r_i is Euclidean distance of control points. A is a matrix which is related to the control points. The control points determine the pattern of movement of certain points and the deformation of the grid.

Fig. 3. Deformation of a grid which tries to move all the points, closer to the primary centers.

How this transform can be used in clustering? As it is shown in the previous section, the centers of the clusters can be found with the subtractive clustering method. If we try to transform the data (like the scatter plot in figure 1) in such a way, that all the points move to the primary clusters

(which is defined by the subtractive clustering), then we have achieved a novel method that helps the algorithm for a better clustering. In order to distinguish the overlapping points within two clusters, the overlapping points must be moved more than others, in other words a non linear transform or non rigid transform must be used as shown in figure 3.

However, first the control points must be determined.

IV. SELECTION OF CONTROL POINTS

First the center of the primary centers is calculated, then lines are drawn from this point to all the other centers. After this, the control points are selected using these two methods:

- 1) The control points are selected such that they move from the 1.2 and 0.8 times of the radius (figure 4).
- 2) The control points are selected such that they move from half of the angle (bisector) with the adjacent center to the desired center (figure 5).

Fig. 4. Movement of control points from .8 and 1.1 to centers.

Fig. 5. Movement of control points from bisector to the primary centers.

To assure these control points and TPS transform do not distort the data, after the selection of the control points, cluster validation criteria must be met.

V. CLUSTER VALIDATION

Cluster validation shows how much *between class distance* is large, and how much *within class distance* is small. In the next section we show that our method has improved these factors. For the assessment of the validity of our method a random scatter plot is generated, where the points are labeled in this plot. Then the points are clustered by the FCM method, and finally the error labels are counted. For the comparison we also first transform the random plot scatters and then cluster the scatter plot with the FCM method. This time, misclassification errors will also be counted.

VI. RESULTS

We generate the random scatter plot 100 times then we measured the mean of errors, between and within class distances. In order to assess our method the results of Kappa

measurements without our method (clustering with FCM) and with the new method are presented in table I and table II. These tables are the result of data analysis by SPSS 16.0 software.

TABLE I: KAPPA MEASUREMENT, BEFORE AND AFTER APPLYING THE NEW METHOD

Kappa	Value	Asymp. Std. Error	Approx. T	Approx. Sig.
Kappa before our method	0.87	0.003	150.767	0
Kappa after our method	0.891	0.003	154.369	0

Although some distances are larger than before applying the new method but paired samples test shows they are generally smaller with a good P-Value. As it shown in table II the clusters are more compact.

TABLE II: PAIRED SAMPLE TEST WITH SPSS

Test	Mean	N	Std. Deviation	Std. Error Mean
After Method	70.5484	100	27.4504	2.7450
Before Method	87.4166	100	28.6353	2.8635

Our results show that tests are normal and misclassification error is reduced at least by half i.e. without the method the mean of errors is 6 and after the method is 3. For 100 times test the Kappa factor (measurement of agreement) improves from 0.87 to 0.891 which shows the reduction of error.

VII. A REAL APPLICATION

This method can be used in online clustering of the neural spikes. For this application we first extract the features of neural spikes (scatter plot) and then transform data points with the TPS, and finally cluster with the FCM method.

VIII. CONCLUSION

In this paper we presented a new method to improve the clustering algorithm (FCM) and we showed that our method improves the clustering method with a TPS transformation on the input data points. It also helps the FCM to work well and it reduces the different clustering by FCM

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