DOFCM: A Robust Clustering Technique Based upon Density

Kaur Prabhjot, Lamba I. M. S., and Gosain Anjana

Abstract—Robust clustering methods reduce the impact of outliers on cluster centroids. Definition of outlier depends on the data structure and applied detection methods. Noise Clustering (NC) is a robust technique, which defines outliers in terms of a distance, called noise distance. NC identifies outliers during clustering process and modifies various parameters, required for creating clusters, thus affecting clustering output. Its main motive is to reduce the influence of outliers on cluster centroids rather than identifying it hence could not result into original clusters. However, in many applications, identification of outliers is important, as they may contain important information. Density Oriented Fuzzy C-Means (DOFCM) is a robust technique, which identifies outlier before clustering, on the basis of density of data-set. According to DOFCM, outliers are defined as the points that are not in the dense part of the data-set. In this paper, we have compared both the techniques for outlier identification and clustering. The results obtained through comparison, by implementing various tests, concluded that DOFCM based upon density approach identifies outliers very well and gives efficient clustering results than NC technique which identify outliers based upon distance.

Index Terms—Data mining, Density-Oriented approach, Fuzzy clustering, Outlier identification, Robust clustering.

I. INTRODUCTION

Data Mining comprises of dependency detection, class identification, class description, and outlier/exception identification, the last focuses on a very small percentage of data points, which are often ignored as noise. Some algorithms in machine learning and data mining have considered outliers, but only to the extent of tolerating those in whatever the algorithms are supposed to do. The exact definition of an outlier often depends on hidden assumptions regarding the data structure and the applied detection method [1]-[5]. Cluster analysis has been a fundamental research area in data analysis and pattern recognition. Clustering helps in finding natural boundaries in the data and fuzzy clustering is used to handle the problem of vague boundaries of clusters. In fuzzy clustering, the requirement of crisp partition of the data is replaced by a weaker requirement of fuzzy partition, where the association among data is represented by fuzzy relations. Outlier identification and clustering are interrelated processes. The fuzzy clustering identifies groups of similar data, whereas the outlier identification extracts noise from the data which does not belong to any cluster. Hawkins [1] defines outlier as an observation that deviates so much from other observations as to arouse suspicion that it was generated by a different mechanism. Barnett & Lewis [2] indicate that an outlying observation or outlier is one that appears to deviate markedly from other members of the sample in which it occurs. Outlier identification is referred to as outlier mining, which has a lot of practical applications in many different areas. Outlier mining actually consists of two sub-problems: first, what data is deemed to be exceptional in a given data-set and second, find an efficient algorithm to obtain such data [4]. In Noise clustering (NC) [12],[13], Dave gave a concept of noise cluster. Data points whose distances to all cluster centroids exceed a certain threshold are considered as noise and they belong to noise cluster, and the distance is called noise distance. Calculation of noise distance is crucial point in NC. Moreover, it identifies outliers during the clustering process. Proposed technique identifies outliers before creating clusters, on the basis of density of data-set. After comparing both the techniques, it is proposed that DOFCM, a density-oriented approach to identify outlier is better than NC which is a distance-oriented technique.

The organization of the paper is as follows: Section II, briefly review Fuzzy C-Means (FCM) [6] and Noise Clustering (NC) algorithms. The properties of robust clustering techniques are defined in Section III. Section IV described the proposed algorithm, DOFCM. Both the techniques are compared and the results are shown in Section V, followed by concluding remarks in Section VI.

II. FUZZY CLUSTERING TECHNIQUES

This section briefly discusses the Fuzzy C-Means (FCM) and Noise Clustering (NC). In this paper, the data-set is denoted by ‘X’, where X=$\{x_1, x_2, x_3, \ldots, x_n\}$ specifying ‘n’ points in M-dimensional space. Centroids of clusters ‘k’ are denoted by $v_k$, $d_k$ is the distance between $x_i$ and $v_k$ and ‘c’ is the number of clusters present in the data-set.

A. The Fuzzy C-Means Algorithm

FCM [6] is the most popular fuzzy clustering algorithm. It assumes that number of clusters ‘c’ is known in priori and minimizes the objective function $(J_{FCM})$ as:

$$J_{FCM(U,V)} = \sum_{k=1}^{c} \sum_{i=1}^{n} u_{ik}^{m} d_{ik}^{2},$$  \hspace{1cm} (1)

where $d_{ik} = \|x_i - v_k\|$, and $u_{ik}$ is the membership of $x_i$ in cluster ‘k’, which satisfies the following relationship:

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\[
\sum_{k=1}^{c} \mu_{ki} = 1, i = 1, 2, \ldots, n
\]  

(2)

Here \( m \) is known as the fuzzifier (or fuzziness index) and any norm \( || \cdot || \) can be used for calculating \( d_{ik} \) (we used Euclidean norm.). Minimization of \( J_{\text{FCM}} \) is performed by a fixed point iteration scheme known as the alternating optimization technique. The conditions for local extreme for “(1)” and “(2)” are derived using Lagrangian multipliers:

\[
\mu_{ki} = \frac{1}{\sum_{j=1}^{n} \left( \frac{d_{kj}}{d_{ji}} \right)^{m-1}} \quad \forall \; k, i
\]  

(3)

where 

\[ 1 \leq k \leq c \]

\[ 1 \leq i \leq n \]

and

\[
u_k = \frac{\sum_{i=1}^{n} (\mu_{ki}^m x_i)}{\sum_{i=1}^{n} (\mu_{ki}^m)} \quad \forall \; i
\]  

(4)

Outliers are the points in the data-set ‘X’ which are so distant from the rest of the points that it would be unreasonable to assign high membership values to the outliers in any of the ‘c’ clusters. FCM assigns memberships to ‘\( x_i \)’ in the ‘c’ clusters inversely proportional to the relative distance of ‘\( x_i \)’ to the {\( v_k \)} centroid. Let \( c = 2 \), if ‘\( x_i \)’ is equidistant from two centroids, the membership of ‘\( x_i \)’ to these clusters will have the same value (0.5), irrespective of the absolute value of the distance of this point from other points in each of the clusters. Hence the problem with FCM is that it gives equal membership to the noisy points/outliers far from the central structure of the two clusters. It is unable to detect outliers and its centroid attraction is somewhat towards outliers rather than at the center of the cluster.

B. Noise Clustering (NC)

Noise clustering has been introduced by Dave [13], [14] to overcome the major deficiency of the FCM algorithm i.e. its noise sensitivity. He gave the concept of “noise prototype”, which is a universal entity such that it is always at the same distance from every point in the data-set. Let \( v_k \) be the noise prototype and ‘\( x_i \)’ be any point in the data-set such that \( v_k, x_i \in \mathbb{R}_c \). Then noise prototype is the distance \( d_i \) given by:

\[ d_{ki} = \delta, \forall i \]

The NC algorithm considers noise as a separate class. The membership \( \mu_{i} \), of \( x_i \) in a noise cluster is defined as:

\[ \mu_{i} = 1 - \sum_{k \neq i} \mu_{ki} \]

NC reformulates FCM objective function:

\[
J(U, V) = \sum_{i=1}^{c+1} \sum_{k=1}^{N_i} (\mu_{ki}^m) \left( d_{ki} \right)^p
\]  

(5)

where ‘\( c+1 \)’ consists of ‘\( c \)’ good clusters and one noise cluster and for \( k = n = c+1 \). Where

\[
\delta^2 = \lambda \left[ \frac{\sum_{i=1}^{N} \sum_{k=1}^{n} (d_{ki})^2}{N \cdot c} \right]
\]

(6)

and membership equation is

\[
u_{ji} = \left( \frac{\sum_{k=1}^{n} \left( \frac{d_{kj}}{d_{ji}} \right)^{\frac{1}{m-1}}}{\sum_{k=1}^{n} \left( \frac{d_{kj}}{d_{ji}} \right)^{\frac{1}{m-1}}} \right)^{-1}
\]

Noise clustering is a better approach than FCM, PCM, and PFCM. Although, it identifies outliers in separate clusters but could not result into efficient cluster shapes because it fails to identify those outliers which are located in between the centroids (refer Section V). Its main emphasis is to reduce the influence of outliers on the clusters rather than exactly identifying it. Real-life data-sets usually contain cluster structures that differ from our assumption of hyper-spherical clusters. The cluster structures must be approximated by several centroids. If the number of clusters is increased for the same data-set, NC does not detect outliers, because in that scenario the average distance between points and regular clusters decreases and the noise distance remains almost constant [11]. NC assigns only those points to noise cluster whose distance from regular clusters is more than the noise distance.

III. PROPERTIES OF NOISELESS CLUSTERING TECHNIQUE

Property P1: RCT must assign lower memberships to all the outliers for all the clusters [15].

Property P2: Centroids generated by RCT on a noisy data-set should not deviate significantly from those generated for the corresponding noiseless set, obtained by removing the outliers [15].

Property P3: RCT must be independent of any number of outliers i.e. able to identify outliers by changing the number of clusters for the same data-set [11].

Property P4: RCT should be independent of any amount of outliers i.e. Centroids generated by Clustering Technique should not deviate by increasing the number of outliers (refer section V).

Property P5: RCT should be independent of the location of outliers in the data-sets i.e. it should be able to find out outliers whether they are within the data-set or away from it (refer Section V).

IV. THE PROPOSED TECHNIQUE, DOFCM

We attempt to decrease the noise sensitivity in fuzzy clustering by identifying outliers before the clustering process. Like NC technique DOFCM results in ‘\( n+1 \)’ clusters with ‘\( n \)’ good clusters and one invalid cluster of outliers. Proposed algorithm identifies outliers on the basis of density of data-set. It has used FCM technique (by modifying membership) to create clusters. It identifies outliers on the basis of the number of other points in its neighborhood. DOFCM defines density factor, called neighborhood membership, which measures density of an object in relation to its neighborhood. As per the technique, the neighborhood of a given radius of each point in a data-set has to contain at least a minimum number of other points to become a good point(non-outlier). Shape of the neighborhood is determined by the choice of a distance function for two points \( x_i \) and \( x_j \) denoted by \( \text{dist}(x_i, x_j) \) e.g. when using Manhattan distance in the 2D space, the neighborhood shape is rectangle and by
using Euclidean distance it is spherical. The proposed scheme uses Euclidean distance.

Neighborhood membership of a point \( i \) in the data-set \( X \) is defined as:

\[
M^i_{\text{neighborhood}}(X) = \frac{\eta^i_{\text{neighborhood}}}{\eta_{\text{max}}}
\]

where \( \eta^i_{\text{neighborhood}} \) = Number of points in the neighborhood of point \( i \)

\( \eta_{\text{max}} \) = Maximum number of points in the neighborhood of any point in the data-set

Let \( 'q' \) is in the neighborhood of point \( 'i' \), so \( 'q' \) will satisfy:

\[
\{ q \in X \mid \text{dist}(i,q) \leq r_{\text{neighborhood}} \}
\]

where \( r_{\text{neighborhood}} \) is the radius of neighborhood, \( \text{dist}(i,q) \) is the distance between point \( 'i' \) and \( 'q' \).

Selection of the Threshold value \( '\alpha' \):

Ideally, a point will be outlier only if no other point is present in its neighborhood. However, in the proposed scheme, a point is considered as an outlier when its neighborhood membership is less than \( '\alpha' \). So, as per the analysis, Outlier could now be defined as a point in the data-set \( X \) whose neighborhood membership is less than the threshold value \( '\alpha' \). Let \( 'i' \) be a point in the data-set \( X \), then if:

\[
M^i_{\text{neighborhood}} = \begin{cases} < \alpha; \text{o}}r\text{utlier} \\ \geq \alpha; \text{non-outlier} \end{cases}
\]

\( '\alpha' \) can be selected from the range of \( M_{\text{neighborhood}} \) values after observing the density of data-set and should be close to zero.

**TABLE-I EFFECT OF CHANGING THRESHOLD VALUE**

<table>
<thead>
<tr>
<th>Data set ( D^n )</th>
<th>( \eta_{\text{max}} )</th>
<th>Threshold value ( '\alpha' )</th>
<th>No. of outliers</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>0.0</td>
<td>6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.09</td>
<td>9</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.14</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.21</td>
<td>12</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>0.0</td>
<td>12</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.0625</td>
<td>12</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.125</td>
<td>29</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.1875</td>
<td>42</td>
<td></td>
</tr>
</tbody>
</table>

* Where \( \eta_{\text{max}} \) is the maximum number of points in the neighborhood of any point in the data-set.

Once the outliers are identified by the algorithm, clustering follows:

Let \( X = \{ x_n \} \) be the data-set after identification of outliers. DOFCM partitions \( X \) by minimizing objective function as:

\[
\min_{\omega} \sum_{i=1}^{K} \sum_{j=1}^{n} \omega_{ij} d_{ij}^2
\]

where \( d_{ij}^2 \) is the distance between point \( i \) and \( j \) and \( \omega_{ij} \) is the membership of point \( i \) to cluster \( j \).
$J_{DOFCM}(U,V) = \sum_{k=1}^{c} \sum_{i=1}^{n} u_{ik}^m d_{ki}^2$  (10)

where $d_{ki} = \|x_i - v_k\|$ and membership function $u_{ki}$ is:

\[
u_{ki} = \begin{cases} 
\frac{1}{\sum_{l=1}^{c} (\frac{d_{ki}}{d_{kl}})^{\frac{1}{M-1}}} & \text{if } M_{\text{neighborhood}} \geq \alpha \\
0 & \text{if } M_{\text{neighborhood}} < \alpha 
\end{cases} \quad (11)
\]

And $m = \text{Fuzziness Index}$

It is seen from above equations that the fuzzy membership depends on local membership ($M_{\text{neighborhood}}$) and threshold value ($\alpha$). If a point is identified as an outlier, DOFCM assigns zero fuzzy membership to it so that it could not affect the location of centroids which is a limitation with the FCM algorithm. Updating of centroid is the same as than in FCM. The constraint on fuzzy membership is now extended to:

$$0 \leq \sum_{k=1}^{c} u_{ki} \leq 1 : i=1, 2, 3, \ldots, n$$  (12)

instead of the following in conventional FCM algorithm.

$$\sum_{k=1}^{c} u_{ki} = 1$$

The FCM algorithm has a constraint that it avoids a situation that the membership value becomes zero. FCM gives meaningful results in applications where memberships are interpreted as probabilities or degree of sharing. The proposed algorithm removes the effect of outliers by assigning them a membership value equal to zero.

V. COMPARISON BETWEEN NOISE CLUSTERING AND DENSITY ORIENTED FUZZY C MEANS FOR OUTLIER IDENTIFICATION

We compared various aspects of NC and DOFCM with synthetic data-sets. For all data-sets we assumed the following computational protocols: $\varepsilon = 0.00001$, Total number of iterations = 100. MATLAB Version 7.0 is used to produce the results.

To prove the properties P1, P2, and P4, we are considering three data-sets: D11, D^412, and D^814 (referred from 11). D11 is a noiseless data-set of points $\{x_i\}_{i=1}^{14}$. D^412 is the union of D11 and an outlier D^412, and D^814 is the union of D11 and 3 outliers D^812, D^813, and D^814. Fig. 2a, Fig. 2b and TABLE-II show clustering results of NC and DOFCM, identification of outliers by NC and DOFCM with $\lambda=1$ and $\alpha=0.09$, with the data-sets D^412 and D^814 respectively. '+' shows outliers identified by DOFCM and 'o' shows outliers identified with NC.

True centroids of D11 are: $v_{true}^{true} = \begin{bmatrix} -3.34 \\ -3.34 \\ 0 \end{bmatrix}$. From the figures and Table-2, it has been seen that both the techniques are able to identify outliers. However, the performance of NC degrades by increasing number of outliers. DOFCM satisfies property P2 and P4, as the centroids generated with DOFCM are same with both data-sets and even more accurate compared to NC. TABLE-III shows memberships generated with DOFCM and NC for the outliers. It is clear from table that memberships generated with DOFCM are lower than the NC; hence DOFCM also satisfies property P1.

TABLE-II: CENTROIDS PRODUCED BY NC AND DOFCM FOR D^812 AND D^14, NO. OF CLUSTERS=2

<table>
<thead>
<tr>
<th></th>
<th>NC (m=2, $\lambda=1$)</th>
<th>DOFCM (m=2, $\alpha=0.09$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>D12 x</td>
<td>y</td>
<td>x y</td>
</tr>
<tr>
<td>-3.131</td>
<td>0.4</td>
<td>3.048</td>
</tr>
<tr>
<td>-3.131</td>
<td>0.4</td>
<td>3.085</td>
</tr>
<tr>
<td>D14 x</td>
<td>y</td>
<td>x y</td>
</tr>
<tr>
<td>3.167</td>
<td>0</td>
<td>3.167</td>
</tr>
<tr>
<td>3.167</td>
<td>0</td>
<td>3.167</td>
</tr>
</tbody>
</table>

Here, noise distance depends upon distance measure, number of assumed clusters, and $\lambda$, which is the value of multiplier used to obtain $\delta^2$, from the average of distances. From the equation, it is interpreted that if the numbers of clusters are increased, $\delta^2$ assumes high values. As in NC, outliers are those data points whose distances to all cluster centroids exceed a certain threshold distance based upon $\delta$. So, if we increase the number of clusters for the same data-set, it did not identify outliers, because the average distance between points and regular clusters decreases with the increase in the number of clusters and the noise distance remains almost constant or assumes relatively high values [11]. Whereas, DOFCM identifies outliers very well and it is independent of increasing the number of clusters in the same data-set, because it identifies outliers before clustering.
process and does not involve any parameter that could affect
clustering in any manner. Fig. 3a shows the results of NC and
DOFCM with the data-set containing two clusters with some
noise (refer to APPENDIX-A). NC partitioned the data-set
into two clusters with $\lambda=0.51$. The centroids of the clusters
are plotted in the figure with ‘$\Delta$’ symbol and the outliers are
plotted with ‘o’. DOFCM partitioned it into two clusters with
$\alpha=0.14$. Centroids are plotted with the symbol ‘*’ and
outliers with ‘+’. If we compare the results of these two
techniques, it is visually verified that density-oriented
technique can identify outliers more efficiently than
distance-oriented.

Outliers contain important information in many
applications and their identification is crucial. The main
emphasis of NC is to reduce the influence of outliers on the
clusters rather than identifying it, whereas, from the results, it
is clear that DOFCM satisfies all the properties required for a
robust technique and identifies outliers very well.

VI. CONCLUSIONS

In this paper, we compared density-oriented and
distance-oriented approaches for outlier identification and
clustering. Various tests are performed on two approaches
and it has been notified from the simulation and results that
density-oriented approach (DOFCM) is much better than
distance-oriented approach (NC) for outlier identification.
Main concern of DOFCM is, not only to reduce the influence
of outliers on the location of cluster centroids, but also to
identify them. Density-oriented approach is independent of
the number of clusters for the data-set and does not involve
any parameter that can affect the result of clustering.
TABLE-III MEMBERSHIPS GENERATED BY DOFCM AND NC FOR D^12 AND D^14

<table>
<thead>
<tr>
<th>Sr No.</th>
<th>Feature 1</th>
<th>Feature 2</th>
<th>D^12 Membership</th>
<th>D^14 Membership</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DOFCM (m=2, α = 0.09)</td>
<td>NC (m=2, λ=1)</td>
<td>DOFCM (m=2, α = 0.09)</td>
<td>NC (m=2, λ=1)</td>
</tr>
<tr>
<td></td>
<td>Neighborhood Membership</td>
<td>Cluster 1</td>
<td>Cluster 2</td>
<td>Cluster 1</td>
</tr>
<tr>
<td>x^1</td>
<td>0</td>
<td>38</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>x^2</td>
<td>0</td>
<td>27</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>x^3</td>
<td>-7</td>
<td>23</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>x^4</td>
<td>10</td>
<td>25</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

APPENDIX-A

Synthetic data-set with 115 points (2 clusters with noise)

<table>
<thead>
<tr>
<th>x</th>
<th>y</th>
<th>x</th>
<th>y</th>
<th>x</th>
<th>y</th>
<th>x</th>
<th>y</th>
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<tbody>
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<td>-1.33</td>
<td>7.76</td>
<td>-8.1</td>
<td>4.28</td>
<td>1.14</td>
<td>34</td>
<td>4</td>
</tr>
<tr>
<td>14.75</td>
<td>-2.09</td>
<td>6.36</td>
<td>-9.1</td>
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<td>-1.82</td>
<td>35</td>
<td>3</td>
</tr>
<tr>
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<td>-1.03</td>
<td>8.1</td>
<td>-7.6</td>
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<td>6.71</td>
<td>-1</td>
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</tr>
<tr>
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<td>-0.87</td>
<td>4</td>
<td>-4</td>
<td>38.79</td>
<td>5.04</td>
<td>0</td>
<td>-10</td>
</tr>
<tr>
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<td>5</td>
<td>-5</td>
<td>26.78</td>
<td>1.07</td>
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<td>-6.86</td>
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<td>-8</td>
</tr>
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<td>4</td>
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REFERENCES


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