Journal of Intelligent & Fuzzy Systems 34 (2018) 525–536
DOI:10.3233/JIFS-17678
IOS Press

DFC: Density Fragment Clustering without Peaks

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Abstract. The density peaks clustering (DPC) algorithm is a novel density-based clustering approach. Outliers can be spotted and excluded automatically, and clusters can be found regardless of the shape and of dimensionality of the space in which they are embedded. However, it still has problems when processing a complex data set with irregular shapes and varying densities to get a good clustering result with anomaly detection. A density fragment clustering (DFC) algorithm without peaks algorithm is proposed with inspiration from DPC, DBSCAN and SCAN to cope with a larger number of data sets. Experimental results show that our algorithm is more feasible and effective when compared to DPC, AP and DBSCAN algorithms.

Keywords: Density peak, fragment clustering, anomaly detection

1. Introduction

Clustering is known as unsupervised classification in pattern recognition, or nonparametric density estimation in statistics [1–3]. The goal of clustering is to separate a finite unlabeled objects into different clusters with characteristics of internal homogeneity and external separation. Clustering has been applied in a wide variety of fields, ranging from engineering (machine learning, artificial intelligence, pattern recognition, mechanical engineering, electrical engineering), computer sciences (web mining, spatial database analysis, textual document collection, image segmentation), life and medical science (genetics, biology, microbiology, psychiatry, clinic, pathology), to earth sciences (geography, geology, remote sensing), social sciences (sociology, psychology, education), and economics (marketing, business) [4, 5].

Traditional methods in clustering can be broadly categorized into hierarchical, partitioning, density-based, model-based, grid-based, and soft-computing methods [6]. Many density-based clustering methods [7–9] have been proposed and inspired by DBSCAN [7] because its capability of discovering clusters with arbitrary shapes with an overall average runtime complexity of $O(n \times lgn)$. In addition, DBSCAN can detect the number of clusters automatically. However, choosing an appropriate density threshold can be nontrivial. It is very sensitive to the user-defined threshold values, often producing very different clustering results in a data set even for slightly different threshold settings [10].

Density peaks clustering (DPC) algorithm is based on the idea that cluster centers are characterized by a higher density than their neighbors and by a relatively

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large distance from points with higher densities [11]. Concretely speaking, DPC adopts the idea of local density maxima from mean-shift [12] and the basic idea of only one parameter of the distance between data points from K-Medoids [13]. The DPC algorithm is effective with two assumptions that cluster centers are surrounded by neighbors with lower local density and that they are a relatively large distance from any points with a higher local density [11]. Several researches [14–23] have been going on around this method.

As illustrated in Table 1, DPC still has some limitations: (1) The number of clusters cannot be determined automatically. It is determined by its decision graph in two dimensional space with a cutoff distance d_c and its density ρ. Du M. et al. [14] have figured out that DPC cannot detect the number of clusters when clusters are in the lower-left corner. Unfortunately, it cannot be changed with human interference. (2) Like DBSCAN [7], relative thin clusters would not be detected by its decision graph. Especially, when a path-based data set consists of a circular cluster with an opening near the bottom and two Gaussian distributed clusters inside, the number of clusters cannot be found via DPC [16] correctly. (3) It is not reasonable that there must be a density peak and only one centroid in each cluster. Otherwise, DPC will split natural groups [16].

The proposed DFC algorithm has solved these above problems via applying both *density fragment* and *network structural similarity* that inspired by DPC [11], SCAN [24] and DBSCAN [7] algorithms. When compared with clustering algorithms such as DBSCAN [7], AP [2] and DPC [11] illustrated in Table 1, the proposed novel DFC algorithm has the capability of determining the number of clusters automatically, clustering more reasonable clusters, and detecting anomalies.

We test the novel DFC algorithm in the most popular clustering benchmarks to demonstrate its feasibility. Our algorithm has overcome these above problems with satisfactory results when compared with DPC, SCAN and DBSCAN algorithms on some UCI and synthetic data sets. The rest of this paper is organized as follows. In Section 2, we describe principles of DPC, DBSCAN and SCAN algorithms. In Section 3, we propose the novel density fragment clustering without peaks algorithm. In Section 4, we present experimental results on synthetic data sets and some UCI data sets. In Section 5, some discussions are made to explain the major reasons. Finally, we make conclusions.

2. Related work

The proposed DFC algorithm is inspired by DPC, DBSCAN and SCAN. Brief reviews of these three algorithms should be given in the following subsections.

2.1. DPC: A density peaks clustering approach

Density peaks clustering (DPC) algorithm is based on the idea that cluster centers are characterized by a higher density than their neighbors and by relatively large distance from points with higher density [11]. Cutoff distance d_c is the only parameter in this method. For each data point x_i, it computes two quantities: its local density ρ_i and its distance δ_i from points of higher density.

$$d_{ij} = distance(x_i, x_j) \tag{1}$$

Where the distance can be measured by distance functions, e.g. Euclidean distance.

$$\rho_i = \sum_j \chi \times (d_{ij} - d_c) \tag{2}$$

Where $\chi(x) = 1$ if $x < 0$ and $\chi(x) = 0$ otherwise, and d_c is the only user defined parameter to describe its cutoff distance. As a rule of thumb, one can choose d_c so that the average number of neighbors is around 1 to 2% of the total number of points in a data set [11]. ρ_i, similar to *MinPoints* in DBSCAN [7], is defined as the number of neighbour points to point x_i in Equation 2.

Table 1
Advantages of DFC when compared with DBSCAN, AP and DPC, where '×' refers to disable, '√' means able and '∂' is partial

Algorithms	Varying sizes	Irregular shapes	Varying densities	♯ of clusters	Anomaly detection
DBSCAN	∂	∂	∂	∂	∂
AP	√	×	∂	∂	×
DPC	√	∂	√	∂	∂
DFC	√	∂	√	√	√

Another local density of a point x_i is presented in Equation 3, as follows:

$$\rho_i = \sum_j exp\left(-\frac{d_{ij}^2}{d_c^2}\right) \tag{3}$$

$$\delta_i = \min_{j:\rho_j > \rho_i} d_{ij} \tag{4}$$

Note that δ_i is measured by computing the minimum distance between point x_i and any other points with relative higher density.

The DPC algorithm can be summarized from Rodriguez et al. [11] and Du et al. [14] in Algorithm 1.

Algorithm 1 The DPC algorithm

Input: Initial nodes $X \in R_{N\times M}$, d_c

Output: The label vector of cluster index: $y \in R_{N\times M}$

Step 1: Calculate d_c

1.1 Calculate d_{ij} from $R_{N\times M}$ based on Equation 1;

1.2 Sort d_{ij} in an ascending order;

1.3 Determine d_c by finding value of 1 to 2% position in the above order.

Step 2: Detect cluster centroids by density peaks

2.1 Calculate ρ_i based on Equation 2 or 3;

2.2 Calculate δ_i based on Equation 4;

2.3 Sort nodes based on ρ in a descending order;

2.4 Detect centroids with relative high ρ and δ.

Step 3: Assign each node to different clusters

3.1 Detect halo nodes based on its density;

3.2 Determine its affiliation of relative high density nodes by δ_i to each cluster.

As illustrated in Algorithm 1, there is an inspiration that each node to be a centroid has two major characteristics: one is relative high density, and the other is relative long distance from its higher density nodes.

2.2. DBSCAN: A density-based clustering approach with noise

DBSCAN is a time proved and efficient clustering algorithm with the following features. (1) It is significantly effective in discovering clusters of arbitrary shapes. (2) It is easy for anomaly detection. (3) It is efficient in clustering process [7].

The DBSCAN can determine a cluster if two parameters *Eps* and *Min Pts* are satisfied. Therefore, it is easy to figure outliers out. The capability of finding arbitrary shaped cluster is achieved by its characteristics of *directly-density-reachable*, *density-reachable* and *density-connected*. It is the inspiration that each cluster is consisted of reachable core nodes and their boundary nodes classified by density parameters of *Eps* and *Min Pts*. Furthermore, the density within the areas of noise is lower than the density in any of the clusters.

2.3. SCAN: A structural network clustering approach

The SCAN algorithm is a famous structural network clustering approach to discover underlying structures in networks. It can detect clusters, hubs and outliers in networks with the following features [24]:

- It detects clusters, hubs and outliers by using the structure and the connectivity of the vertices as clustering criteria.
- It is fast with its running time of $O(m)$ on a network with n vertices and m edges.

Similar to DBSCAN algorithm, SCAN algorithm inherits the ideas of node density, such as definitions of *directly density-reachable*, *density-reachable*, and *density-connected*. Different from DBSCAN, each edge between two vertices is measured by *network structural similarity* in Equation 5.

$$\sigma(v, w) = \frac{|\Gamma(v) \cap \Gamma(w)|}{\sqrt{|\Gamma(v)||\Gamma(w)|}} \tag{5}$$

In SCAN algorithm, *network structural similarity* in Equation 5 is adopted to determine core and member vertex in a cluster. It is the inspiration that *network structural similarity* is an efficient measurement to determine the role of each vertex in a network. In other words, network-based modelling maybe a good way to aggregate clusters.

3. Methods

The proposed DFC algorithm inherits the strengths of DPC, DBSCAN and SCAN. *Density fragment* can be defined as the set of density decreasing nodes with relative nearby distance. DFC assumes that (1) a cluster is consisted of many density fragments; (2) two density fragments can be merged together if their *network structural similarity* is relative high. As illustrated in Algorithm 2, DFC includes three major steps: density decreasing, density fragment generation and density fragment aggregation.

Algorithm 2 The DFC algorithm.

Input: Initial nodes $X \in R_{N\times M}$, d_c, ρ
Output: All clusters and outliers are found
Step 1: Similarity matrix(d) calculation
1.1 Calculate d_{ij} from $R_{N\times M}$ based on Equation 1;
1.2 Sort d_{ij} in an ascending order.
Step 2: Density(ρ) calculation
2.1 Determine d_c value with principles of DPC;
2.2 Calculate ρ_i value based on Equations 2 or 3;
2.3 Put all ρ in a descending order.
Step 3: Delta(δ) calculation
for each node i **do**
  $\delta_i = d_{ij}$ based on Equation 1
end for
Step 4: Density fragment generation
4.1 Core node link generation;
for each node i in a descending order **do**
  if $\delta_i < d_c$ **then**
    Node i becomes a core node i;
    Get slot nodes for the core node i that their distances within d_c;
    Connect core node i to its neighbour core node $i+1$;
    Get a core node link based on the above rule;
    Get the core node link and their slot nodes together and then generate a density fragment.
  end if
end for
Step 5: Density fragment aggregation
for each density fragment **do**
  Calculate density fragment similarity based on Equation 7
  for each $DFSim(x, y)$ **do**
    if $DFSim(x, y) > 0.5$ **then**
      Aggregate the fragment x and fragment y as one cluster.
    end if
  end for
end for
Step 6: Anomaly detection
for each core node link **do**
  if $DFSim(x, y) > 0.5$ **then**
    Node i is an outlier.
  else
    if Core node link has no slot nodes **then**
      It is an outlier.
    end if
  end if
end for

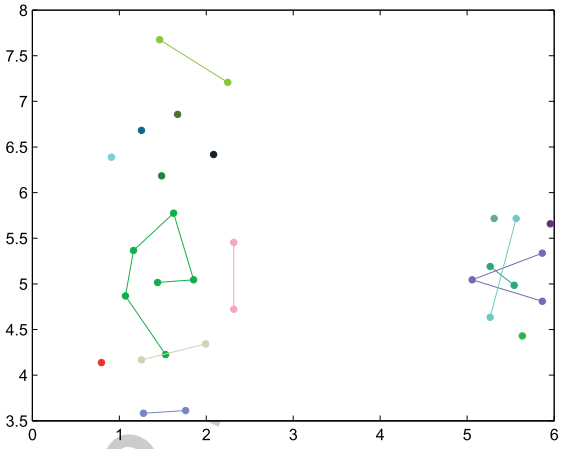


Fig. 1. An example of core node chains.

3.1. Density decreasing

As similar with DPC, a suitable cutoff distance d_c is selected based on principles of density to calculate their local density ρ for sorting these density values in a descending order. δ_i is an Euclidean distance between the $node_i$ and its next $node_{i+1}$ in the density decreasing order depicted in Equation 6.

$$\delta_i = Distance(node_i, node_{i+1}) \tag{6}$$

3.2. Density fragment generation

Density fragment generation is processed in two stages: in stage I, $node_i$ can become a core node if its $\delta_i \leq d_c$, then check its next $node_{i+1}$ with *density-reachability* to form a core node chain illustrated in Fig. 1; in stage II, a core node i can expand its *density-connectivity* to its nearby nodes in the range of d_c. These nearby nodes can be defined as slot nodes. A core node chain and its slot nodes constitute a density fragment. All density fragments can be formed after processing this two stages.

As illustrated in Fig. 1, 40 nodes with two dimensions are generated randomly, core node chains are depicted with solid line, and density fragments are formed by these core node chains and their slot nodes.

3.3. Density fragment aggregation

As described in the sub Section 3.2, *density fragment* is a network structure. *Density fragment aggregation* can be processed by principles

Table 2
7 different types of data sets

Data sets	Nodes	Dimensions	Clusters
Iris	150	4	3
Seeds	210	7	3
Wine	178	13	3
Glass	214	9	6
Flame	240	2	2
Aggregation	788	2	7
Spiral	312	2	3
D	87	2	3

Table 3
F-Measure evaluation

Data sets	DBSCAN	AP	DPC	DFC
Iris	0.7045	0.4851	0.7715	0.7554
Seeds	0.4784	0.3877	0.8026	0.793
Wine	0.5794	0.3142	0.5892	0.5894
Glass	0.3315	0.2874	0.5418	0.5571
Flame	0.6242	0.2874	1	0.9713
Aggregation	0.8140	0.3429	1	0.9909
Spiral	1	0.2853	1	1
D	0.8143	0.6117	0.8780	1

of *network structural similarity* and a priori probability. The network structural similarity of density fragments can be defined in Equation 7. $Frag_x$ and $Frag_y$ refer to density fragment of x and y respectively. The larger of $DFSim(x, y)$ value, the higher probability of aggregation between $Frag_x$ and $Frag_y$. The aggregation of density fragments is processed with a priori probability that the density fragment with higher density has a higher priority to merge other density fragments.

$$DFSim(x, y) = \frac{|Frag_x \cap Frag_y|}{\sqrt{|Frag_x||Frag_y|}} \tag{7}$$

The proposed density fragment clustering approach is depicted in Algorithm 2.

4. Results

To test its feasibility and effectiveness of the proposed DFC algorithm, we compare it with DBSCAN, AP and DPC in the above four UCI data sets and the next three synthetic data sets listed in Table 2. F-Measure can be defined in Equation 10, which is an index to evaluate the performance of clustering results. 7 different data sets (*Iris*, *Seeds*, *Wine*, *Glass*, *Flame*, *Aggregation* and *Spiral*) are selected to evaluate the clustering performance of DBSCAN, AP, DPC and DFC in Table 3 and Fig. 2. The results in Table 3 and Fig. 2 are mean values based on 30 times run.

F-Measure index measures accuracy. It considers both the precision P and the recall R of clustering algorithms: P is the ratio of the number of correct results to the number of all returned results, and R is the ratio of the number of correct results to the number of results that should have been returned. P, R and F-Measure(F) are defined as the following Equations 8, 9 and 10.

$$P = (M_j, C_i) = \frac{|M_j \cap C_i|}{|C_i|} \tag{8}$$

$$R = (M_j, C_i) = \frac{|M_j \cap C_i|}{|M_j|} \tag{9}$$

$$F(M_j, C_i) = \frac{2 \cdot P(M_j, C_i) \cdot R(M_j, C_i)}{P(M_j, C_i) + R(M_j, C_i)} \tag{10}$$

Besides the clustering performance depicted in Fig. 2, many experiments have been done to evaluate the DFC capability with limitations such as varying sizes, irregular shapes, varying densities, number of clusters and anomaly detection.

4.1. Varying sizes

Clusters with varying sizes are normal in a real data set, and they should be detected correctly without interference. *Aggregation*, *Flame* and *D* are selected to evaluate the capability of processing varying sizes of clusters in a data set.

As illustrated in Fig. 3, to test the accuracy of the DBSCAN algorithm without any other factors, the number of cluster is controlled to the true cluster number ($Eps = 0.9$, $MinPts = 5$). AP's *preference* is set to the medium value of the similarity matrix according to the original AP algorithm. DPC's d_c value is set to 2.7212 and DFC's $DFSim$ is set to 0.3024 when they can get their best result. This figure shows that both DFC and DPC can find clusters correctly while AP cannot cluster in an intuitive way. And some points are close to their actual clusters while DBSCAN cannot recognize them. And the parameters in these four algorithms are set for the same purpose in the following data sets. Figures 5 and 8 show the same result that DFC has the ability to detect data sets with varying size while most algorithms can not.

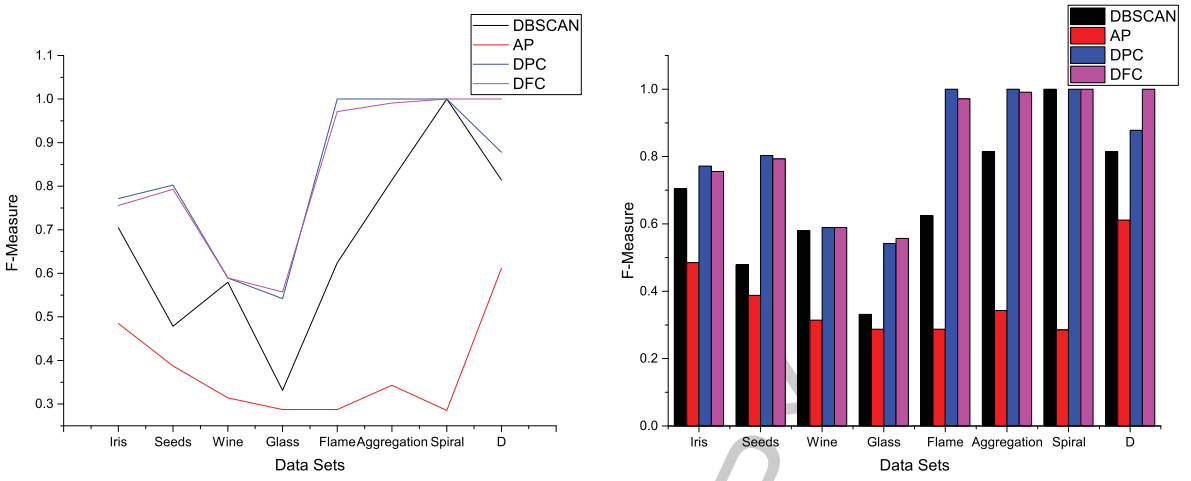
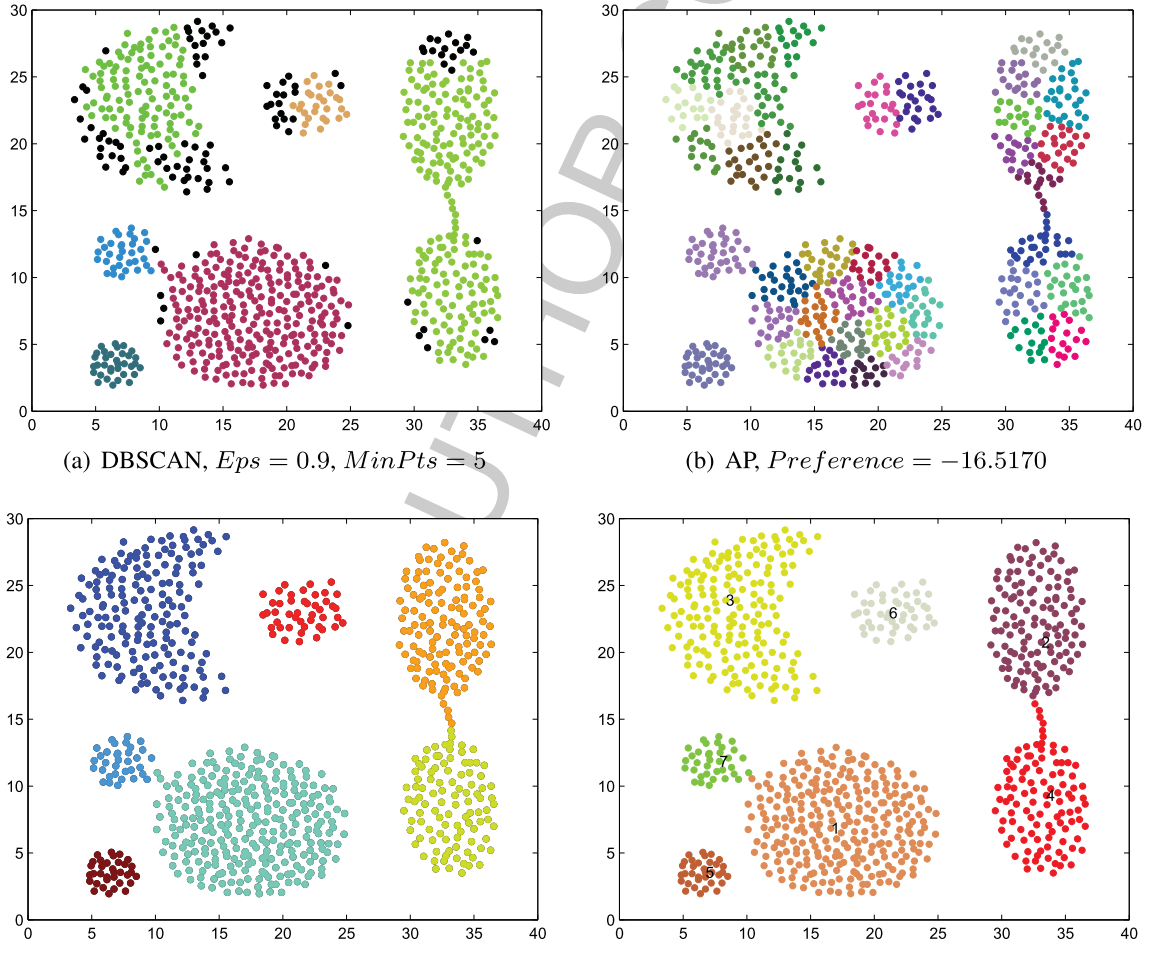


Fig. 2. F-Measure with 7 different data sets.



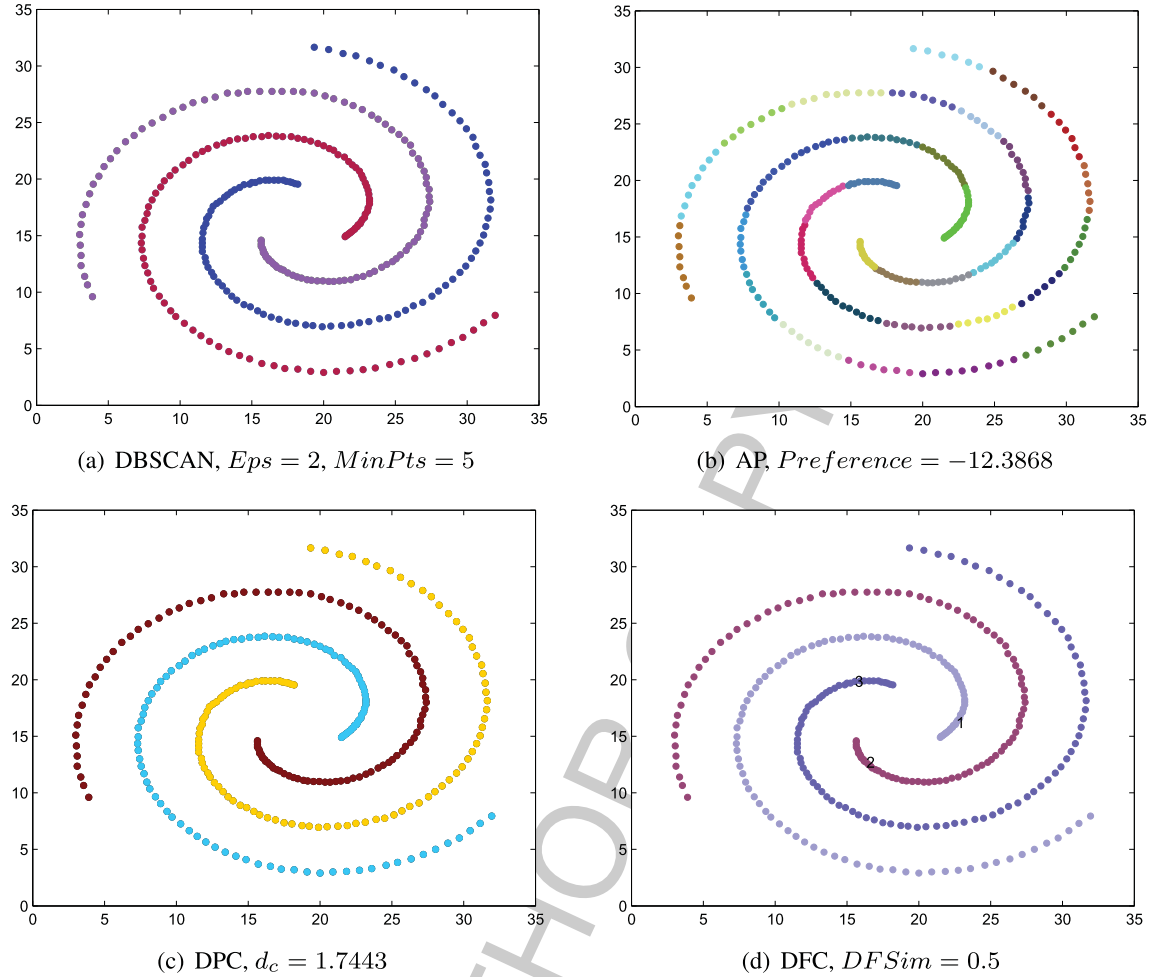
(a) DBSCAN, $Eps = 0.9$, $MinPts = 5$

(b) AP, $Preference = -16.5170$

(c) DPC, $d_c = 2.7212$

(d) DFC, $DFSim = 0.3024$

Fig. 3. Clustering the data set of *Aggregation* with varying sizes and irregular shapes.



(a) DBSCAN, $Eps = 2$, $MinPts = 5$

(b) AP, $Preference = -12.3868$

(c) DPC, $d_c = 1.7443$

(d) DFC, $DFSim = 0.5$

Fig. 4. Clustering the data set of *Spiral* with irregular shapes.

4.2. Irregular shapes

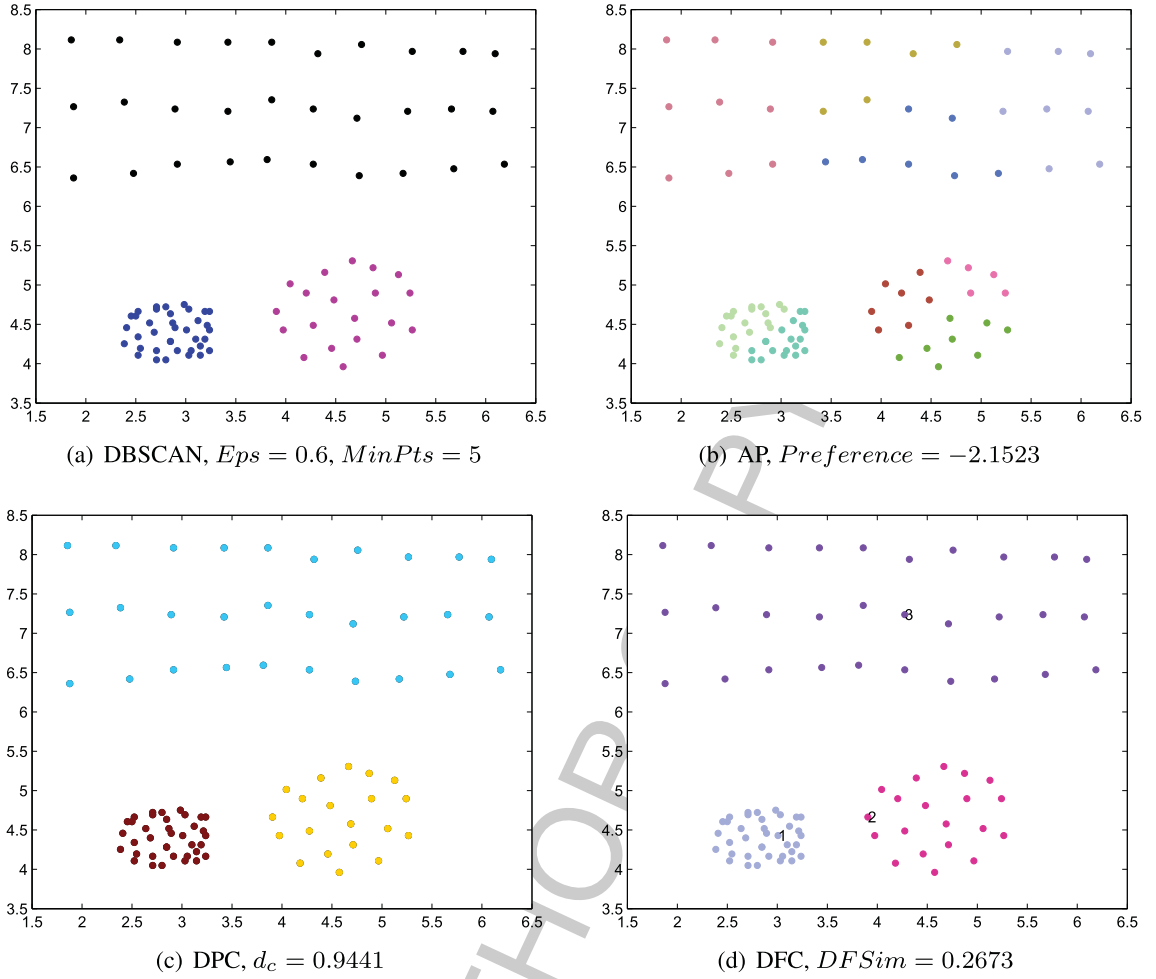
In general, density-based clustering algorithm has advantage of processing data sets with irregular shapes. *Aggregation*, *Spiral* and *Flame* can be adopted to evaluate its capability of processing irregular shapes. When compared with the DPC algorithm, the proposed DFC algorithm has the equal capability of clustering irregular shaped clusters shown in Figs. 3, 4 and 8. Compared with AP in these three data sets, DFC has the superior performance. DBSCAN gets a good result on *Spiral* clustering the same as the DPC and DFC in Fig. 4. However, DBSCAN cannot deal with the data sets such as *Aggregation* and *Flame* due to its incorrect anomaly detection. The DFC can detect the linear data like *Spiral* and also has the ability to handle irregular spherical data like *Aggregation* and *Flame*.

4.3. Varying densities

Data set D in Fig. 5 is used to test the advantage of the DFC in varying densities clustering. AP cannot solve this kind of data set when it gets the right cluster number. DBSCAN only detect the two cluster centers while the data set has the three centers actually, and all the points in the third cluster are recognized as anomalies which shown black color in Fig. 5. The DPC and DFC have a good performance in the data set D.

4.4. Number of clusters

The DPC has the advantage of finding cluster number by its decision graph [11]. However the DPC doesn't work well in data sets *Iris* or *Glass* which shown in Figs. 6 and 7, because it is difficult to select the suitable cluster centroids. The proposed



(a) DBSCAN, $Eps = 0.6$, $MinPts = 5$

(b) AP, $Preference = -2.1523$

(c) DPC, $d_c = 0.9441$

(d) DFC, $DFSim = 0.2673$

Fig. 5. Clustering with varying densities on *D* data set.

DFC can achieve reasonable clusters without human intervention.

4.5. Anomaly detection

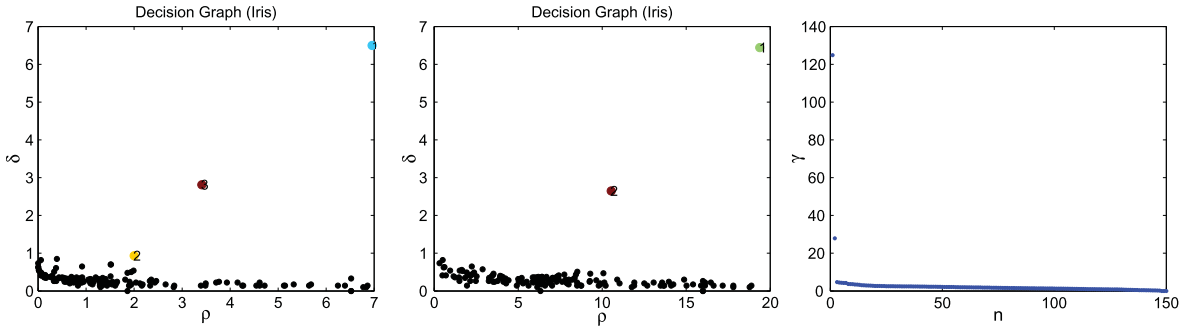
Anomaly detection is a basic function for any clustering algorithm. DBSCAN adopts *MinPts* and *density-reachability* to detect outliers, but this algorithm meets unsatisfied anomaly detection which shown in Figs. 3, 5 and 8. DPC takes outliers as halos without anomaly detection. As illustrated in Figs. 8 and 9, only the proposed DFC algorithm can figure these two outliers correctly in the top left corner in data set *Flame*.

5. Discussion

With the aggregation principle in DFC, clusters are formed by merging *density fragments* based on *network structural similarity* and *density decreasing sequence*. To analyse the strengths and weaknesses of the proposed DFC algorithm, the elaborate analysis of simulation results shown in Section 4 are made to know its capability of processing data sets with varying sizes, irregular shapes and varying densities, of detecting the number of clusters and outliers.

5.1. Analysis of processing varying sizes

As illustrated in Section 4.1, both DFC and DPC can detect clusters correctly with varying sizes.In DBSCAN algorithm, the true cluster cannot be found when there is a close line, and the wrong anomaly detecting disturb border points to reach their correct clusters. In AP algorithm, it is difficult to adjust global parameters to satisfy the data distribution in Fig. 3(b). To overcome the limitation of global parameters, each cluster in DPC is formed by determining its centroid



(a) 3 Centroids (b) 2 Centroids (c) γ distribution

Fig. 6. Decision graph of DPC with *Iris* data set.

and by absorbing lower density nodes based on inter-distances δ_i in Equation 6. The proposed DFC also has this capability because that the size of each cluster is determined by *network structural similarity* among *density fragments*.

5.2. Analysis of detecting irregular shapes

As illustrated in Figs. 3, 4 and 8, irregular shapes in data sets *Aggregation*, *Spiral* and *Flame* are extracted correctly by DPC and DFC algorithms. The DBSCAN algorithm gets good result in *Spiral* while fault in clustering *Aggregation* and *Flame*. The AP algorithm can get many fragments of each clusters, however it cannot combine them together to a reasonable cluster as depicted in Fig. 4(b). The DPC algorithm can get the correct clusters because each centroid is in the front part of a cluster and the following density decreasing nodes are near to them iteratively shown in Fig. 4(c). Similar as illustrated in Figs. 3 and 8, the reason for successful clustering in DFC is that density fragments are materials of any irregular shaped cluster and the merging principle is based on *network structural similarity* and *priori probability* without any direction guidance.

5.3. Analysis of processing varying densities

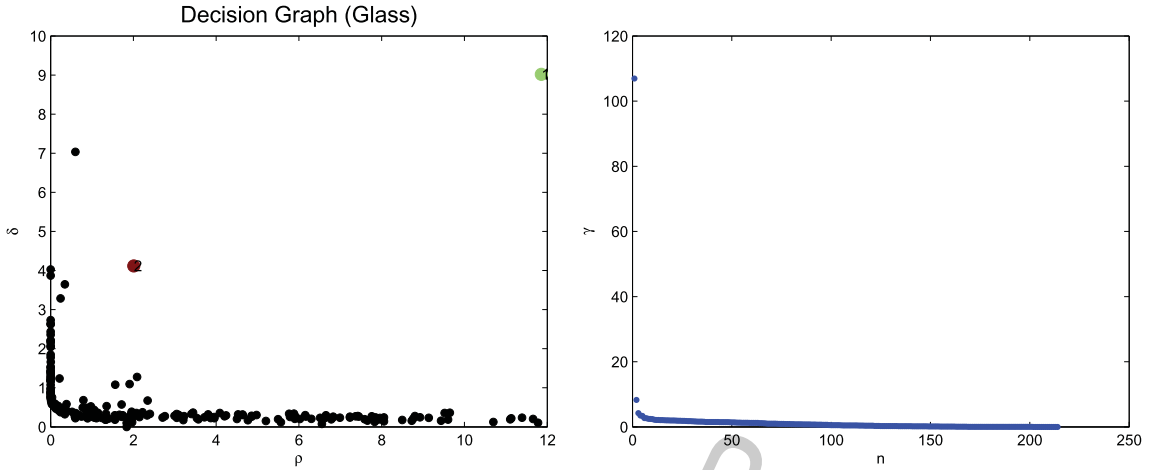
Generally speaking, it is an important capability of handling data sets with varying densities. DBSCAN algorithm cannot handle varying density data sets because it is distance-based clustering approach. As principles in DBSCAN, a node will be absorbed to a cluster if it is *density-reachable* or *density-connectivity* [7]. However, it is difficult to set the global density parameter in DBSCAN. Both DPC and DFC can handle data sets with varying densities because both of them do not adopt density principles in the stage of cluster generation. A cluster in DPC is formed by finding its centroid to absorb decreasing density nodes one by one [11]. The proposed DFC forms its cluster by merging density fragments with scalability in Equation 7.

5.4. Analysis of detecting the number of clusters

As illustrated in Figs. 6 and 7 in Section 4.4, the DPC algorithm will determine the number of clusters with human involvement. However, it is difficult for experts to determine the number of centroids in the decision graphs of Fig. 6(a) and (b). However, the proposed DFC algorithm has a relative advantage of detecting the number of clusters automatically when compared with DPC. The reason is that it will be unreasonable if the centroids of clusters are determined in a priori. In other words, more reasonable number of clusters should be determined by *density-reachability* and *density-connectivity* as DBSCAN. The proposed DFC algorithm does not determine each centroid of a cluster, while it forms a cluster by merging density fragments as SCAN.

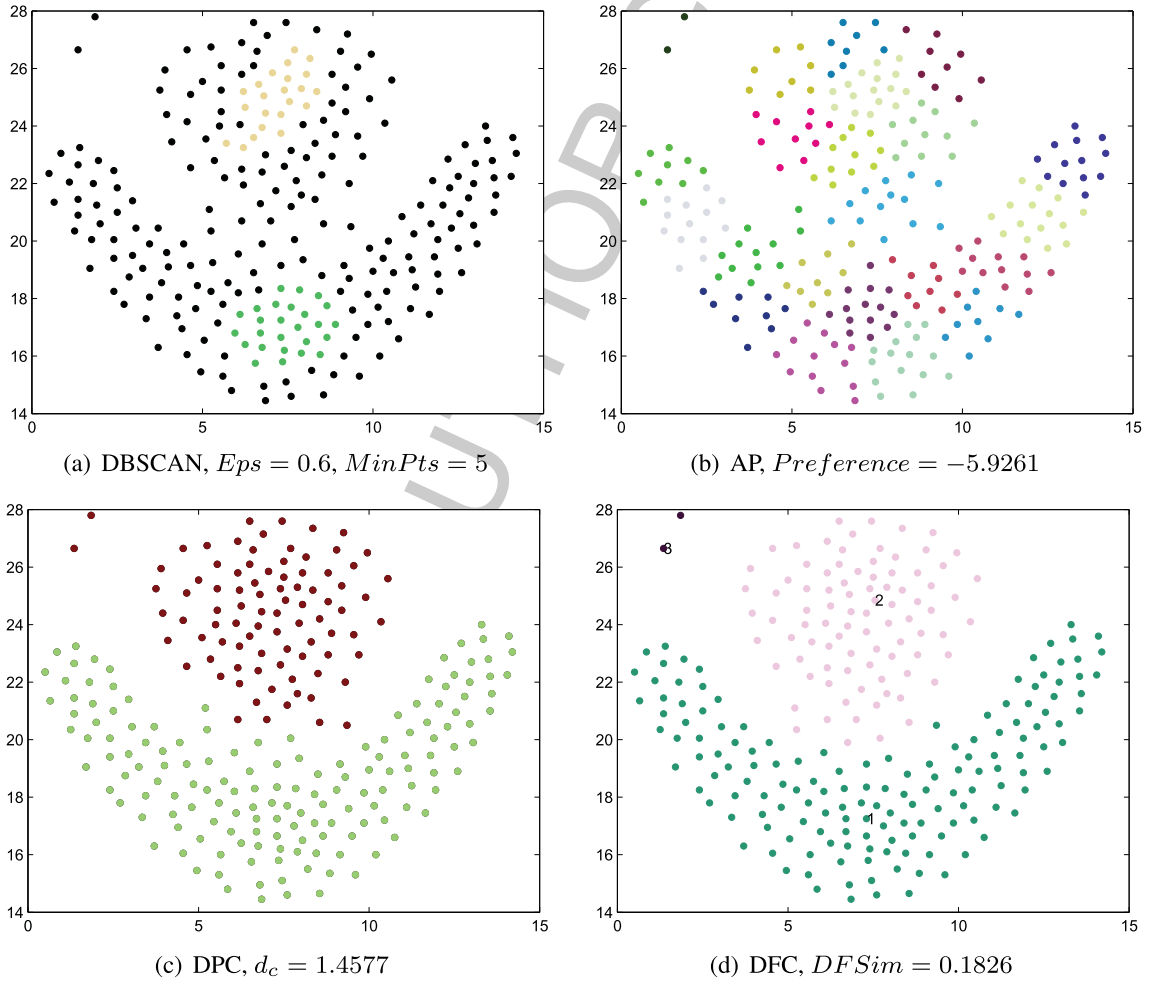
5.5. Analysis of anomaly detection

Compared with DPC, AP and DBSCAN shown in Figs. 8 and 9, only the proposed DFC algorithm can figure these two outliers correctly in the left top corner in the data set of *Flame*. DBSCAN algorithm has problems of finding outliers, and AP algorithm cannot find these two outliers with optimization by large amount of iterations. The state-of-the-art DPC algorithm cannot detect outliers when the distance between outliers and relative higher density nodes is less than d_c. However, the d_c will not be a small value to find a centroid of a cluster in a data set.



(a) Decision graph (b) γ distribution

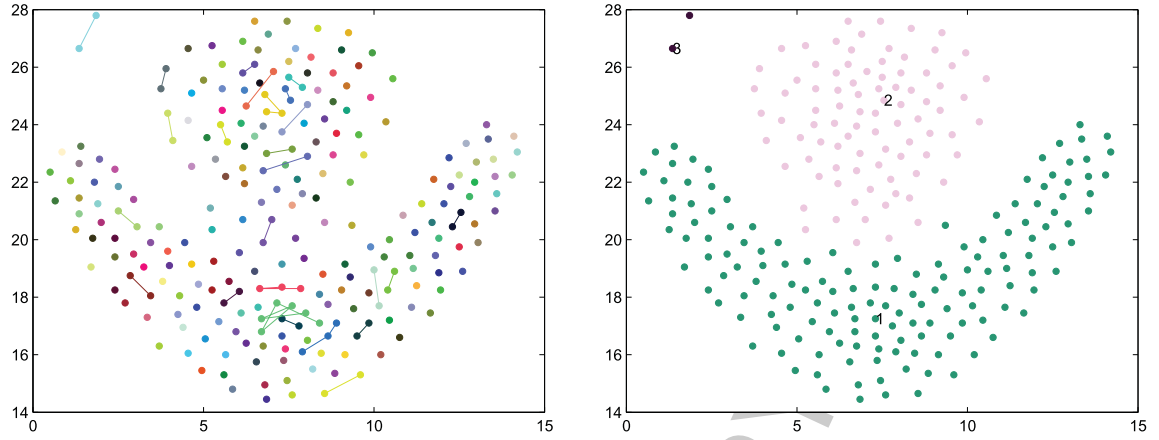
Fig. 7. Decision graph of DPC with *Glass* data set.



(a) DBSCAN, $Eps = 0.6$, $MinPts = 5$ (b) AP, $Preference = -5.9261$

(c) DPC, $d_c = 1.4577$ (d) DFC, $DFSim = 0.1826$

Fig. 8. Irregular shapes and anomaly detection of *Flame* data set.



(a) Core chian of density fragment (b) DFC

Fig. 9. Anomaly detection with DFC of *Flame* data set.

However, outliers are detected by density fragments and their density connectivity in our proposed DFC algorithm. Therefore, DFC has its advantage to detect outliers.

6. Conclusion

With inspiration by DPC, DBSCAN and SCAN algorithms, the proposed DFC is processed by merging *density fragments* with principles of *network structural similarity* and *density decreasing sequence* to improve its capability with varying sizes, varying densities and irregular shapes, with detecting the number of clusters and outliers. In this paper, the proposed DFC algorithm shows the power in some synthetic data sets. Besides the good feasibility, the DFC gets better clustering performances when compared with some classical methods, such as DBSCAN, AP and DPC in UCI data sets.

However, the proposed DFC algorithm does not perform well in a path-based data set such as Pathbase. Future research is to improve the performance of DFC algorithms on more complex data sets.

Acknowledgments

The authors are grateful to the financial support by the National Natural Science Foundation of China (No. 61572225), the Foundation of Jilin University of Finance and Economics (No. 2016P46) and the Foundation of Education Department of Jilin Province in China (No. JJKH20170119KJ).

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