Physica A 514 (2019) 25–35

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

DPC-LG: Density peaks clustering based on logistic distribution and gravitation☆

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HIGHLIGHTS

- New density calculation method based on logistic distribution is proposed.
- The capability of aggregating some non-spherical clusters is enhanced effectively.
- The density order is improved more reasonable.

ARTICLE INFO

Article history:
Received 1 June 2018
Received in revised form 28 August 2018
Available online 5 September 2018

Keywords:
Density peaks
Logistic distribution
Gravitation theory

MSC:
00-01
68T10

ABSTRACT

The Density Peaks Clustering (DPC) algorithm, published in *Science*, is a novel density-based clustering approach. Gravitation-based Density Peaks Clustering (GDPC) algorithm, inherited the advantages of DPC, is an improved algorithm. GDPC is able to detect outliers and to find the number of clusters correctly. However, it still has some problems in: (1) processing some data sets of varying densities; (2) processing some data sets of irregular shapes. An improved density clustering algorithm, named as DPC-LG, is proposed to overcome some weakness of GDPC. It can be seen from experimental results that the DPC-LG algorithm is more feasible and effective, compared with AP, DPC and GDPC.

1. Introduction

Clustering is aimed at grouping a set of objects in a way that objects are classified into categories on the basis of their similarity [1–3]. The approach has been applied in a wide variety of fields, including engineering, computer sciences, life and medical sciences, earth sciences, social sciences and economics [4–8].

Broadly, traditional methods in clustering can be categorized into: hierarchical method, partitioning method, density-based method, model-based method, grid-based method, and soft-computing method [9–11]. W.E. Wright [12] introduced gravitational clustering inspired by the motion of particles in space due to their gravitational attraction between each other. Gravitational clustering method can generate better clustering results, especially for border-line points, which has contributed significantly to the evaluation of clustering procedures [12]. Previously, agglomerative hierarchical clustering

☆ The authors are grateful to the financial support by the National Natural Science Foundation of China (no. 61572225), the Social Science Foundation of Jilin Province, China (no. 2018B79) and the Natural Science Foundation of the Science and Technology Department of Jilin Province, China (no. 20180101044JC).
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https://doi.org/10.1016/j.physa.2018.09.002
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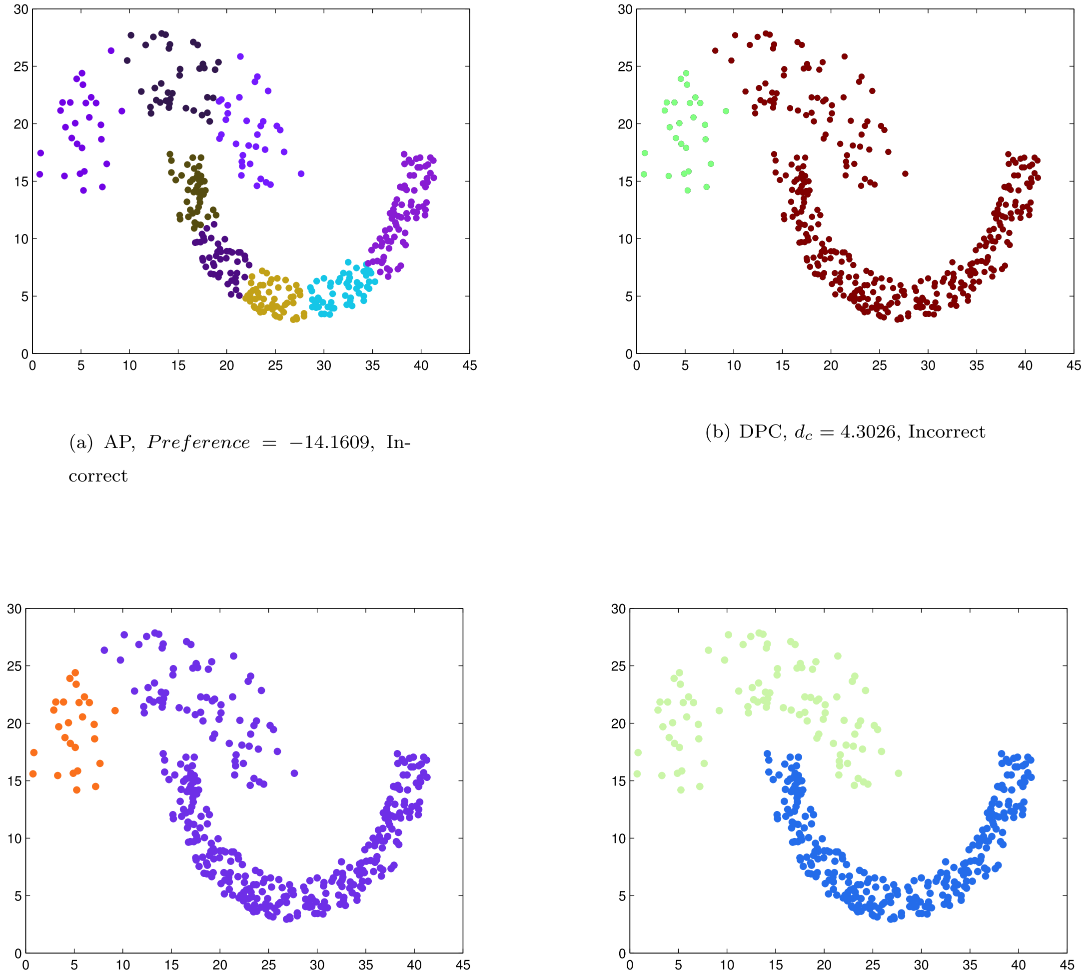


(a) AP, $Preference = -14.1609$, Incorrect

(b) DPC, $d_c = 4.3026$, Incorrect

(c) GDPC, $d_c = 5.4509$, Incorrect

(d) DPC-LG, $d_c = 5.1658$, Correct

Fig. 1. Aggregate the data set of *Jain*.

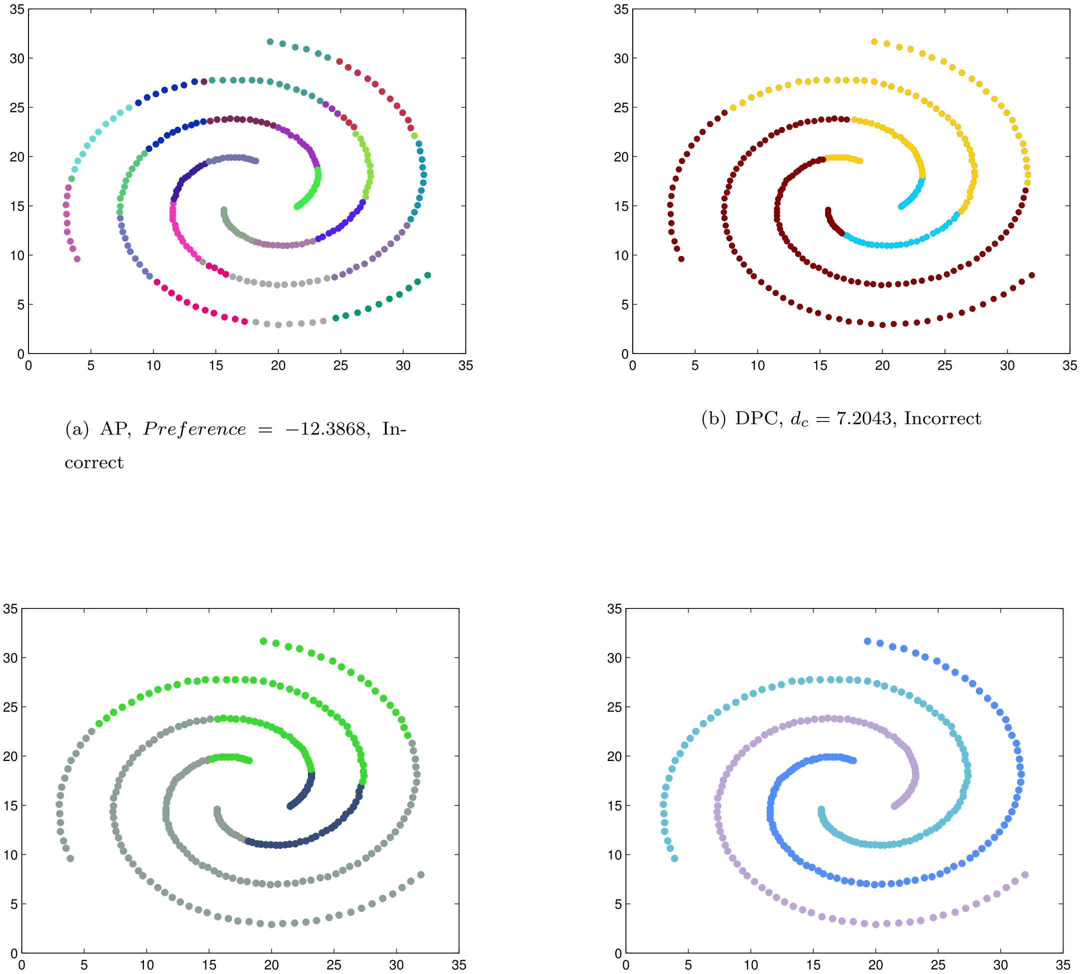
methods, based on Gaussian probability models, had shown great promise in a variety of applications [13]. The Gaussian probability model can provide efficiency for agglomerative hierarchical clustering algorithms [13].

A novel clustering algorithm, named as Density Peaks Clustering (DPC), was published in the journal *Science* [14]. DPC is a density-based clustering algorithm based on the idea that cluster centers are characterized by a higher densities and a relatively larger distance [14]. It is able to discover cluster centers rapidly, to recognize some shaped data sets, and to detect clusters regardless of varying size and varying densities. Focusing on this method, several researches [15–23] have been carried out to improve its capabilities.

However, DPC still has its deficiency in detecting outliers automatically and finding the number of clusters correctly [15,19,22], to which GDPC is well qualified. Inspired by DPC and Newton's law of gravitation, GDPC is an enhanced algorithm based on gravitation theory and nearby distance to identify centers and anomalies accurately [22]. However, it still has some problems in:

1. processing some data sets of varying densities;
2. processing some data sets of irregular shapes.

For example, GDPC cannot process *Jain* data set successfully presented in Fig. 1(c) though it found two cluster centers correctly. GDPC is also unable to aggregate the clusters well in *Spiral* data set. As is shown in Fig. 2(c), GDPC can detect the number of clusters, but it cannot achieve good cluster results. In Fig. 3, data points are marked in density order and NO.1 represents the data point of the highest density. The assignment rules of GDPC algorithm is the same to DPC algorithm; each point except for cluster centers is assigned to its nearest neighbor of higher density within the same cluster [14]. This can be explained by the assignment of data point NO.45. First, find data points with higher densities than data point NO.45; second,



(a) AP, $Preference = -12.3868$, Incorrect

(b) DPC, $d_c = 7.2043$, Incorrect

(c) GDPC, $d_c = 7.7345$, Incorrect

(d) DPC-LG, $d_c = 2.5812$, Correct

Fig. 2. Aggregate the data set of *Spiral*.

calculate distance between these data points and NO.45, and select the minimum distance. Thus, three points NO.24, NO.31, and NO.44 are discovered, $d_{(24,45)}$, $d_{(31,45)}$, and $d_{(44,45)}$ represent the minimum distance between point NO.45 and the above three points respectively, which is shown by the three colored lines as three possible cluster assignation. It is obvious that the red line is shorter than the other two, for which data point NO.45 is assigned to the second cluster. Clearly, the unreasonable distribution of data points contributes to the failure of cluster aggregation, caused by unreasonable order of the local density ρ. In GDPC method, density calculation can affect the order of ρ, because the local density ρ_i is simply computed by the number of neighbor points whose distances to point i are less than d_c. As a result, the local density ρ is a discrete value lacking smoothness.

In order to overcome the two problems, we are inspired by Gaussian probability models [13] to adopt logistic distribution to enhance GDPC. The local density is calculated by the probability density function (PDF) of the logistic distribution, instead of the number of neighbor points around point i. The approach is able to rationalize the order of ρ and aggregate the clusters effectively.

Thus a developed algorithm, named DPC-LG, is proposed. The approach is applied to *Iris*, *Breast* data sets and five shaped data sets, namely *Compound*, *Flame*, *Spiral*, *Jain* and *R15*. Compared with AP, DPC and GDPC, the enhanced DPC-LG has four advantages:

1. aggregate clusters with varying densities efficiently;
2. process non-spherical clusters effectively;
3. detect the number of clusters correctly;
4. discover outliers accurately.

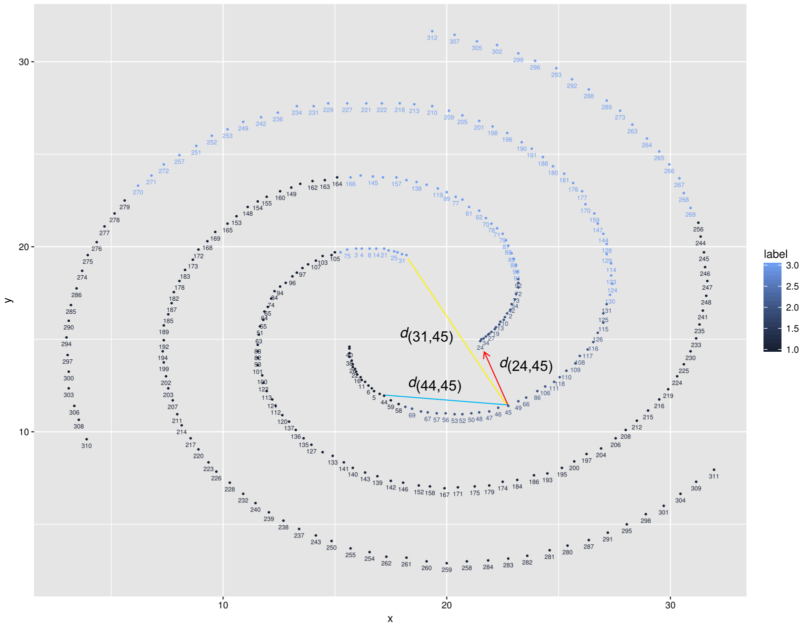


Fig. 3. Sorting density by **GDPC** on *Spiral* data set, $d_c = 7.7345$, **Incorrect**.

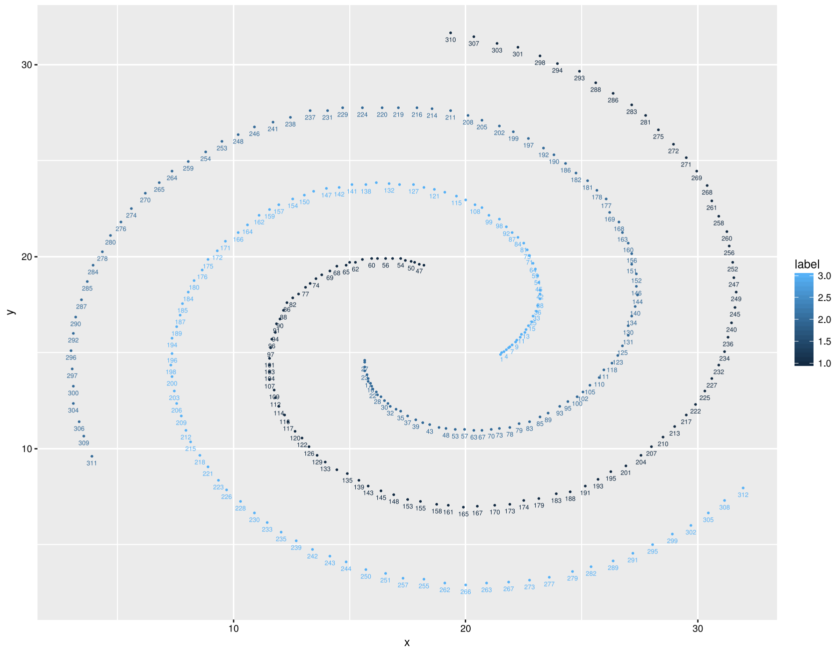


Fig. 4. Sorting density by **DPC-LG** on *Spiral* data set, $d_c = 2.5812$, **Correct**.

The rest of this paper is organized as follows. In Section 2, the DPC algorithm, GDPC algorithm and logistic distribution are described. In Section 3, density peaks clustering based on logistic distribution and gravitation algorithm is proposed. In Section 4, experimental results on some data sets are presented. In Section 5, some discussions are made to explain the major reasons. And some conclusions are drawn in the last Section.

2. Related work

The proposed DPC-LG algorithm is inspired by DPC [14], GDPC [22] and logistic distribution [24]. Brief reviews should be given in the following subsections.

Table 1
Mapping between Newton's law of gravitation and parameters from DPC [22].

Parameters from Gravitation	Parameters from DPC
m_i	ρ_i
m_j	ρ_j
r_i	δ_i

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 a relatively larger distance from points with higher density [14]. For each data point i, it computes two quantities: its local density ρ_i and its distance δ_i from points of higher density. These two quantities are relied on distance d_{ij} between data points.

$$d_{ij} = distance(i, j) \tag{1}$$

where the distance can be measured by distance functions, e.g. Euclidean distance. The local density of point i is given by Eq. (2).

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

where $\chi(d_{ij} - d_c) = 1$ if $(d_{ij} - d_c) < 0$ and $\chi(d_{ij} - d_c) = 0$ otherwise, cutoff distance d_c is the only user-defined parameter. 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 [14]. For the point i with the highest density, its distance δ_i is given by Eq. (3).

$$\delta_i = max(d_{ij}) \tag{3}$$

For the rest of points, distance δ_i is defined by Eq. (4).

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

2.2. GDPC: gravitation-based density peaks clustering algorithm

GDPC inherits the advantage of DPC, combined with law of gravitation. The GDPC assumes that cluster centers are characterized by a higher density than their neighbors and by a relatively lower gravitation to a point with higher density [22]. The GDPC requires three quantities: density ρ, distance δ and gravitation F. The calculation of density ρ and distance δ are similar to DPC. According to law of gravitation, gravitation F between object i and object j is given by Eq. (5).

$$F_{(i,j)} = G \times \frac{m_i \times m_j}{r_i^2} \tag{5}$$

As presented in Table 1. GDPC algorithm proposed the mapping between Newton's law of gravitation and parameters from the DPC.

According to Table 1, the function of gravitation F [22] is defined by Eq. (6).

$$F_{(i,j)} = G \times \frac{\rho_i \times \rho_j}{\delta_i^2} \tag{6}$$

2.3. The probability density function of the logistic distribution

In probability theory and statistics, the logistic distribution is a continuous probability distribution [24]. The probability density function (PDF) of the logistic distribution is given by Eq. (7).

$$f(x; \mu, \delta) = \frac{\pi}{\sqrt{3}\delta} \frac{e^{-\pi(x-\mu)/\sqrt{3}\delta}}{\{1 + e^{-\pi(x-\mu)/\sqrt{3}\delta}\}^2} \tag{7}$$

The corresponding cumulative distribution function is defined by Eq. (8).

$$F(x; \mu, \delta) = \frac{1}{1 + e^{-\pi(x-\mu)/\sqrt{3}\delta}} \tag{8}$$

when $\mu = 0$ and $\delta = 1$, the PDF of the logistic distribution is presented by Eq. (9).

$$f(x; 0, 1) = \frac{\pi}{\sqrt{3}} \frac{e^{-\pi x/\sqrt{3}}}{(1 + e^{-\pi x/\sqrt{3}})^2} \tag{9}$$

The corresponding cumulative distribution function is shown in Eq. (10).

$$F(x;0,1)=\frac{1}{1+e^{-\pi x/\sqrt{3}}} \tag{10}$$

This is the standardized form of the logistic distribution. When variable $z=-\pi x/\sqrt{3}$, the PDF of standard form is given by Eq. (11).

$$f(z)=\frac{1}{e^{z}+2+e^{-z}} \tag{11}$$

It is clear that the logistic density function in Eq. (11) is symmetric about zero, and it is similar to the normal distribution [24]. Its corresponding cumulative distribution function is given by Eq. (12).

$$F(z)=\frac{1}{1+e^{-z}} \tag{12}$$

3. Methods

The proposed DPC-LG algorithm inherits the strengths of GDPC and logistic distribution. Its main idea is similar to GDPC algorithm, but the calculation of local density ρ is different. As a rectification of GDPC, the DPC-LG algorithm includes three major steps: (1) calculate density and distance of points; (2) generate decision graph of gravitation; (3) aggregate clusters with gravitation.

3.1. Calculate density and distance of points

Like DPC method, a suitable cutoff distance d_c is selected to calculate the local density ρ_i, but the formula for density ρ_i is different from DPC algorithm. The probability density function of the standardized logistic distribution is adopted as shown in Eq. (11) that random variable z is distributed as logistic with mean 0 and variance $\pi^2/3$. So $u_{ij}=\frac{d_{ij}}{d_c}$ and the local density ρ_i is given by Eq. (13).

$$\rho_i=\sum_j \frac{1}{e^{u_{ij}}+2+e^{-u_{ij}}} \tag{13}$$

Distance δ_i is depended on density ρ_i and Euclidean distance shown in Eq. (1). Density of all data points are sorted in a descending order so that the point of the highest density can be found. Like DPC algorithm, for the point of the highest density, δ_i is measured by the maximum distance between the point and all other points in Eq. (3). For other points i, δ_i is defined by calculating the minimum distance between point i and all other points with relative higher density as shown in Eq. (4).

3.2. Generate decision graph of gravitation

According to Eq. (6), gravitation F is calculated. We adopt the reciprocal of gravitation F as the vertical axis and density ρ as the horizontal axis of decision graph. Cluster center is characterized by a higher density and by a relatively lower gravitation, so it is easy to find cluster centers which are prominent in the decision graph of gravitation.

3.3. Aggregate clusters with gravitation

Cluster centers are selected by decision graph and the remaining points i is assigned to each cluster. Finally, we can get the clusters that are aggregated by assignment process. The density peaks clustering based on logistic distribution and gravitation algorithm is depicted in Algorithm 1.

4. Results

To test its feasibility and effectiveness of the proposed DPC-LG algorithm, we compare it with AP, DPC and GDPC on *Iris*, *Breast* data sets and five shaped data sets, that is *Compound*, *Flame*, *Spiral*, *Jain* and *R15*. The attributes of these data sets are listed in Table 2.

F-Measure is used for testing the performance of AP, DPC, GDPC and DPC-LG. *F-Measure* index is the measure of 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* are defined as the following Eqs. (14)–(16). M_j is set of the number of results that should have been returned. C_i is set of the number of all returned results.

$$P(M_j,C_i)=\frac{|M_j\cap C_i|}{|C_i|} \tag{14}$$

Algorithm 1: DPC based on logistic distribution and gravitation algorithm.

Require: Initial points $X \in R_{N\times M}$ ($R_{N\times M}$ is the matrix of $N\times M$ dimensions), d_c (d_c is a cutoff distance)
Ensure: 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 certain percentage position in the above order.
Step 2: Detect cluster centers by density peaks
2.1 Calculate ρ_i based on Equation (13) ;
2.2 Sort points based on ρ in a descending order ;
2.3 Calculate δ_i based on Equation (3) and Equation (4) ;
2.4 Compute gravitation based on Equation (6);
2.5 Form the decision graph with density ρ and the reciprocal of gravitation F;
2.6 Detect centers and outliers from the decision graph.
Step 3: Assign each point to different clusters
3.1 Put outliers to a special cluster;
3.2 Assign each point with *clusterId* by its value of the reciprocal of gravitation F;
3.3 Iterate until all points are clustered.

Table 2
Seven different types of data sets.

Data sets	Points	Dimensions	Clusters
Iris	150	4	3
Breast	699	9	2
Compound	399	2	6
Flame	240	2	2
Spiral	312	2	3
Jain	373	2	2
R15	600	2	15

Table 3
F-Measure evaluation.

Data sets	AP	DPC	GDPC	DPC-LG
Iris	0.4851	0.7715	0.7715	0.7715
Breast	0.5491	0.7442	0.7533	**0.7607**
Compound	0.8303	0.7279	0.7784	**0.8341**
Flame	0.5789	1	1	1
Spiral	0.3008	0.7795	0.7795	**1**
Jain	0.4690	1	0.8038	1
R15	0.9867	0.9916	0.9867	**0.9932**

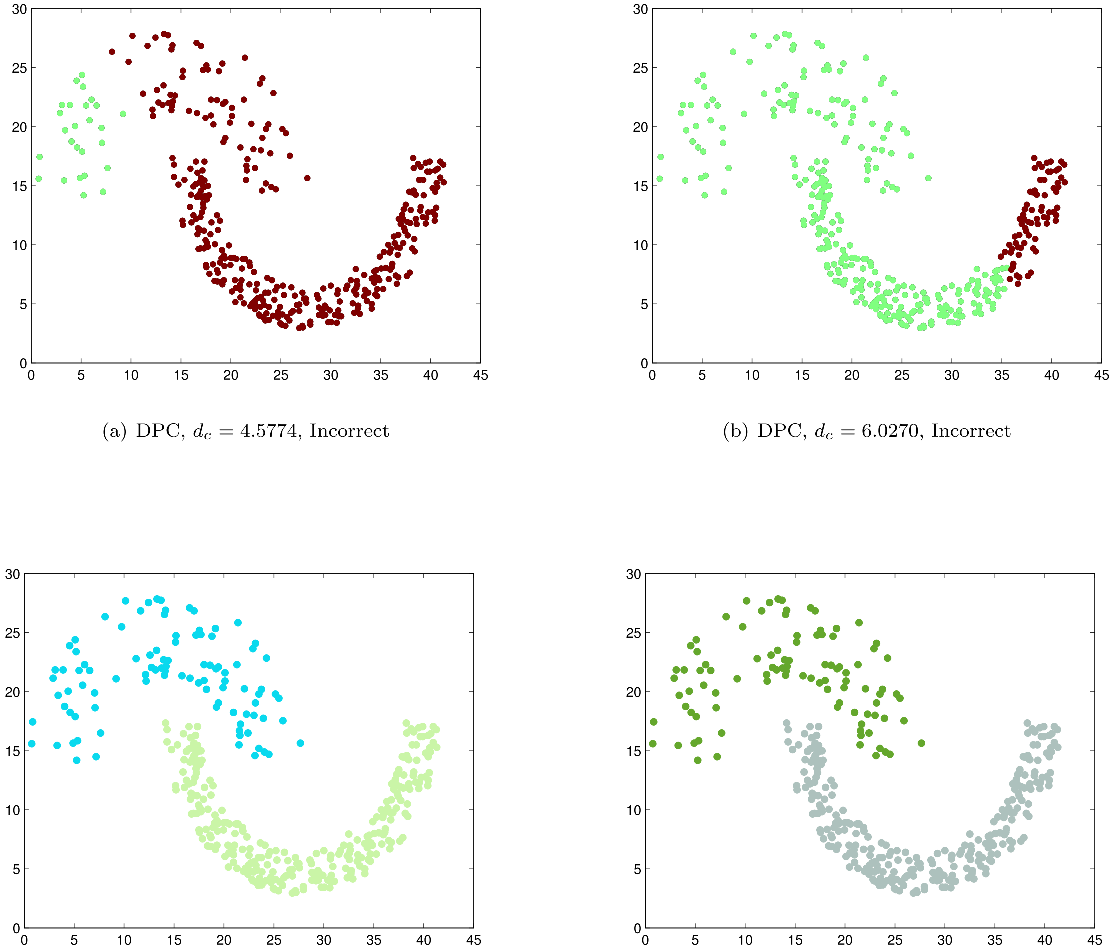
$$R(M_j, C_i) = \frac{|M_j \cap C_i|}{|M_j|} \tag{15}$$

$$F(M_j, C_i) = \frac{2 \times P(M_j, C_i) \times R(M_j, C_i)}{P(M_j, C_i) + R(M_j, C_i)} \tag{16}$$

The score of *F-Measure* is higher, and the performance of algorithm is better. The clustering results are depicted in Table 3, which are mean values based on 30 times run. It is found that DPC-LG obtains the highest *F-Measure* score on data sets of *Breast*, *Compound*, *Spiral* and *R15*. DPC-LG performs better or equally, compared with GDPC. Next, its capability is evaluated in terms of varying densities, irregular shapes, number of clusters and outliers detection.

4.1. Detect clusters of varying densities

The data set *Jain* has two clusters, one with higher densities, and the other with lower densities. *Jain* is applied to test the performance of DPC-LG in detecting clusters of varying densities. We make experiment with varying d_c in *Jain* data set. As is shown in Figs. 1 and 5, AP, DPC and GDPC are unable to find clusters with varying densities. DPC cannot detect *Jain* accurately with varying d_c. However, DPC-LG can achieve it successfully with varying d_c, stable cluster results with varying d_c is achieved. It is shown that the DPC-LG algorithm has stability.



(a) DPC, $d_c = 4.5774$, Incorrect

(b) DPC, $d_c = 6.0270$, Incorrect

(c) DPC-LG, $d_c = 4.5774$, Correct

(d) DPC-LG, $d_c = 6.0270$, Correct

Fig. 5. Aggregate the data set of *Jain* with varying d_c.

4.2. Detect clusters of irregular shapes

Spiral is applied to evaluate the performance of DPC-LG algorithm in processing irregular shapes. In Fig. 2, AP is unable to process *Spiral* data set. DPC and GDPC can find three clusters correctly, but they cannot aggregate *Spiral* data set efficiently and achieve good cluster results. Compared with AP, DPC and GDPC, DPC-LG is able to achieve better performance in *Spiral* data set.

4.3. Detect the number of clusters

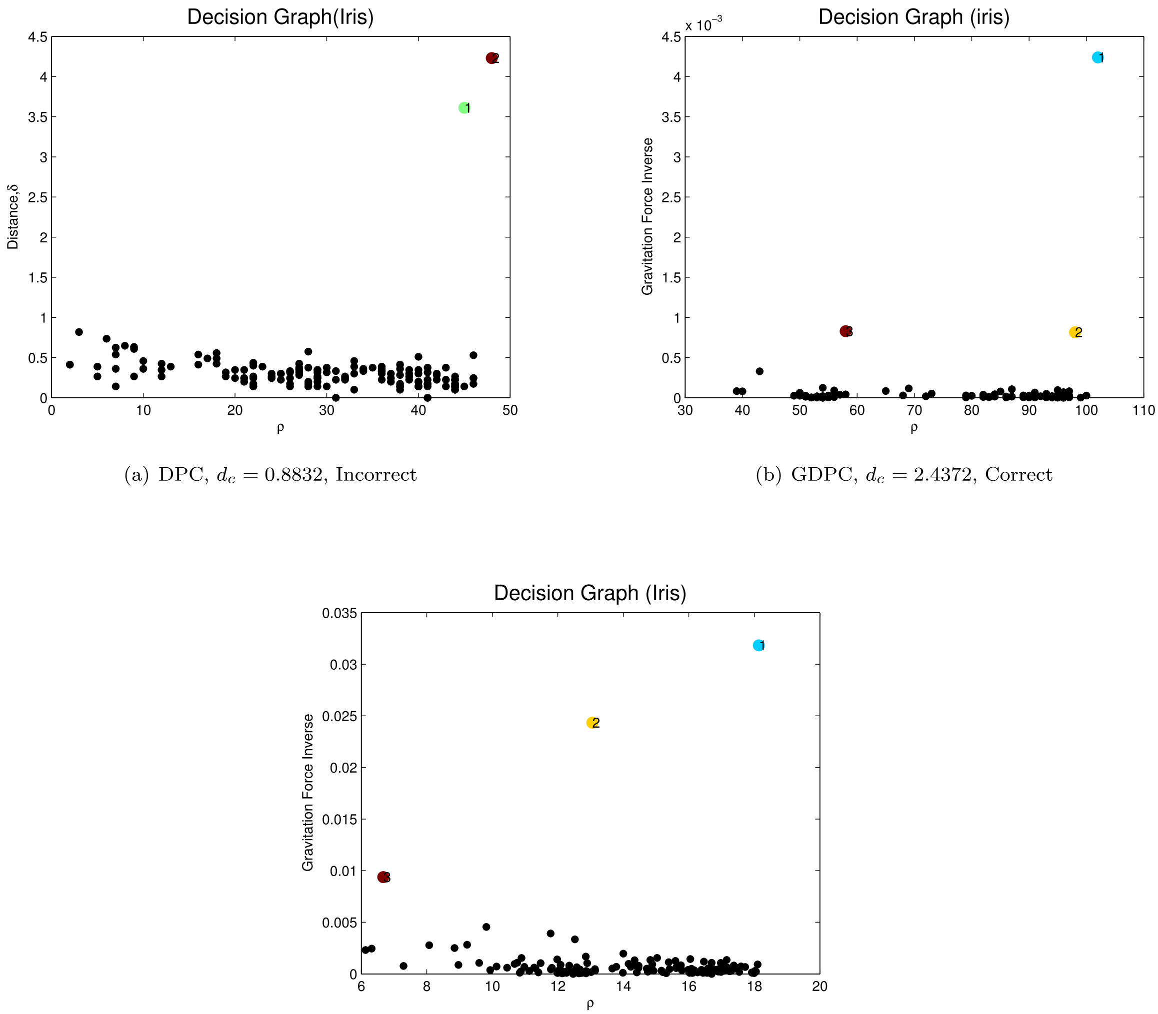
As illustrated in Fig. 6, it appears that GDPC and DPC-LG are superior to DPC in detecting the number of clusters. DPC can only distinguish two cluster centers, and it is difficult to recognize three cluster centers in *Iris*. However, GDPC and DPC-LG can make cluster centers notable in decision graph and find three cluster centers correctly.

4.4. Detect outliers

As is illustrated in Fig. 7, AP and DPC have poor performance in outlier detection. GDPC is able to recognize two points on the upper left corner as outliers. DPC-LG inherits the advantages of the GDPC, so it can also detect outliers successfully in *Flame* data set.

5. Discussion

To analyze the strengths and weaknesses of DPC-LG algorithm, its performance is discussed in cluster detection.



(a) DPC, $d_c = 0.8832$, Incorrect

(b) GDPC, $d_c = 2.4372$, Correct

(c) DPC-LG, $d_c = 0.8832$, Correct

Fig. 6. The decision graph of *Iris*.

5.1. Analysis of detecting varying densities

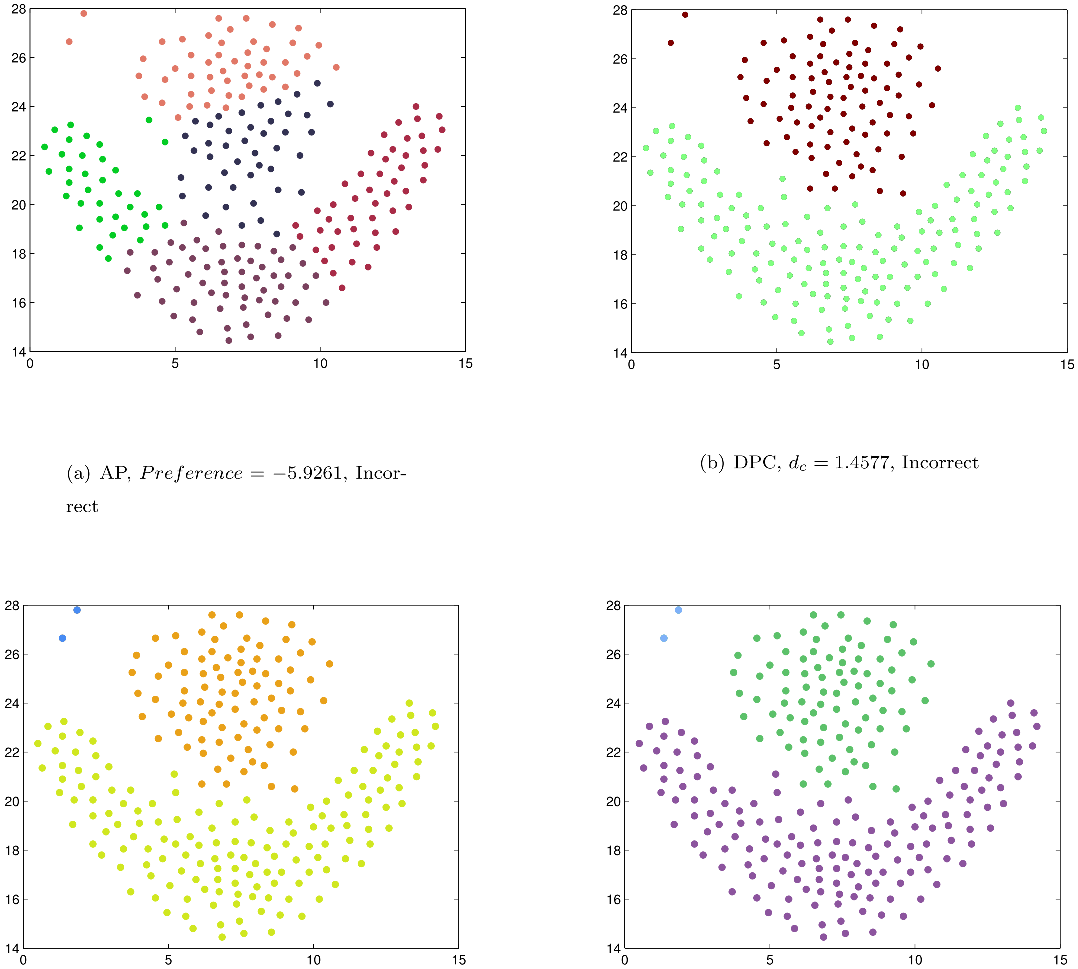
As is illustrated in Fig. 1, AP failed to discover two clusters, it detects seven clusters. AP is unable to identity correct clusters of varying densities. GDPC is also unable to aggregate the clusters of *Jain* data set correctly though it found two clusters successfully. From the experiment results of *Jain* data set, DPC cannot get good result, but DPC-LG can achieve greater performance in *Jain* with varying d_c. It is shown that the DPC-LG algorithm has stability. The reason why DPC-LG can aggregate *Jain* correctly with varying d_c is that the calculation of local density ρ is improved by logistic distribution.

5.2. Analysis of detecting irregular shapes

In Fig. 2, AP, DPC and GDPC cannot get good results, only DPC-LG can get correct clusters. As is illustrated in Fig. 3, it is found that GDPC clusters *Spiral* data set with unreasonable density, therefore, according to assignment rules of GDPC algorithm, data point NO.45 is assigned to the second cluster because the red line is shorter than the other two. As shown in Fig. 4, these data points are assigned to correct clusters successfully.

5.3. Analysis of detecting the number of clusters

In Newton's law of gravitation, the force is proportional to the product of the two masses and inversely proportional to the square of the distance between them. In Eq. (6), the law states the following: in a data set, each density point attracts



(a) AP, $Preference = -5.9261$, Incorrect

(b) DPC, $d_c = 1.4577$, Incorrect

(c) GDPC, $d_c = 1.8682$, Correct

(d) DPC-LG , $d_c = 0.9301$, Correct

Fig. 7. Detect outliers on the data set of *Flame*.

every single density of other points by the attractive force of gravity, the force is proportional to the data set of the densities of two points and inversely proportional to the square of the distance between them. For a normal point i except cluster centers, it has a relatively lower density and a relatively small distance to point j with higher density than point i. The force between point i and point j is large because δ_i is smaller and the force is inversely proportional to the square of δ_i. Conversely, the gravity of cluster center is small, and the reciprocal of its gravity is large. Therefore, its decision graph can make cluster centers notable and it is capable to find the number of clusters correctly.

5.4. Analysis of detecting outliers

In Fig. 7(a) and Fig. 7(b), neither DPC or AP has the ability to identify these two outliers. DPC algorithm cannot detect outliers when the distance between outliers and relatively higher density points is less than d_c. As presented in Fig. 7(c) and Fig. 7(d), both GDPC and DPC-LG can find these two outliers correctly in the left top corner, and they have great capability of outlier detection. The metric of *gravitation force inverse* can reduce the influence from d_c value [22].

6. Conclusion

It can be seen from experimental results that the DPC-LG algorithm is more feasible and effective, compared with AP, DPC and GDPC. Inspired by GDPC, DPC-LG overcomes the weakness of unreasonable density ordering by improving density calculation. DPC-LG has good performance in processing clusters of varying densities, clusters of irregular shapes, the number of clusters and outliers. GDPC applies law of gravitation to DPC algorithm, overcoming the weakness of detecting outliers and the number of clusters [22]. Absorbing logistic distribution function, DPC-LG achieves reasonable density ordering to ensure the stability of the algorithm. Therefore, on top of detecting outliers and the number of clusters, DPC-LG has greater ability to process clusters of varying densities correctly and process clusters of irregular shapes successfully.

However, the DPC-LG algorithm does not perform well in *Pathbased* [25] data set. It is necessary to make further research to improve the performance of DPC-LG algorithm on more complex data sets.

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