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# REDPC: A Residual Error-based Density Peak Clustering Algorithm

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## Abstract

The density peak clustering (DPC) algorithm was designed to identify arbitrary-shaped clusters by finding density peaks in the underlying dataset. Due to its aptitudes of relatively low computational complexity and a small number of control parameters in use, DPC soon became widely adopted. However, because DPC takes the entire data space into consideration during the computation of local density, which is then used to generate a decision graph for the identification of cluster centroids, DPC may face difficulty in differentiating overlapping clusters and in dealing with low-density data points. In this paper, we propose a residual error-based density peak clustering algorithm named REDPC to better handle datasets comprising various data distribution patterns. Specifically, REDPC adopts the residual error computation to measure the local density within a neighbourhood region. As such, comparing to DPC, our REDPC algorithm provides a better decision graph for the identification of cluster centroids and better handles the low-density data points. Experimental results on both synthetic and real-world datasets show that REDPC performs better than DPC and other algorithms.

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*Keywords:* clustering, density peak clustering, anomaly detection, residual error, low-density data points

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## 1. Introduction

Clustering algorithms aim to analyze data by discovering their underlying structure and organize them into different categories according to certain characteristic measures, such as internal homogeneity and external bifurcation, without priori-knowledge. Successful applications of clustering techniques are evident in various domains, such as pattern recognition in general [1–4], image understanding [5, 6], bioinformatics [7], lifestyle identification [8], disease diagnosis [9], cyber security [10], risk analysis [11] [12], etc. Moreover, some emerging topics, such as big data [13], virtual reality [14], and Internet of Things (IoT) [15], also avail from clustering methods. In general, clustering methods can be broadly categorized into five groups based on their dynamics, namely partitioning [16] [17], hierarchical [18], density-based [19] [20], model-based [21], and grid-based [22].

Density-based clustering algorithms have been widely applied to form arbitrary-shaped clusters by detecting high-density regions in the data space. Basically, the region with high-density, or a set of densely connected data points, is treated as a cluster. Density-based spatial clustering of applications with noise (DBSCAN) [23] is probably the most well-known density-based clustering algorithm engendered from the basic notion of local density. Recently, density-based clustering methods have attracted more attention since Rodriguez and Liao proposed their density peak clustering (DPC) algorithm [24] in 2014. The desirable features of DPC include i) relatively low computational complexity, ii) small number of control parameters in use, and iii) identification of cluster centroids of varying cluster sizes based on the generated decision graph.

Nonetheless, the performance of DPC highly relies on the value of the cutoff distance parameter  $C_d$ , which serves as a threshold to distinguish the level of

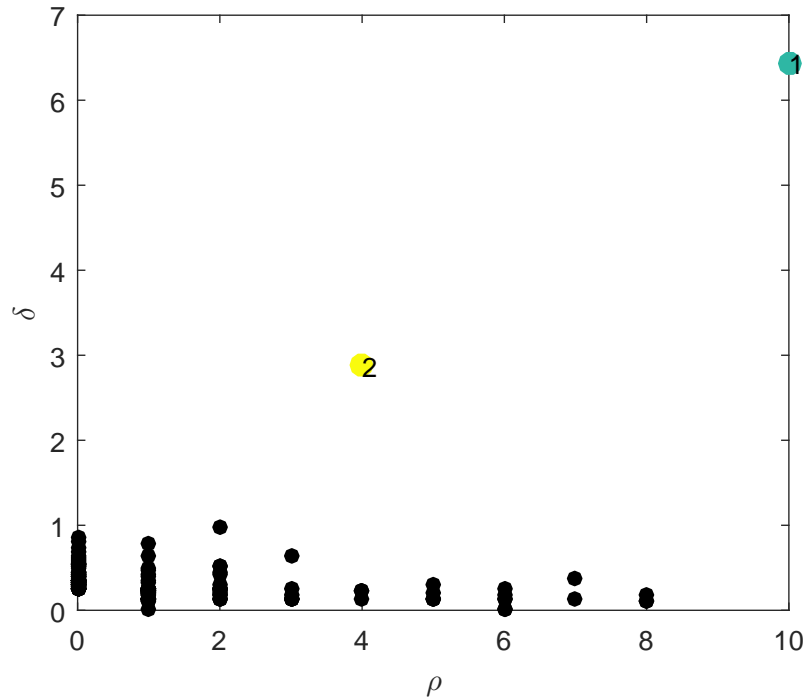


Figure 1: The decision graph generated by DPC on the *Iris* dataset ( $C_d = 0.2449$ ).

density in terms of distance between data points. Specifically, the identification of cluster centroids in DPC is performed manually with the facilitation of a generated decision graph, which is regulated by the value of  $C_d$  (see Section 2.2 for more technical details). For example, it is clearly shown in Figure 1 that only two cluster centroids (indexed as ‘1’ and ‘2’ with different colors) in the well-known 3-cluster *Iris* dataset are straightforwardly identified by the decision graph generated by DPC, even if the value of  $C_d$  is assigned in a systematic manner (cutoff at 1% of the sorted distances among all data points, see Section 2.2 for more technical details). As such, the performance of DPC is sometimes limited by its way of generating decision graphs.

Moreover, DPC does not perform well on anomaly detection, which is a beneficial function of clustering algorithms that the presence of anomalies indicates possible erroneous conditions that may lead to significant performance degrada-

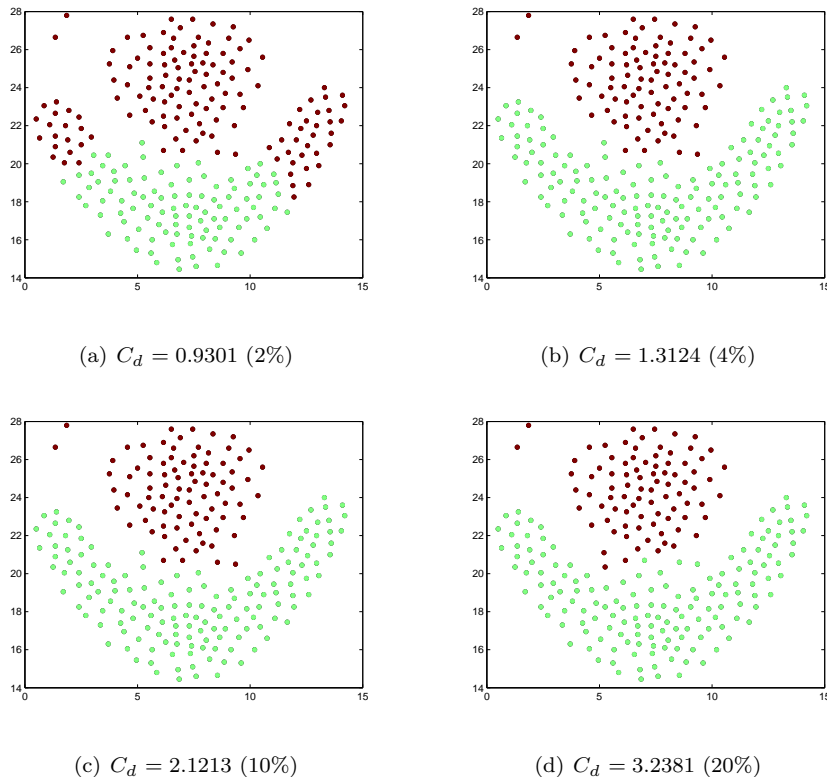


Figure 2: Clusters identified by DPC with different  $C_d$  parameter values on the *Flame* dataset.

tion [25]. As shown in Figure 2, DPC does not well handle the uneven cluster  
distribution (also pointed out in [26]) that the two anomalies (in the top left  
corner) are always considered as part of a larger cluster regardless of different  
 $C_d$  values in use, because there is no “noise-signal cutoff” used in DPC [24]. In  
such cases, DPC faces the difficulty in identifying the outliers even with varying  
 $C_d$  values and it may not be able to find clusters of small sizes or consisting of  
outliers (relatively speaking) only.

Therefore, to generate better decision graphs for cluster centroid identifica-  
tions by adopting more effective density measurement, and to better detect  
anomalies for comprehensive clustering results by further examining the border-  
line data points, in this paper, we propose a density-based clustering method

named Residual Error-based Density Peak Clustering (REDPC). Specifically, REDPC adopts the residual error computation to measure the local density within a neighbourhood region so that the generated decision graphs are better suited for cluster centroid identifications (see Section 3.1 for more technical  
55 details). Moreover, REDPC treats low-density data points as *halo points* (see Section 3.3 for more technical details) and further processes them to detect anomalies.

The term *halo* was originally defined by Rodriguez and Laio in [24] as a set of data points in certain *halo* regions that are “suitable to be considered as noise”  
60 (see Section 2.2). In this paper, we adopt the similar usage that let *halo points* refer to the set of low-density data points that require further analysis. Due to the further analysis applied to halo points, REDPC is shown to be capable of better identifying and handling various types of anomalies manifested in different patterns in different datasets (see Section 4).

In terms of performance evaluations, we apply REDPC on four UCI datasets  
65 and five synthetic datasets (two synthetic datasets are own-defined but publicly available online). For comparison purposes, we also apply K-Means [27], affinity propagation (AP) [18], DBSCAN [23] and DPC [24] on the same datasets. Experimental results show that our algorithm achieves the best performance on  
70 most datasets (specifically, best on eight out of nine datasets and the second best on the remaining dataset).

Our main contributions in this paper are listed as follows:

1. We adopt the residual error computation to measure local density within a neighbourhood region. As such, the generated decision graphs are better  
75 suited for cluster centroid identifications.
2. We perform further analysis on low-density data points after obtaining the intermediate clustering results. As such, the anomalies and borderline data points are better distinguished.
3. We empirically show with the experimental results on nine datasets that  
80 our proposed REDPC clustering method performs better than DPC and

other benchmarking clustering algorithms.

The rest of the paper is organized as follows. We briefly introduce the dynamics of DBSCAN and DPC as related work in Section 2. We present our proposed residual error-based clustering method in Section 3. We report the experimental results with comparisons and discussions in Section 4. We draw the conclusion and propose future work in Section 5.

## 2. Related Work

In this literature review section, we present the technical concepts and dynamics of two density-based clustering methods, which are closely related to ours. Specifically, we introduce the pros and cons of DBSCAN [23] and DPC [24] in the following two subsections, respectively.

### 2.1. DBSCAN: Density-Based Clustering Approach with Noise

DBSCAN is probably the most well-known and widely applied density-based clustering algorithm due to its following desirable features: i) efficient identification of arbitrary-shaped clusters, ii) scalability to large datasets [19], iii) small number of control parameters in use, iv) no predetermination on the number of clusters *a priori*, and v) ability to identify outliers. The dynamics of DBSCAN are based on the notion that clusters are defined as regions of considerably higher density, wherein the density, represented by the number of data points in the neighbourhood, exceeds a predefined threshold value. Moreover, the region with relatively lower density is kept outside the cluster and denoted as outliers. Definitions used in DBSCAN are given as follows:

**Definition 1:** *Eps*-neighbourhood of a data point

The *Eps*-neighbourhood of a data point  $p$  is defined as follows:

$$N_{Eps}(p) = \{q \in D \mid dist(p, q) \leq Eps\}, \quad (1)$$

where  $q$  denotes another data point in the dataset  $D$  and  $dist(\cdot)$  denotes the function used to compute distance between two data points.



105 **Definition 2:** Directly density-reachable

A data point  $p$  is directly density-reachable from another data point  $q$  with respect to  $N_{Eps}(p)$  and  $MinPts$  (minimum number of data points in the  $Eps$  neighbourhood of that data point), if  $p \in N_{Eps}(q)$  and  $N_{Eps}(q) \geq MinPts$ .

**Definition 3:** Density-reachable

110 A data point  $p$  is density-reachable from another data point  $q$  with respect to  $N_{Eps}(p)$  and  $MinPts$ , if there exists a chain of data points  $p_1, p_2, \dots, p_n, p_1 = q, p_n = p$  such that  $p_i + 1$  is directly density-reachable from  $p_i$ .

**Definition 4:** Density-connected

A data point  $p$  is density-connected to another data point  $q$  with respect to 115  $N_{Eps}(p)$  and  $MinPts$ , if there exists a data point  $o$  such that both  $p$  and  $q$  are density-reachable from  $o$  with respect to  $N_{Eps}(p)$  and  $MinPts$ .

**Definition 5:** Cluster

Let  $D$  be a set of data points. A cluster  $C$  with respect to  $N_{Eps}(p)$  and  $MinPts$  is a non-empty subset of  $D$  satisfying the following two conditions:

- 120
1.  $\forall p, q$ : if  $p \in C$  and  $q$  is density-reachable from  $p$  with respect to  $N_{Eps}(p)$  and  $MinPts$ , then  $q \in C$  (maximality).
  2.  $\forall p, q \in C$ :  $p$  is density-connected to  $q$  with respect to  $N_{Eps}(p)$  and  $MinPts$  (connectivity).

**Definition 6:** Noise

125 Let  $C_1, C_2, \dots, C_k$  denote the clusters identified in  $D$  with respect to  $Eps$  and  $MinPts$ , then we can define the noise as the set of data points in  $D$  not belonging to any cluster  $C_i, i = 1, \dots, k$ , i.e., noise =  $p \in D \mid \forall i : p \notin C_i$ .

During cluster formation, *direct density-reachability*, *density-reachability* and *density-connectivity* (see Definitions 2-4) are used by DBSCAN to characterize 130 symmetric and asymmetric relations between core points (i.e., high-density data points within clusters) and borderline points. Based on the pre-determined density parameters  $Eps$  and  $MinPts$ , clusters are formed comprising reachable core points and their corresponding borderline points. When there are no more data points that can be further added into any cluster, DBSCAN terminates. Re-

135 cently, an efficient distributed clustering scheme is proposed in [28], which uses  
only the borderline data points identified by DBSCAN to assist the clustering  
across multiple datasets that may be stored in local sites.

DBSCAN has two major advantages in identifying arbitrary-shaped clusters  
with outlier detection, namely the formation of a chain structure of high-density  
140 data points (i.e., core points) and the identification of outliers as low-density  
data points. However, DBSCAN is sensible to the user-defined parameter values  
and does not perform well on highly overlapped dense regions [29].

## 2.2. DPC: Density Peak Clustering

In a nutshell, DPC generates clusters by assigning data points to the same  
145 cluster of its nearest neighbour with higher density. Specifically, DPC uses  
the decision graph approach to identify cluster centroids that have the highest  
density. A decision graph is derived based on the following two fundamental  
properties of each data point  $x_i$ : i) local density  $\rho_i$  and ii) individual distance  
of each data point from other data points of higher density  $\delta_i$ .

Assume a dataset consists of  $X_{Y \times Z} = [x_1, x_2, \dots, x_Y]^T$ , where  
 $x_i = [x_{1i}, x_{2i}, \dots, x_{Zi}]$  denotes a vector with  $Z$  number of attributes and  $Y$  de-  
notes the total number of data points. The distance between two data points  
 $x_i$  and  $x_j$  is computed as follows:

$$d(x_i, x_j) = \|x_i - x_j\|, \quad (2)$$

150 where  $\|\cdot\|$  denotes Euclidean distance.

The local density of a data point  $x_i$ , denoted as  $\rho_i$ , is then defined as:

$$\rho_i = \sum_j \chi(d(x_i, x_j) - C_d), \quad (3)$$

$$\chi(a) = \begin{cases} 1, & \text{if } a < 0, \\ 0, & \text{otherwise,} \end{cases} \quad (4)$$

where  $C_d$  denotes the cutoff distance that user specified to distinguish the level  
of density. In DPC, the value of  $C_d$  can be autonomously determined in a

systematic way as follows:

$$C_d = D_{Y_d \times \frac{p}{100}}, \quad (5)$$

where  $Y_d = \binom{Y}{2}$ ,  $D_{Y_d \times \frac{p}{100}} \in D = [d_1, d_2, \dots, d_{Y_d}]$ , wherein  $D$  denotes the set of all the distances between every pair of two data points in a dataset, sorted in ascending order, and  $p$  denotes the user specified cutoff percentile.

On the other hand,  $\delta_i$  is defined as the shortest distance from any other data point that has a higher density value than  $x_i$ . If  $x_i$  has the highest density value,  $\delta_i$  is assigned to the longest distance to any other data point. Specifically,  $\delta_i$  is computed as follows:

$$\delta_i = \begin{cases} \min_{j: \rho_j > \rho_i} d(x_i, x_j), & \text{if } \exists j \text{ s.t. } \rho_j > \rho_i, \\ \max_j d(x_i, x_j), & \text{otherwise.} \end{cases} \quad (6)$$

After the computation of  $\rho_i$  and  $\delta_i$  for each data point in the given dataset, DPC autonomously generates a decision graph based on the computed  $\rho$  and  $\delta$  values (see Figure 3) and subsequently asks the user to determine cluster centroids. As a rule of thumb, data points with higher  $\rho$  and higher  $\delta$  values should be selected as cluster centroids. However, as shown previously in Figure 1 that because DPC considers all the data points during the computation of local density (see (3)), it may not perform well on overlapping clusters.

In terms of dealing with the cluster boundaries, for each cluster, DPC defines a border region, which is a set of data points that are assigned to the underlying cluster but within certain distance (i.e.,  $C_d$ ) from any data point belonging to another cluster. Furthermore, DPC locates the data point with the highest density within this border region of the corresponding cluster and makes use of its computed density  $\rho_b$ . Subsequently, “the points of the cluster whose density is higher than  $\rho_b$  are considered as part of the cluster core (robust assignment)” and “the others are considered as part of the cluster halo (suitable to be considered as noise)” [24]. However, according to the definition, a halo point has to be close to at least one data point belonging to another cluster. Therefore, DPC may not well handle certain low-density data points, especially

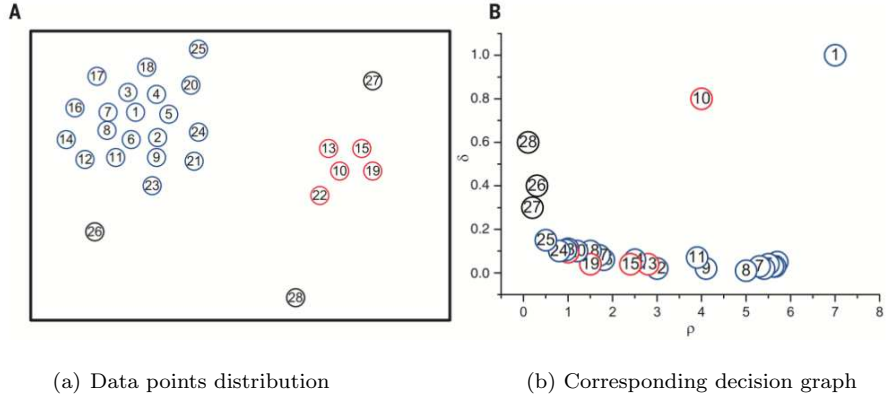


Figure 3: An example of DPC’s decision graph (excerpted from [24]).

if they are not near to other identified clusters. As shown previously in Figure 2, the two data points in the top left corner are always considered as part of a larger cluster regardless of different  $C_d$  values in use.

### 3. REDPC: Residual Error-based Density Peak Clustering Algorithm

180 To better deal with overlapping clusters and low-density data points, we propose Residual Error-based Density Peak Clustering (REDPC) algorithm. Specifically, we learn from DPC in using decision graphs to identify cluster centroids, learn from DBSCAN in determining density connectivities within a neighbourhood, and learn from the residual error theory in measuring density.

185 The overall process of REDPC consists of the following four stages and each stage is elaborated in the following four subsections, respectively:

1. *Preprocessing*: Firstly, the residual errors of individual data points are computed as local density measurement and then  $\delta$  (see the following subsection) is computed as distance measurement.
- 190 2. *Initial assignment*: Secondly, the decision graph is generated, cluster centroids are identified, and data points are intermediately assigned to the respective clusters.

3. *Halo identification*: halo points (consists of both borderline points and anomalies) are identified.
- 195 4. *Anomaly refinement*: Finally, anomalies are isolated from *halo points* and further processed before presenting the final clustering result.

### 3.1. Preprocessing

To construct better decision graphs for more distinguishable cluster centroid identifications, we adopt the residual error computation to measure the density  
 200 of each data point within its neighbourhood region. Specifically, the residual error  $e_{ij}$  between data point  $x_i$  to its neighbour  $x_j$  is computed as follows:

$$e_{ij} = \frac{\|x_i - x_j\|}{N}, \quad (7)$$

where  $N$  is a user-defined constant parameter denoting the neighbourhood size. Specifically,  $N$  is an integer used to find  $N$  number of the nearest neighbours of  $x_i$ , wherein Euclidean distance is used as the same as DPC (see (2)). Furthermore, the residual error of  $x_i$  can be computed as follows:

$$e_i = \sum_j e_{ij} = \sum_j \frac{\|x_i - x_j\|}{N}. \quad (8)$$

Comparing (8) to (3), it is obvious that by adopting the residual error computation, when measuring the local density, REDPC only takes the data points within the neighbourhood into consideration. In contrast, DPC takes all the  
 205 data points in the entire dataset into consideration. By only considering the local regional density, REDPC is capable of generating better decision graphs for cluster centroid identifications (see Section 4).

Moreover, we use  $\delta_i$  to denote the minimum distance of data point  $x_i$  to another data point with lower residual error. Specifically,  $\delta_i$  is computed as  
 210 follows:

$$\delta_i = \begin{cases} \min_{j:e_j < e_i} \|x_i - x_j\|, & \text{if } \exists j \text{ s.t. } e_j < e_i, \\ \max_j \|x_i - x_j\|, & \text{otherwise.} \end{cases} \quad (9)$$

The dynamics of the preprocessing procedures in REDPC are summarized in Algorithm 1.

---

**Algorithm 1** The preprocessing procedures in REDPC

---

**Input:** Dataset  $D$  comprising  $n$  number of data points and user predefined neighbourhood size  $N$

**Output:** Euclidean distance matrix  $DM$  of size  $n * n$ , residual error vector  $e$ ,  $sortd\_e$  ( $e$  sorted in ascending order), minimum distance vector  $\delta$ , and index vector of the nearest neighbour of each data point  $NNeigh$

Compute the Euclidean distance between data points to obtain  $DM$ ;

**for** each data point  $x_i$  in  $D$  **do**

    find its neighbours  $N_i$  based on  $DM$  and  $N$ ;

**for** each data point  $x_j$  in  $N_i$  **do**

        compute  $e_{ij}$  (see (7));

**end for**

**end for**

aggregate  $e_{ij}$  to obtain  $e$  and sort  $e$  in ascending order to obtain  $sortd\_e$ ;

compute  $\delta$  (see (8) and (9));

obtain  $NNeigh$  based on  $sortd\_e$ ;

---

### 3.2. Initial Assignment

After preprocessing, REDPC then generates a decision graph based on  $e_i$  (see (8)) and  $\delta_i$  (see (9)) computed for each data point  $x_i$  in the underlying dataset (see Figure 7(a) in Section 4). As a rule of thumb, data points with lower  $e_i$  values and higher  $\delta_i$  values should be selected as cluster centroids. After the identification of cluster centroids, based on the shortest distance between any unassigned data point  $x_j$  to any data point  $x_i$  that has been assigned with its corresponding cluster label, assign  $x_j$  to the same cluster as  $x_i$ . Repeat this assignment procedure until all the data points have been assigned with certain cluster labels. As such, we obtain the initial assignments of all data points.

The dynamics of initial assignment procedures in REDPC are summarized in Algorithm 2.

---

**Algorithm 2** The initial assignment procedures in REDPC

---

**Input:** user identified cluster centroids  $CC$ ,  $sortd\_e$  and  $NNeigh$  obtained from Algorithm 1

**Output:** cluster labels assigned to all the data points  $Cl$

assign cluster labels to all cluster centroids in  $CC$  to obtain initial  $Cl$ ;  
**while** there still exists a data point with no cluster label assigned **do**  
    based on  $Cl$ ,  $sortd\_e$  and  $NNeigh$ , find data point  $x_i$  to be assigned;  
    assign  $x_i$  with the cluster label of its nearest neighbour;  
    update  $Cl$  accordingly;  
**end while**

---

225 *3.3. Halo Identification*

After the initial assignment of cluster labels, we first identify the halo points from each intermediate cluster for later anomaly detections (in the final stage). To identify the halo points, we need to determine the value of the cutoff parameter  $C_d$ . In REDPC,  $C_d$  is defined as the same as that in DPC (see (5)), which  
230 is systematically determined based on the user specified cutoff percentile  $p$ .

Subsequently, for each data point  $x_i$  in cluster  $A$ , if there exists a data point  $x_j$  in cluster  $B$  and  $B \neq A$  that the distance between  $x_i$  and  $x_j$  is less than the cutoff threshold, i.e.,

$$\|x_i - x_j\| < C_d, \quad (10)$$

then we compute the mean of the residual values of the two data points as follows:

$$mean\_e_{ij} = \frac{1}{2}(e_i + e_j). \quad (11)$$

For each identified cluster  $K$ , we use a variable named residual threshold  $rt_K$  to denote the threshold for the residual value of each corresponding cluster.

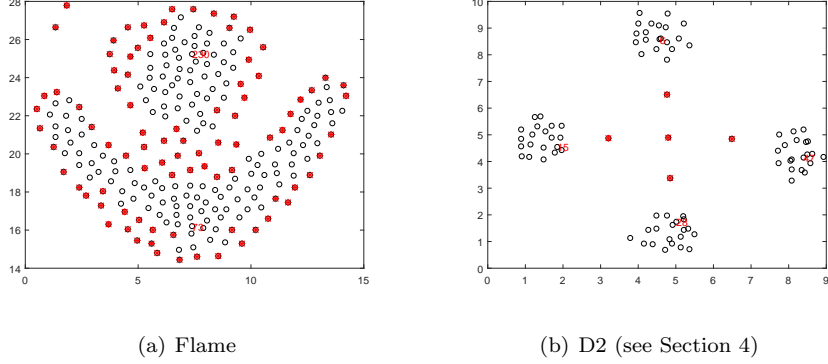


Figure 4: Illustrations of identified halo points, represented with asterisks in red color.

The value of  $rt_K$  is initialized to a large number. If  $x_i$  is found in cluster  $A$ ,  $x_j$  is found in cluster  $B$ , and they fulfil the inequality defined in (10), then the residual thresholds for both clusters are updated as follows:

$$rt_K = \text{mean}_{.e_{ij}}, \text{ if } rt_K > \text{mean}_{.e_{ij}}, K = A, B. \quad (12)$$

After updating  $rt$  for all the clusters, we can then determine the set of halo points in each cluster, denoted as  $halo_{set}$ , by adopting the following criterion:

$$halo_{set}_K = halo_{set}_K \cup x_i, \text{ iff } e_i > rt_K. \quad (13)$$

The dynamics of halo identification procedures in REDPC are summarized in Algorithm 3. The exact mechanisms adopted can be simply described as using borderline data points to determine the level of overlap between adjacent clusters, and subsequently identify the halo points in the border regions for further identification of possible anomalies. As illustrated in Figure 4, halo points are well identified by REDPC around the cluster borders.

### 3.4. Anomaly Refinement

It is of great importance to distinguish the anomalies from other normal data points in the identified clusters because anomalies highly likely represent the abnormal patterns or malicious activities in real-world scenarios. For example, unusual road traffic patterns may suggest nearby accidents or emergencies, unusual



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**Algorithm 3** The halo identification procedures in REDPC

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**Input:** dataset  $D$ ,  $Cl$  obtained from Algorithm 2,  $C_d$  computed according to (5) and  $e_{ij}$  obtained from Algorithm 1

**Output:** the set of halo points  $halo\ set$

initialize residual threshold  $rt$  to a large value for each cluster in  $Cl$ ;

**for** each data point  $x_i$  in  $D$  **do**

**for** each data point  $x_j$  in  $D$ ,  $i \neq j$  &&  $Cl(i) \neq Cl(j)$  **do**

**if** distance between  $x_i$  and  $x_j$  is within  $C_d$  (see 10) **then**

            compute the mean residual  $mean\_e_{ij}$  (see 11);

            update  $rt_{Cl(i)}$  and  $rt_{Cl(j)}$  if necessary (see 12);

**end if**

**end for**

**end for**

initialize  $halo\ set$  to  $\phi$ ;

**for** each data point  $x_i$  in  $D$  **do**

**if** halo point identification criterion is met (see 13) **then**

        update  $halo\ set$  accordingly;

**end if**

**end for**

---

credit card transactions may indicate identity theft, unusual computer network loads should alert the cyber security division, etc. Therefore, in REDPC, we further detect the anomalies and highlight them during visualization.

During anomaly detection, a halo point with high residual error and low  $\delta$  value is recognized as an anomaly and highlighted with a special symbol for clearer graphical representation (e.g., see Figure 8(f) in Section 4.2). The threshold values used to distinguish  $e$  and  $\delta$  are heuristically determined. Specifically, the threshold for residual error  $th_e$  is defined as

$$th_e = mean(e_i) + \frac{1}{2}(min(e_i) + max(e_i)) \quad (14)$$

and the threshold  $th_\delta$  is defined as

$$th_\delta = \frac{1}{2}(\min(\delta_i) + \max(\delta_i)). \quad (15)$$

Therefore, after the determination of  $th_e$  and  $th_\delta$  values, we can then identify the set of anomalies in the dataset, denoted as  $anaset$ , by adopting the following criterion:

$$anaset = anaset \cup x_i, \text{ iff } e_i > th_e \ \&\& \ \delta_i < th_\delta. \quad (16)$$

245 Moreover, if  $anaset$  is non-empty, we further investigate the most possible cluster label of each detected anomaly. This refinement is also intuitively designed that for each anomaly in  $anaset$ , we first find its nearest neighbours with the neighbourhood size as the same as  $N$  defined in (7). Furthermore, if within the neighbourhood of an anomaly, there exist other anomalies, we then  
 250 remove these anomalies from the neighbour because their cluster labels are not yet properly assigned. At last, we assign the cluster label of each anomaly to the majority cluster label in its neighbourhood (if the majority ties, we assign the cluster label of the nearest data point belonging to any of the tying clusters). Due to the incorporation of such refinement of the identified anomalies,  
 255 not only the clustering results may be improved, but also these anomalies are highlighted visually for human inspections (see Section 4).

The dynamics of anomaly refinement procedures in REDPC are summarized in Algorithm 4).

### 3.5. Overall REDPC Dynamics and Its Computational Complexity

260 The dynamics of REDPC is depicted in Figure 5, wherein the information flow among the underlying dataset, user inputs, and the REDPC algorithms are explicitly shown. Moreover, the computational complexity of REDPC is shown in Table 1, wherein  $n$  denotes the number of data points in the underlying dataset and  $m$  denotes the number of halo points obtained from Algorithm 3.  
 265 In normal circumstances,  $m \ll n$ .

Comparing to other clustering algorithms benchmarked in this paper, REDPC has a middle level of computational complexity as shown in Table 2,

---

**Algorithm 4** The anomaly refinement procedures in REDPC

---

**Input:**  $DM$ ,  $e$  and  $\delta$  obtained from Algorithm 1,  $Cl$  obtained from Algorithm 2,  $halo\text{set}$  obtained from Algorithm 3 and user specified neighbourhood size  $N$

**Output:** the set of anomalies  $an\text{oset}$  and refined  $Cl$

```

initialize  $an\text{oset}$  to  $\phi$ ;
compute thresholds  $th_e$  and  $th_\delta$  (see (14) and (15));
for each data point  $x_i$  in  $halo\text{set}$  do
    if  $x_i$  fulfils the anomaly criterion then
        append  $x_i$  to  $an\text{oset}$  (see (16));
    end if
end for
for each data point  $x_j$  in  $an\text{oset}$  do
    find the neighbours  $N_j$  according to  $N$ ;
    remove anomalies (both assigned and yet-to-be-assigned) from  $N_j$ ;
    assign the cluster label of  $x_j$  to the majority cluster label in  $N_j$ ;
end for

```

---

Table 1: Computational complexity of REDPC

Stage:	Algo. 1	Algo. 2	Algo. 3	Algo. 4	Overall Algo
Complexity:	$O(n^2)$	$O(n \log n)$	$O(n^2)$	$O(mn)$	$O(n^2)$

wherein  $I$  denotes the number of iterations and  $K$  denotes the user predefined number of clusters. Moreover, in the following experiment section, we also compare the computational time taken by all the clustering algorithms.

#### 4. Experiments

To evaluate the performance of REDPC, we apply it on four UCI datasets, namely *Iris*, *Seeds*, *Wine* and *Thyroid*, three widely used synthetic datasets,

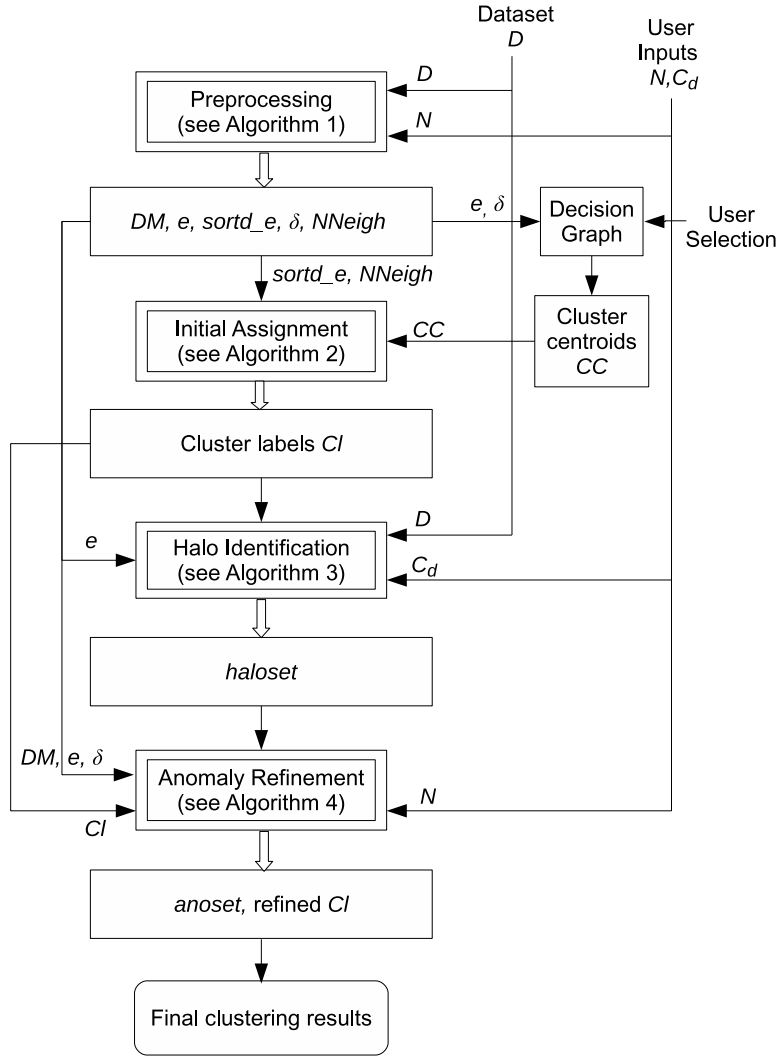


Figure 5: Dynamics of the overall REDPC algorithm.

Table 2: Computational complexity comparisons

Algorithm:	K-means	AP	DBSCAN	DPC	REDPC
Complexity:	$O(Kn)$	$O(In^2)$	$O(n \log n)$	$O(n^2)$	$O(n^2)$

Table 3: Properties of the UCI and synthetic datasets

Datasets	Properties		
	# Points	# Dimensions	# Clusters
Iris	150	4	3
Seeds	210	7	3
Wine	178	13	3
Thyroid	215	5	3
Flame	240	2	2
Aggregation	788	2	7
Spiral	312	2	3
D1	87	2	3
D2	85	2	4

namely *Flame*, *Aggression* and *Spiral*, and two own-defined datasets  $D1$ <sup>1</sup> and  
275  $D2$ <sup>2</sup>. The properties of these nine datasets are listed in Table 3. Moreover,  
we conduct experiments using K-Means [27] (to minimize the difference caused  
by randomness, averaged results of 10 independent runs are reported), AP [18],  
DBSCAN [23] and DPC [24] on the same datasets for comparisons.

In this paper, we use  $F$ -score to measure the accuracy of the clustering  
280 results. The performance comparisons among all the benchmarking models are  
reported in Table 4 and visualized in Figure 6. It is encouraging to find that  
REDPC achieves the highest  $F$ -score on eight out of nine datasets. Although  
REDPC only achieves the second best on *Aggregation*, the difference between  
the winner (DPC) and REDPC’s result is as small as  $1 - 0.9983 = 0.0017$  or  
285 0.17%. When we further examine the difference in terms of the number of  
correctly labelled data points, we find that the difference between DPC and  
REDPC is as small as 1 (out of the total number of 788 data points). As such,

<sup>1</sup>The  $D1$  dataset (with cluster labels) is available online: [https://www.dropbox.com/s/f3ynvm153i2500u/D1\\_with\\_label.csv?dl=0](https://www.dropbox.com/s/f3ynvm153i2500u/D1_with_label.csv?dl=0)

<sup>2</sup>The  $D2$  dataset (with cluster labels) is available online: [https://www.dropbox.com/s/899xltgq3gg09bg/D2\\_with\\_label.csv?dl=0](https://www.dropbox.com/s/899xltgq3gg09bg/D2_with_label.csv?dl=0)

Table 4: Performance Comparison

Datasets	K-Means	AP	DBSCAN	DPC	REDPC
Iris	0.8149	0.3924	0.7462	<b>0.8404</b>	<b>0.8404</b>
Seeds	0.8091	0.2833	0.6137	0.8025	<b>0.8106</b>
Wine	0.5896	0.2521	0.5052	0.5699	<b>0.5900</b>
Thyroid	0.7251	0.1814	0.6933	0.7545	<b>0.7890</b>
Flame	0.7432	0.1538	0.8833	<b>1</b>	<b>1</b>
Aggregation	0.7890	0.2117	0.8885	<b>1</b>	0.9983
Spiral	0.3278	0.1505	<b>1</b>	<b>1</b>	<b>1</b>
D1	0.8352	0.5445	<b>1</b>	<b>1</b>	<b>1</b>
D2	0.9976	0.9332	0.9332	0.9756	<b>1</b>

although DPC achieves slightly better performance than REDPC in terms of clustering accuracy, this small amount of difference may not be significant. In the following subsections, we elaborate on the performance of REDPC in various aspects, respectively.

In addition, the computational time spent by each algorithm (average of 10 runs for all models) is shown in Table 5. The comparison results are consistent with Table 2 that DBSCAN with the lowest computational complexity achieves the shortest computational time and REDPC with a middle level of computational complexity achieves a middle level of computational time. Comparing to DPC, although they both have the same computational complexity of  $O(n^2)$ , REDPC is always approximately 20 ms slower. This is mainly due to the additional refinement procedures taken by REDPC to better handle the anomalies (see Algorithms 3 and 4). However, this compensation on computational time greatly improves REDPC’s performance (see Table 4). Note that all the clustering algorithms were implemented using MATLAB and the experiments were conducted using the same 64-bit computer installed with Intel(R) Core(TM) i3-4160 CPU at 3.60 GHz and 8 GB RAM.

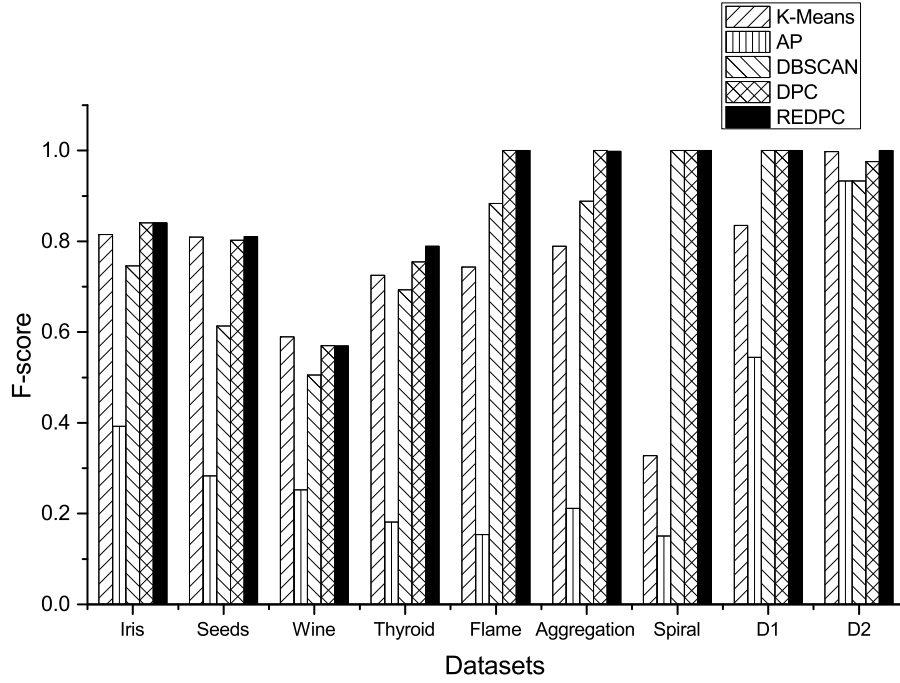


Figure 6: Visualization of performance comparison on nine datasets.

Table 5: Comparisons on computational time spent (in ms)

Datasets	K-Means	AP	DBSCAN	DPC	REDPC
Iris	148.2681	67.6571	1.9672	70.6112	93.5109
Seeds	148.0411	95.5450	1.8822	71.4411	82.6917
Wine	156.5255	70.2968	1.4468	69.4427	90.1444
Thyroid	149.1138	5551.4389	3.3243	70.8240	102.1959
Flame	150.5154	119.2546	1.7628	72.8839	92.1913
Aggregation	174.6097	1853.7493	10.2566	123.0901	148.9328
Spiral	160.1743	180.8485	3.1349	89.5048	105.0130
D1	149.6506	34.3190	1.1136	67.6673	90.7307
D2	146.9794	32.2693	0.8710	68.8392	92.7008

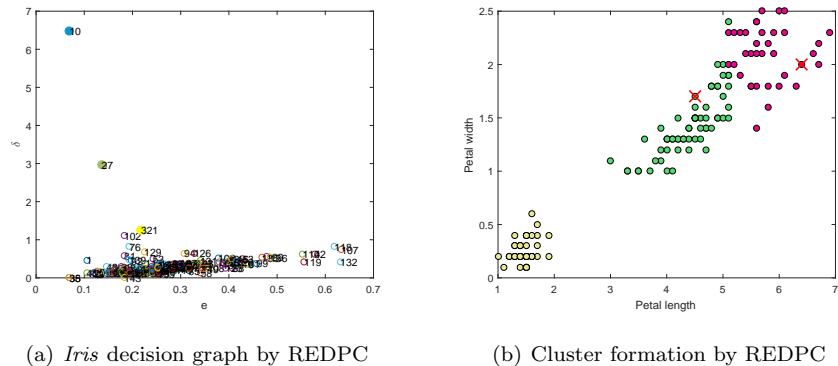


Figure 7: Determination of cluster centroids and the resulting cluster formation based on the decision graph generated by REDPC on *Iris* dataset.

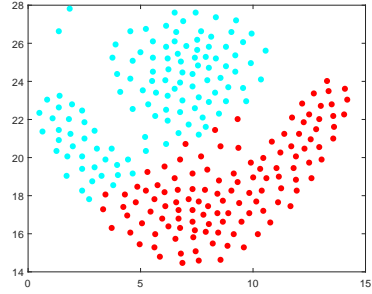
305 *4.1. Identifying Cluster Centroids*

As aforementioned that the performance of DPC is sometimes limited by its generated decision graph. In comparison, REDPC employs the residual error computation to measure the local density within a neighbourhood region. As a result, REDPC generates decision graphs that are better suited for cluster centroid identifications. As shown in Figure 7(a), the third cluster centroid in the *Iris* dataset is relatively more identifiable in the decision graph generated by REDPC comparing to that generated by DPC (see Figure 1).

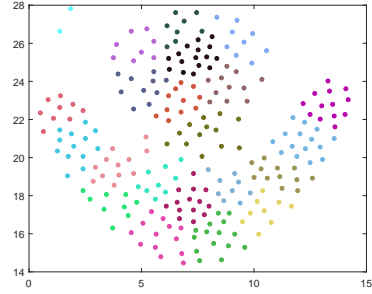
*4.2. Identifying Clusters with Anomalies*

To illustrate the capability of REDPC in anomaly detection, we present the clustering results of all clustering methods on the *Flame* and *D2* datasets in Figures 8 and 9, respectively. The two anomalies in *Flame* are located in the top left corner and the five anomalies in *D2* are located in the center. It is clearly shown that K-Means and AP fail in identifying anomalous data points. DBSCAN [23] adopts *MinPts* and *density-connectivity* to detect outliers, but along with outliers, it detects much more borderline data points incorrectly on *Flame* dataset. DPC does not perform anomaly detections as aforementioned.

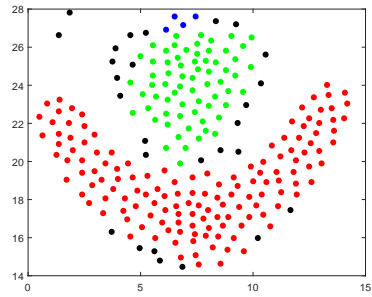




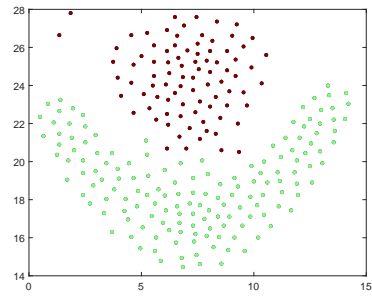
(a) K-Means,  $K = 2$



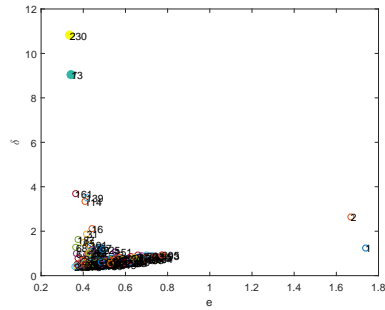
(b) AP,  $preference = -5.9261$



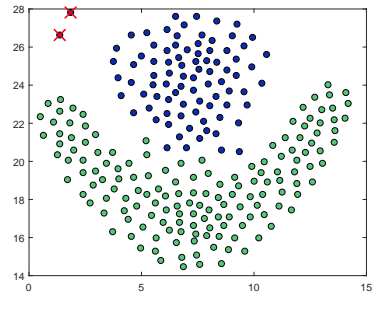
(c) DBSCAN,  $Eps = 0.85$ ,  $MinPts = 5$



(d) DPC,  $C_d = 8\%$



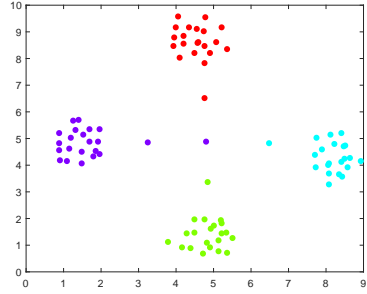
(e) *Flame* decision graph by REDPC



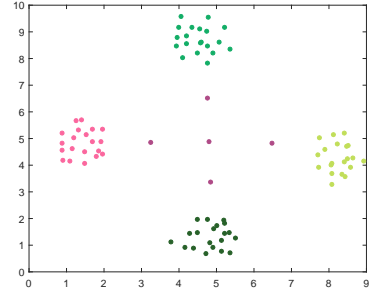
(f) REDPC,  $N = 4$ ,  $C_d = 1\%$  (#clusters = 2, #anomalies = 2)

Figure 8: Cluster formation results on *Flame* dataset.

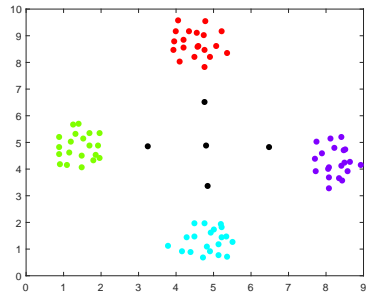
On the other hand, as shown in Figures 8(f) and 9(f), REDPC consistently detects the correct possible anomalies.



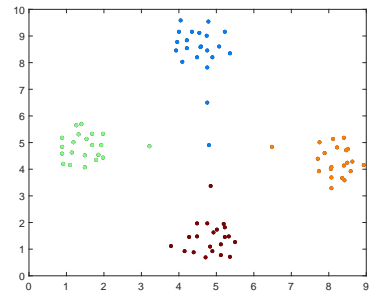
(a) K-Means,  $K = 4$



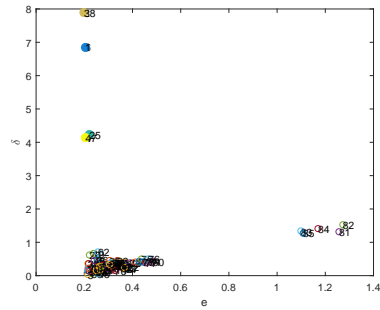
(b) AP,  $preference = -4.8674$



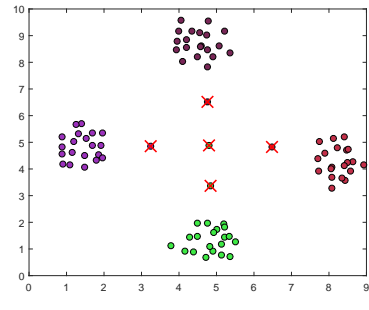
(c) DBSCAN,  $Eps = 1$ ,  $MinPts = 5$



(d) DPC,  $C_d = 5\%$



(e)  $D2$  decision graph by REDPC



(f) REDPC  $N = 5$ ,  $C_d = 1\%$  (#clusters = 4, #anomalies = 5)

Figure 9: Cluster formation results on  $D2$  dataset.

### 4.3. Identifying Clusters of Varying Sizes

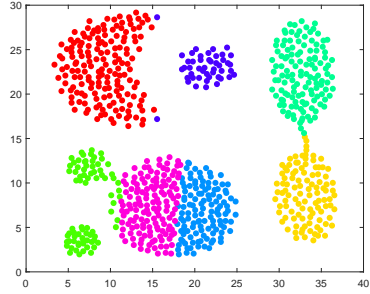
325 To illustrate the performance of REDPC on datasets comprising of clusters  
of varying sizes, such as *Aggregation* and *D1*, we refer you to Figures 10 and  
11, respectively. It is clearly shown in these two figures that both K-means and  
AP do not perform well on these datasets. The performance of DBSCAN is  
much better, however, it still faces problems in a small set of borderline points  
330 (see Figure 10(c)). In comparison, DPC correctly identifies all the clusters of  
varying sizes and REDPC only mislabels one data point.

### 4.4. Identifying Clusters of Irregular Shapes

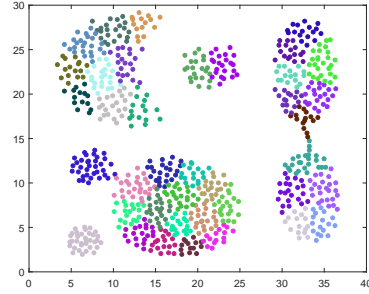
Density-based clustering algorithms have been shown to perform well in  
identifying arbitrary-shaped clusters in the literature. In this subsection, we  
335 use Figures 8, 10 and 12 to show REDPC’s performance in identifying irregular  
shaped clusters. K-means and AP are partition based clustering methods and  
hence cannot well handle such datasets. DBSCAN performs perfectly in *Spiral*  
(see Figure 12(c)), however, not so well in the other datasets. In comparison,  
both DPC and REDPC are shown to be capable of correctly identifying the  
340 natural clusters of irregular shapes.

### 4.5. Identifying Clusters of Different Densities

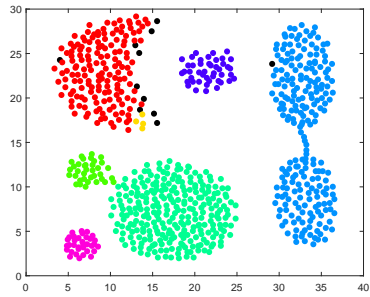
Among all the datasets used in this paper, our own-defined synthetic dataset  
*D1* best illustrates the scenario of having clusters of different densities (see  
Figure 11). It is clearly shown in the figure that K-Means and AP do not well  
345 handle a dataset of varying densities. DBSCAN only detects two clusters and  
deems the third cluster as a set of outliers (i.e., the top cluster in Figure 11(c)  
only consists of outliers, which is due to the relatively low density of those data  
points that they do not fulfil the density-reachability definition, see Section 2.1).  
In comparison, both DPC and REDPC correctly identify all the natural clusters  
350 (the two anomalies reported by REDPC are assigned to the correct cluster after  
refinement, see Algorithm 4).



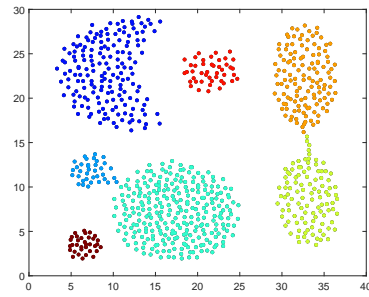
(a) K-Means,  $K = 7$



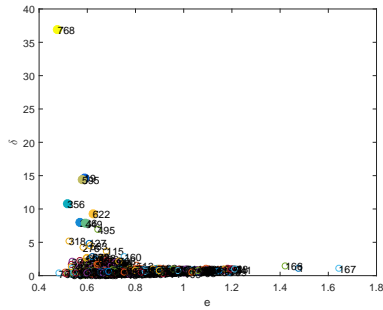
(b) AP,  $preference = -16.5170$



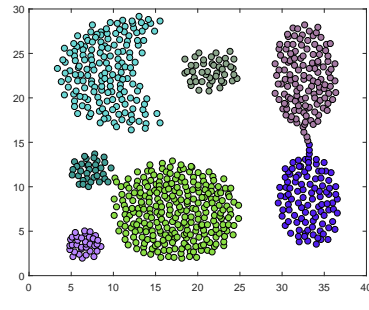
(c) DBSCAN,  $Eps = 1.1$ ,  $MinPts = 5$



(d) DPC,  $C_d = 5\%$

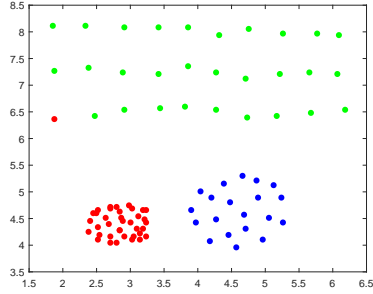


(e) Aggregation decision graph by REDPC

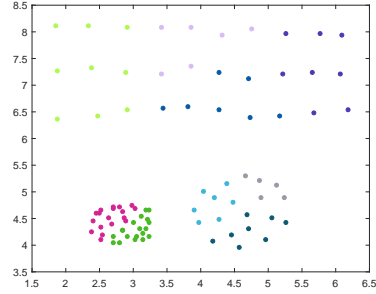


(f) REDPC,  $N = 7$ ,  $C_d = 1\%$  (#clusters = 7)

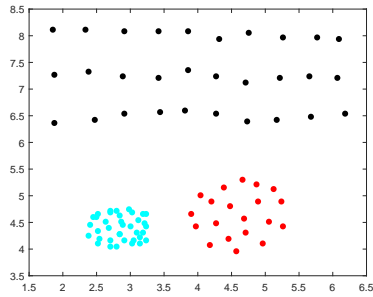
Figure 10: Cluster formation results on *Aggregation* dataset.



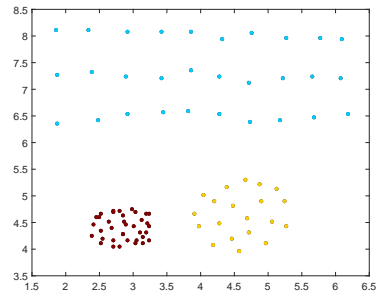
(a) K-Means,  $K = 3$



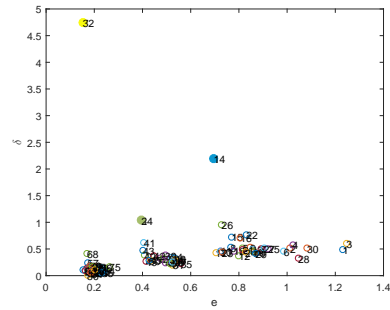
(b) AP,  $preference = -2.1523$



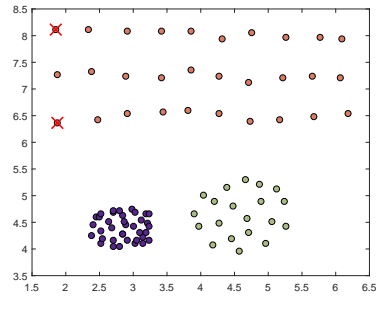
(c) DBSCAN,  $Eps = 0.5$ ,  $MinPts = 5$



(d) DPC,  $C_d = 20\%$



(e)  $D1$  decision graph by REDPC

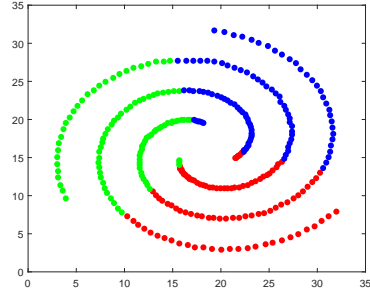


(f) REDPC  $N = 11$ ,  $C_d = 1\%$  (#clusters = 3, #anomalies = 2)

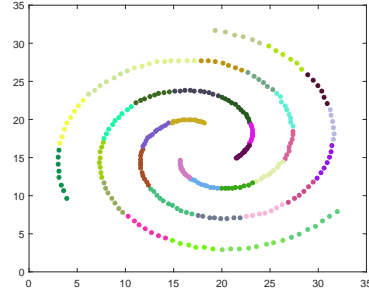
Figure 11: Cluster formation results on  $D1$  dataset.

#### 4.6. Overall Comparison of All Benchmarking Models

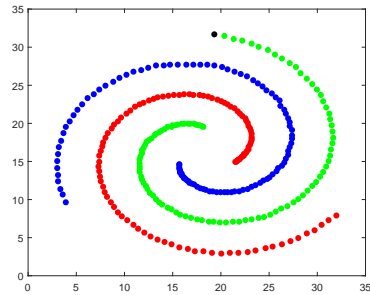
Our proposed REDPC algorithm has shown to perform better than the other benchmarking models in identifying clusters of various properties in the previous



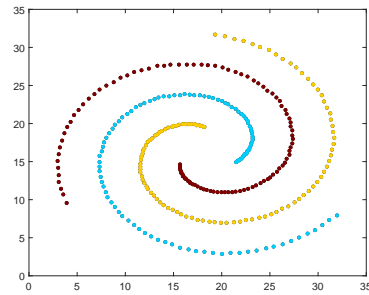
(a) K-Means,  $K = 3$



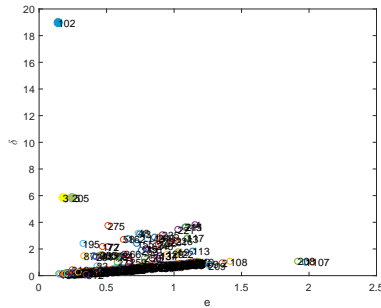
(b) AP,  $preference = -12.3868$



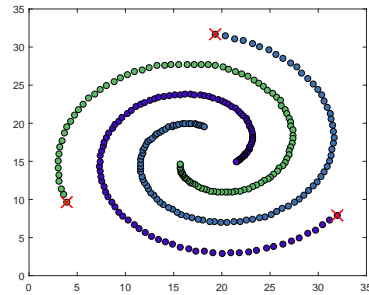
(c) DBSCAN,  $Eps = 2.5$ ,  $MinPts = 5$



(d) DPC,  $C_d = 5\%$



(e) *Spiral* decision graph by REDPC



(f) REDPC,  $N_i = 5$ ,  $C_d = 1\%$  (#clusters = 3, #anomalies = 3)

Figure 12: Cluster formation results on *Spiral* dataset.

355 subsections, respectively. In this subsection, we summarize the performance of  
all clustering algorithms on each property of the clusters in Table 6. As shown

Table 6: Overall Performance Comparison on Different Cluster Properties

Property	Algorithm				
	K-Means	AP	DBSCAN	DPC	REDPC
Centroid detection	✓	×	∂	✓	✓
Anomaly detection	∂	×	✓	✓	✓
Variable sizes	∂	×	✓	✓	✓
Variable shapes	×	×	✓	✓	✓
Variable densities	✓	×	✓	✓	✓

Symbols ‘×’ denotes poor performance, ‘∂’ denotes acceptable performance, and ‘✓’ denotes excellent performance, respectively. The assignment criteria are based on whether the clustering algorithm performs well on all the datasets used when analyzing the corresponding property (see Sections 4.1 to 4.5). Specifically, ‘×’ is assigned if the  $F$ -score on any dataset is less than 0.6, ‘✓’ is assigned if the  $F$ -scores on all datasets are greater than 0.8, otherwise, ‘∂’ is assigned.

in the table, it is fair to say that REDPC is a well-designed algorithm working well in various performance evaluation aspects.

Another note on the comparison between DPC and REDPC is that although  
 360 REDPC uses one more parameter than DPC does, which is the neighbourhood  
 size  $N$  (they both use the distance cutoff parameter  $C_d$ ), in practice, we spend  
 almost equally amount of effort in determining the best performing parameter  
 values for both methods. The reason is because for REDPC, we always fix the  
 value of  $C_d$  at 1% and tune  $N$  in an incremental manner. On the other hand, in  
 365 order to get DPC’s best clustering accuracy, we need to tune  $C_d$  with varying  
 values. Therefore, in terms of conducting the experiments shown in this paper,  
 both methods require the tuning of only one parameter.

## 5. Conclusion

In this paper, we propose the Residual Error-based Density Peak Clustering  
 370 (REDPC) algorithm by using residual error computation to measure the local  
 density within a neighbourhood region and further process the identified low-

density data points. As such, REDPC may generate better decision graphs for cluster centroid identifications and better identify the possible anomalies. The experimental results on both synthetic and real-world UCI datasets demonstrate  
375 that REDPC performs better than DPC and other algorithms.

Going forward, we will improve REDPC for better autonomy in parameter value determination and apply it to more complex and challenging datasets.

### Acknowledgements

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380 of China No. 61772227 and Science & Technology Development Foundation of Jilin Province under the grant No. 20160101259JC, 20180201045GX. This research is also supported in part by the National Research Foundation, Prime Minister's Office, Singapore under its IDM Futures Funding Initiative.

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