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Particle swarm Optimized Density-based Clustering and Classification: Supervised and unsupervised learning approaches

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ABSTRACT

Two pattern recognition technologies in the field of machine learning, clustering and classification, have been applied in many domains. Density-based clustering is an essential clustering algorithm. The best known density-based clustering method is Density-Based Spatial Clustering of Applications with Noise (DBSCAN), which can find arbitrary shaped clusters in datasets. DBSCAN has three drawbacks: firstly, the parameters for DBSCAN are hard to set; secondly, the number of clusters cannot be controlled by the users; and thirdly, DBSCAN cannot directly be used as a classifier. In this paper a novel Particle swarm Optimized Density-based Clustering and Classification (PODCC) is proposed, designed to offset the drawbacks of DBSCAN. Particle Swarm Optimization (PSO), a widely used Evolutionary and Swarm Algorithm (ESA), has been applied in optimization problems in different research domains including data analytics. In PODCC, a variant of PSO, SPSO-2011, is used to search the parameter space so as to identify the best parameters for density-based clustering and classification. PODCC can function in terms of both Supervised and Unsupervised Learnings by applying the appropriate fitness functions proposed in this paper. With the proposed fitness function, users can set the number of clusters as input for PODCC. The proposed method was evaluated by testing ten synthetic datasets and ten benchmarking datasets selected from various open sources. The experimental results indicate that the proposed PODCC can perform better than some established methods, especially with respect to imbalanced datasets.

1. Introduction

Clustering Analysis is a widely used unsupervised pattern recognition technology in the field of data mining [1]. Individual records in datasets can be grouped into clusters based on their similarity without knowing the ground truth partitions. The corresponding supervised procedure is known as Classification, where a classifier predictor is learnt from training data of correctly identified observations [2]. Density-based clustering can find arbitrary shaped clusters by detecting the high-density hyper-spheres and merging the close hyper-spheres into clusters. The best known density-based clustering algorithm is Density-Based Spatial Clustering of Applications with Noise (DBSCAN) [3]. DBSCAN uses two parameters, the radius of the hyper-spheres (ϵ) and the minimum number of points in each hyper-sphere (*Minpts*). However, DBSCAN has three drawbacks. Firstly, the parameters for DBSCAN are hard to set; secondly, the number of clusters cannot be controlled by the user; and thirdly, DBSCAN cannot be directly applied for classification purposes.

The central motivation for the work presented in this paper is the intuition that Evolutionary and Swarm Algorithms (ESAs) [4] can be used as a parameter tuning tool for DBSCAN. The main advantage of ESAs is the highly robust global search performance of such algorithms. The development of ESAs was inspired by the idea of natural selection and animal behavior observations. Numerous categories of ESAs have been proposed, these include: Particle Swarm Optimization (PSO) [5], Artificial Bee Colony (ABC) [6], Ant Colony Optimization (ACO) [7], Genetic Algorithms (GAs) [8] and Differential Evaluation (DE) [9].

In the context of DBSCAN, the clustering approach of interest with respect to the work presented in this paper, there has been some research directed at applying ESAs to optimize the performance of DBSCAN. One example is that of [10] where a hybrid partitioning-based DBSCAN method is proposed that uses a modified ant clustering algo-

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rithm; however [10], did not consider parameter optimization, which is discussed in this paper.

One example where the nature of the parameters used in DBSCAN was considered can be found in Ref. [11] where Genetic Algorithm with a Density-Based Approach for Clustering (GADAC) was proposed to determine the nature of the parameters used by DBSCAN to provide satisfactory clustering results. However, the DBSCAN parameters using in GADAC are not directly optimized by the GA operations.

DE was applied to optimise for the parameters for DBSCAN in Ref. [12]; however, the fitness function applied in Ref. [12] was only applicable to supervised learning, not unsupervised learning. For unsupervised learning, an internal clustering index can be used in the fitness function of the ESA optimized clustering method [13]. The fitness functions on the basis of clustering indices are continuous functions. Since PSO performs better than GA for optimizing continuous functions [14], and is more computationally efficiently than GA [15], PSO is selected as the parameter tuning tool for DBSCAN in this paper. A drawback of applying internal indices as a fitness function is that most of the indices are defined for centroid-based method. It may not perform well for density-based clustering and imbalanced data. The applications of internal indices for DBSCAN are investigated later in this paper.

As a population-based stochastic optimization technique, PSO can be used to find the "good enough solution". From the literature a number of examples can be found where PSO has been used to support clustering. In Ref. [16] two PSO methods were proposed, one to find the centroids of clusters and another that used K-means clustering to seed the initial swarm. In Ref. [17] PSO was applied to search the cluster centres in the arbitrary data set automatically. In Ref. [18] PSO was coupled with the K-means clustering to cluster document collections. In Ref. [19] a hybrid method, FAPSO-ACO-K, was proposed which combined Fuzzy Adaptive Particle Swarm Optimization (FAPSO), Ant Colony Optimization (ACO) and *K*-means so as to find the best cluster partition in the nonlinear partitional clustering problem. In Refs. [20,21] a framework was proposed for Differential Evolution Particle Swarm Optimization (DEPSO) based clustering which combined DE with PSO. However, to the best knowledge of the authors, there has been no work directed at using PSO for the purpose of density-based cluster parameter optimization. The above methods also have other limitations. Firstly, the encoding methods of clustering results based on enumerating all items are complex to search for an optimal solution. Secondly, the method can only be applied to the unsupervised learning. To the best knowledge of the authors, no work using SPSO to optimize the DBSCAN parameters for both supervised and unsupervised learning using fitness functions of the form presented in this paper has been conducted.

Based on the above observations, this paper proposes a novel hybrid approach, Particle swarm Optimized Density-based Clustering and Classification (PODCC), directed at optimizing the performance of density-based clustering by finding the best parameter settings through a search of the entire parameter space using PSO. The Standard Particle Swarm Optimization algorithm defined in 2011 (SPSO-2011) [22] is used to implement PODCC, since the adaptive random topology and rotational invariance featured in SPSO-2011 has been shown to achieve faster convergence to the global optimum than pervious PSO variants.

In this paper, two types of continuous fitness functions are designed on the basis of current clustering validation indices and the penalty functions designed for minimizing the amount of noise and to control the number of clusters. Two categories, unsupervised and supervised PODCC are proposed with different fitness functions.

The rest of this paper is organized as follows. Section 2 reviews the operation of DBSCAN and highlights the limitation of DBSCAN using a toy example. Section 3 then presents the proposed PODCC approach directed at addressing the limitations of DBSCAN identified in the previous section. Section 4 proposes various fitness functions for PODCC. Section 5 presents the experimental design and the results achieved. Section 6 presents the simulations of applying PODCC to 10 open datasets. Section 7 then presents some conclusions concerning the main findings of the research presented in this paper.

2. Operation and limitations of DBSCAN

Density-Based Spatial Clustering of Applications with Noise (DBSCAN) was first proposed in 1996 [3]. DBSCAN can easily find the arbitrary shape of clusters by detecting high-density hyper-spheres and merging neighbouring hyper-spheres into clusters. As already noted, DBSCAN uses two critical parameters, the hyper-sphere radius (ϵ) and the minimum number of points in each hyper-sphere (Minpts). The clustering results of DBSCAN are sensitive to the values of these two parameters. The pseudo code for the DBSCAN algorithm is given in Algorithm 1. The clustering Pattern Result (PR) is a list $[c_1, c_2, \ldots, c_n]$ where each element c_i is a cluster identifier (identifier 0 indicates the noise cluster), n is the number of records in the input dataset $\mathcal{S}$, and the indices indicate individual record numbers for each record s in $\mathcal{S}$. A mark *seen* is used to distinguish between the records which have been processed and those which still need to be processed. $N_\epsilon(s;\mathcal{S})$ is a function that returns the subset of records in $\mathcal{S}$ that are presented in a particular cluster (hyper-sphere) of radius ϵ that $s \in \mathcal{S}$. The function of $card(N_\epsilon(s;\mathcal{S}))$ returns the cardinality of the set $N_\epsilon(s;\mathcal{S})$; whilst $sid(s)$ returns the index in PR of s in $\mathcal{S}$.

Algorithm 1 DBSCAN.
Input: Dataset $\mathcal{S}$, hyper-sphere radius ϵ, the minimum number of points in the hyper-sphere, *MinPts*.
Output: Pattern Result, (PR).
1. Initialise $cid = 0$;
2. For each record in the dataset, i.e. $s \in \mathcal{S}$,
  If s is not marked as "seen",then
    Mark s as "seen" and find $N_\epsilon(s;\mathcal{S})$,
    If $card(N_\epsilon(s;\mathcal{S})) < MinPts$, then
      $(PR)_{sid(s)} = 0$;
    else
      $cid = cid + 1$;
      $(PR)_{sid(s)} = cid$;
      For $s' \in N_\epsilon(s;\mathcal{S})$ and s' is not marked as "*seen*",
        Mark s' as "*seen*";
        Find $N_\epsilon(s';\mathcal{S})$;
        If $card(N_\epsilon(s';\mathcal{S})) \geq MinPts$, then
          $(PR)_{sid(s')} = cid$;
  else
    continue to next point
3. Return (PR).

A number of hybrid and enhanced density-based clustering methods have also been developed on the basis of DBSCAN, namely: *l*-DBSCAN [23], ST-DBSCAN [24], Rough-DBSCAN [25], P-DBSCAN [26], MR-DBSCAN [27], PDS-DBSCAN [28], Revised DBSCAN [29], G-DBSCAN [30], and NG-DBSCAN [31]. However, any type of DBSCAN and its variations above has three drawbacks also mentioned in the introduction section. Firstly, it lacks a method to determine the appropriate settings of the two parameters. Manual tuning seems to be the only option. Secondly, unlike K-means, the number of clusters cannot be controlled by the users since DBSCAN does not support the idea of fixing the number of clusters on start up. Thirdly, DBSCAN cannot be directly used as supervised learning method to perform classification. The drawbacks can be illustrated by a simple example as follows.

Table 1
Sample dataset.

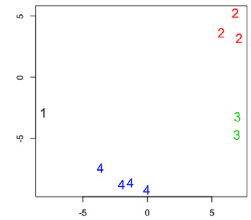
Item ID	Attribute 1	Attribute 2	Cluster Label	Figure
1	−8.055	−2.913	1	
2	7.111	3.188	2	
3	6.953	−4.693	3	
4	−3.627	−7.416	4	
5	5.732	3.648	2	
6	6.988	−3.216	3	
7	−0.041	−9.207	4	
8	−1.983	−8.748	4	
9	6.827	5.266	2	
10	−1.306	−8.633	4	

Table 2
Clustering results of sample dataset.

Case	*PR*	(ϵ, *MinPts*)	CD Coef.	No. of Clusters
1	0 0 0 0 0 0 0 0 0 0	(9, 7)	0.364	0
2	1 2 3 4 5 6 7 8 9 8	(1, 1)	0.182	9
3	1 2 2 1 2 2 1 1 2 1	(7, 0)	0.667	2
4	0 1 0 2 1 0 2 2 1 2	(6, 3)	0.909	2

Example 1. The three drawbacks of DBSCAN can be illustrated by considering a simple problem of clustering a dataset of 10 items as shown in Table 1. Firstly, to demostrate the parameter setting problem, the two parameters are randomly set for four different cases as shown in Table 2. The clustering result for each case, generated using DBSCAN, is shown in Fig. 1. Inspection of Fig. 1 indicates that the known clustering shown in Table 1 is not arrived at. The results are also included in Table 2. The second column gives the clustering pattern result *PR*, the third column gives the parameter settings, the fourth column gives the obtained Czekanowski Dice (CD) coefficient and the last column the number of clusters. Note that with respect to the CD coefficient, the higher the value the better the clustering result in comparison with the ground truth clustering.

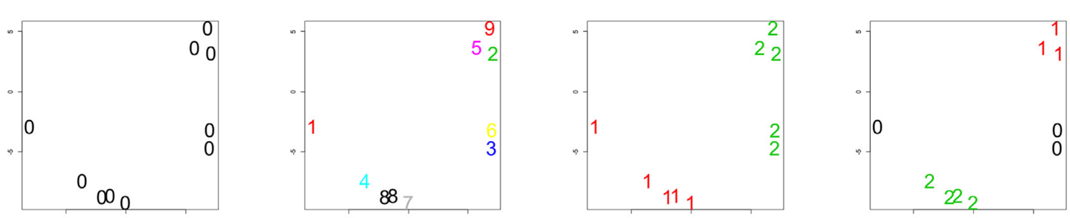
Secondly, to demonstrate the problem of the number of clusters, it can be observed that the numbers of clusters of the four cases are different and not the same as the number of ground truth clusters given in Table 2.

Thirdly, the cluster labels in Table 1 cannot be optionally used in the training to perform a classification.

To overcome the first drawback, this paper proposes Particle swarm Optimized Density-based Clustering and Classification (PODCC) to search for the most appropriated parameters for DBSCAN. To overcome the second and third issues, this paper also presents a number fitness functions used in PODCC.

3. Particle swarm Optimized Density-based Clustering and Classification (PODCC)

The proposed Particle swarm Optimized Density-based Clustering and Classification (PODCC) method is based on the ideas of applying PSO [22] and cluster measurement indices to optimize the input parameter settings for the algorithm. The operation of PODCC is illustrated by the data flow chart given in Fig. 2. A parameter value pair is a particle, which means a possible solution. A group of particles are generated in a 2-dimension search space. Given that the positions ($\overrightarrow{X_i} = (x_{i1}, x_{i2})$) and velocities ($\overrightarrow{V_i} = (v_{i1}, v_{i2})$) of particles, the previous best particles ($\overrightarrow{P_i} = (p_{i1}, p_{i2})$) and the local best particle ($\overrightarrow{L} = (l_1, l_2)$) are initialized, a loop is executed to find the best particle of the highest fitness value. The loop starts with updating $\overrightarrow{X_i}$ and $\overrightarrow{V_i}$. The updated particles are passed to the DBSCAN function to produce a cluster pattern result (*PR*). In this paper, a pattern result means either a clustering result or a classification result. The fitness values of *PRs* are computed by chosen fitness functions. Two types of fitness function, unsupervised and supervised, are considered in this paper (the nature of these functions is considered further in Section 4). The best particles are updated with respect to the fitness values. To ensure that the process terminates, a maximum iteration (*T*) is specified. The loop will be terminated when *T* is reached. Finally $\overrightarrow{L}$ is returned and used in DBSCAN to produce the Best Pattern Results (*BPR*).



(a) Case 1 (b) Case 2 (c) Case 3 (d) Case 4

Fig. 1. Clustering results of DBSCAN by using randomly generated parameters.

Algorithm 2 PODCC.
Input: A fitness function F, dataset $\mathcal{S}$, the swarm size M and maximum iteration number T;
Output: Best Pattern Result BPR;
1. For all particles in the swarm, $\forall i \in \{1, \dots, M\}$
 1.1 Initialise particles' positions $\overrightarrow{X_i}$ and velocities $\overrightarrow{V_i}$;
 1.2 Initialise personal/previous best $\overrightarrow{P_i}$ and local best $\overrightarrow{L}$;
2. For all particles in the swarm, $\forall i \in \{1, \dots, M\}$
 2.1 Update particle's velocity by Eq. (5);
 2.2 Update particle's position by Eq. (9);
 2.3 Generate the Pattern Results by
 $(PR)_{\overrightarrow{X_i}} = DBSCAN(\mathcal{S}, x_{i1}, x_{i2})$;
 $(PR)_{\overrightarrow{P_i}} = DBSCAN(\mathcal{S}, p_{i1}, p_{i2})$;
 $(PR)_{\overrightarrow{L_i}} = DBSCAN(\mathcal{S}, l_1, l_2)$;
 2.4 If $F((PR)_{\overrightarrow{X_i}}) < F((PR)_{\overrightarrow{P_i}})$, then
  Update particle's best-known position $\overrightarrow{P_i} = \overrightarrow{X_i}$;
 2.5 If $F((PR)_{\overrightarrow{P_i}}) < F((PR)_{\overrightarrow{L}})$, then
  Update the neighbourhood's best-known position $\overrightarrow{L} = \overrightarrow{P_i}$;
3. Repeat step 2 until maximum iteration number T or the other stop condition is met;
4. Generate the best Pattern Result,
 i.e. $BPR = (PR)_{\overrightarrow{L}} = DBSCAN(\mathcal{S}, l_1, l_2)$.

The pseudo code for PODCC are presented in Algorithm 2. In this paper the Standard Particle Swarm Optimization algorithm defined in 2011 (SPSO-2011) [22] was used, but clearly alternatives could be substituted. SPSO-2011 was used because the adaptive random topology and rotational invariance featured in SPSO-2011 has been shown to achieve faster convergence to the global optimum than pervious PSO variants.

Returning to Algorithm 2, in Step 1, the particles are initialized using the following equations.

$$x_{i,d} = U(\min_d, \max_d) \tag{1}$$

$$v_{i,d} = \frac{U(\min_d, \max_d) - x^0_{i,d}}{2} \tag{2}$$

$$p_{i,d} = x^0_{i,d} \tag{3}$$

$$l_{i,d} = \min(f(p^0_{i,d})) \tag{4}$$

where $U(\min_d, \max_d)$ is a random value in $[\min_d, \max_d]$ where the subscript $d \in \{1, 2\}$ means the dimension of the particle.

In Step 2.1, the velocity is updated using the following function:

$$\overrightarrow{V_i} = \omega \overrightarrow{V_i} + x' - \overrightarrow{X_i} \tag{5}$$

where $x\prime$ is a random point defined in the hypersphere: $\mathcal{H}_i(\overrightarrow{G_i}, \|\overrightarrow{G_i} - \overrightarrow{X_i}\|)$. For the ith particle, a centre of gravity $(\overrightarrow{G_i})$ is calculated using three points: the current position $(\overrightarrow{X_i})$, a point slightly beyond the best previous personal position $(\overrightarrow{p_i})$, and a point slightly beyond the best previous position in the neighbourhood $(\overrightarrow{l}_i)$, as shown below:

$$\overrightarrow{p_i} = \overrightarrow{X_i} + c_1 \overrightarrow{U_1} \otimes (\overrightarrow{P_i} - \overrightarrow{X_i}) \tag{6}$$

$$\overrightarrow{l}_i = \overrightarrow{X_i} + c_2 \overrightarrow{U_2} \otimes (\overrightarrow{L} - \overrightarrow{X_i}) \tag{7}$$

$$\overrightarrow{G_i} = \frac{\overrightarrow{X_i} + \overrightarrow{p_i} + \overrightarrow{l}_i}{3} \tag{8}$$

where c_1 and c_2 are the cognitive and social acceleration coefficients respectively. $\overrightarrow{U_1}$ and $\overrightarrow{U_2}$ are the predefined independent and uniformly distributed random vectors respectively within the range $[0, 1]$. $\otimes$ means the element-wise vector multiplication. ω is a predefined inertia weight.

In Step 2.2, the position of the ith particle are updated according to the equation:

$$\overrightarrow{X_i} = \overrightarrow{X_i} + \overrightarrow{V_i} \tag{9}$$

In Step 2.3, by using the particles x_{i1} and x_{i2} as ϵ and $MinPts$ respectively, the items in the dataset $\mathcal{S}$ can be clustered or classified by DBSCAN according to Algorithm 1 given in Section 2. In Steps 2.4 and 2.5, the fitness value of the pattern results can be computed by using different fitness functions defined in Section 4 below. After the stop condition is met, the best pair of parameters, l_1 and l_2, are the output in Step 3. Finally, the optimized pattern results are returned by passing the parameters, l_1 and l_2, as ϵ and $MinPts$ in DBSCAN.

4. Design of fitness functions for PODCC

A number of fitness functions are designed for either unsupervised or supervised learning using Particle swarm Optimized Density-based Clustering and Classification (PODCC). The fundamental distinction is that if the ground truth target class values of records in the dataset are not used in PODCC we have unsupervised learning (clustering), if they are used we have supervised learning (classification). Both Internal and External Indices are used to measure clustering results. Class labels (ground truth values) are needed for the calculations of external indices, whilst calculations of internal indices do not require ground truth values. The unsupervised fitness function for PODCC, F_{usp}, is defined as follows:

$$F_{usp} = f_{Int} + f_{NK} \tag{10}$$

where f_{Int} is an internal clustering index function and f_{NK} (Eq. (15)) is the sum of the function to control the number of clusters (f_K) and the noise minimization function (f_{Noise}). Two widely used clustering indices, the Davies-Bouldin (DB) index [32] and Silhouette (SIL) index [33], are used for f_{Int} in this paper. Given a set of N data points $\mathcal{S} = (s_1, \dots, s_N)$ assigned to K clusters $C = \{C_1, \dots, C_i, \dots, C_K\}$ and the centroids of each cluster m_i, $i = 1, \dots, K$. $C_i = \{s^i_1, \dots, s^i_j, \dots, s^i_{n_i}\}$ is the ith cluster, where n_i is the number of data points in C_i. The DB index is calculated as follows:

$$f_{DB} = \frac{1}{K} \sum_{i=1}^{K} \max_{i' \in \{1,\dots,K\}, i' \neq i} \{ \frac{e_i + e_{i'}}{\|m_i - m'_i\|^2} \}, e_i$$
$$= (1/n_i) \sum_{j=1}^{n_i} \|s^i_j - m_i\|^2 \tag{11}$$

where e_i and $e_i\prime$ are the measures of scatter within clusters C_i and C'_i respectively. The silhouette statistic (SIL) is calculated using:

$$f_{SIL} = \frac{1}{K} \sum_{i=1}^{K} \left(\frac{1}{n_i} \sum_{j=1}^{n_i} \frac{b^i_j - a^i_j}{\max(a^i_j, b^i_j)} \right), \text{where} \tag{12}$$

$$a^i_j = \frac{1}{n_i - 1} \sum_{k=1, k \neq j}^{n_i} \|s^i_j - s^i_k\| \tag{13}$$

$$b^i_j = \min_{h \in \{1,\dots,K\}, h \neq i} \left\{ \frac{1}{n_h} \sum_{k=1}^{n_h} \|s^i_j - s^h_k\| \right\} \tag{14}$$

where: (i) a^i_j is the average distance between a data point s^i_j belonging to a cluster C_i and all other data points in C_i, and (ii) b^i_j is the minimum average distance between the jth data point in the cluster C_i and all the data points in the other clusters $\{C_h : h \neq i\}$. The lower the DB index the better the clustering result, whilst the higher the SIL index the better

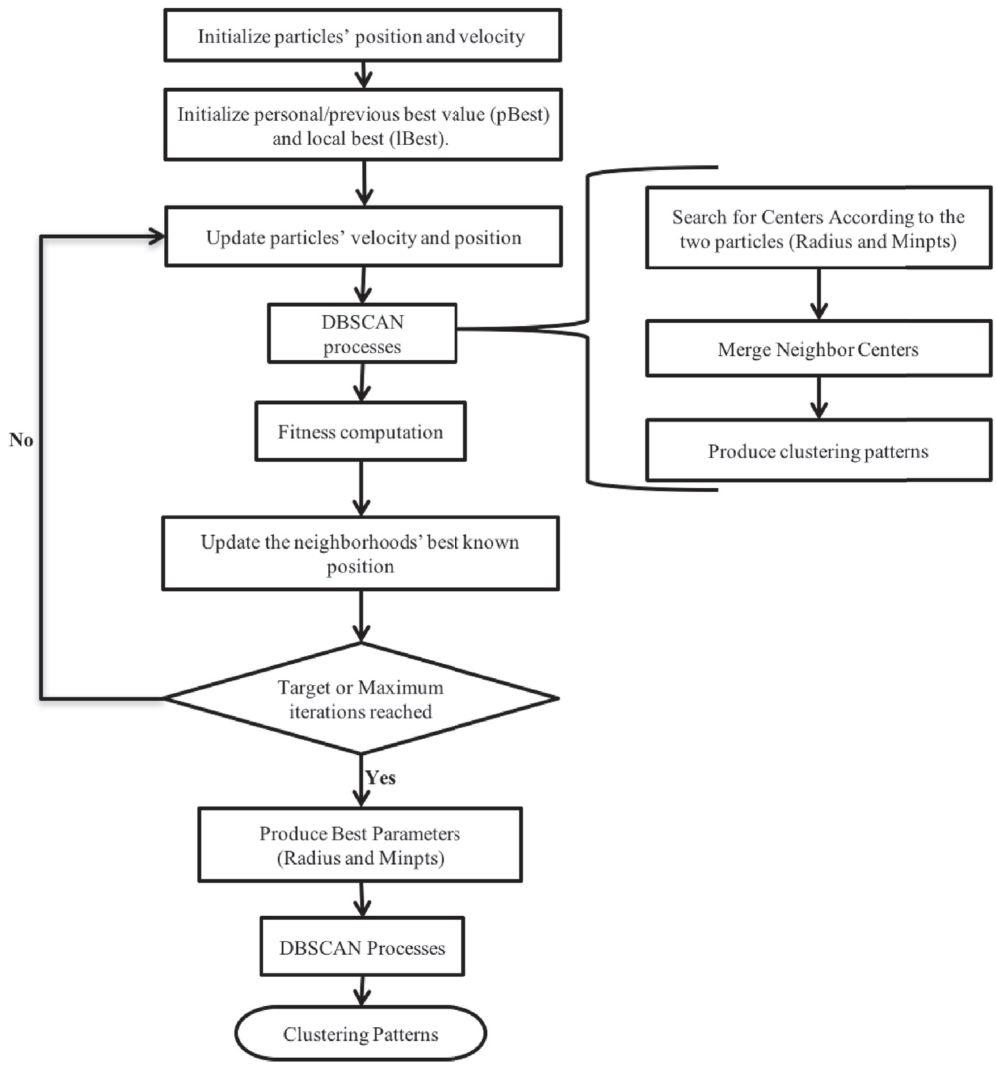


Fig. 2. Data flow diagram outlining the operation of PODCC.

the clustering result. By default, PODCC minimizes the fitness value; therefore f_{Int} is f_{DB} or $-f_{SIL}$.

The function f_{Int} cannot be solely used as a fitness function since the best internal indices for PODCC do not lead to the best pattern results. As shown in Fig. 3, all the data points are clustered in one cluster when either $f_{\text{Int}} = -f_{SIL}$ or $f_{\text{Int}} = f_{DB}$ is the only value to be minimized. The details of the two datasets used in Figs. 3–4 are given in Table 5 in Section 5.

To address this problem f_{NK} is also used, f_{NK} returns the sum of the function for the number of clusters (f_K) and the noise minimization function (f_{Noise}). f_{NK} is defined as follows:

$$f_{NK} = f_K + f_{Noise}, \text{ where} \tag{15}$$

$$f_K = \frac{abs(\max(PR) - K)}{K} \tag{16}$$

$$f_{Noise} = \frac{card(\{PR_i \in PR : PR_i = 0\})}{N} \tag{17}$$

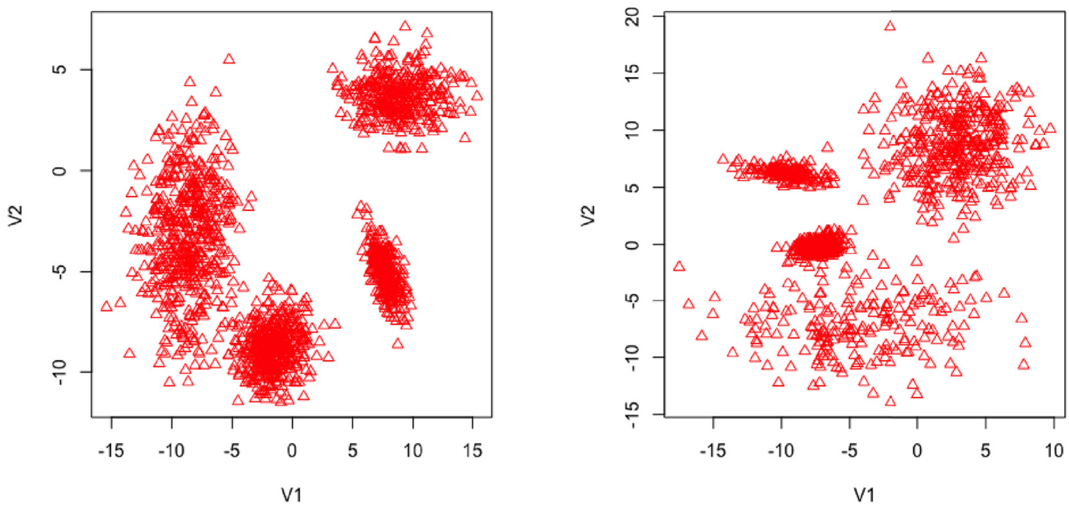
The variable f_K (Eq. (16)) is used to overcome the drawback of DBSCAN, noted in Section 2, that the number of clusters cannot be controlled by users. In some real cases, the K value is a known a priori, but it cannot be used to guide the clustering process in standard DBSCAN. If the K value is unknown, the user can assume some K values as the input of PODCC. By comparing the optimized clustering results of the different input K values, the most suitable number of clusters for the dataset can be found. The variable f_K is used to calculate the ratio of the absolute difference between the number of clusters as PODCC procedures (i.e. $\max(PR)$) and the number of clusters determined by the user to K. The variable f_K can be minimized to 0 when $\max(PR) = K$. Therefore, the number of clusters in PODCC can be control by the user. The variable f_K cannot be solely used as a fitness function since the pattern results shown in Fig. 4 may be generated by PODCC.

The function f_{Noise} is used to compute the percentage of noise in pattern results during PODCC, such that it can be used to minimize the amount of noises in the pattern results. The function f_{Noise} cannot be solely used as a fitness function since all data points are grouped into one cluster (Fig. 3). The function f_{NK} can be used as a fitness function for unsupervised PODCC (i.e. $F_{usp} = f_{NK}$) where no good internal index is suitable for the dataset to be clustered (see more details in Section 5).

If the ground truth target class values of a dataset are used in PODCC, PODCC can perform\classification supervised learning. A supervised fitness function for PODCC, F_{spd}, is defined as follows:

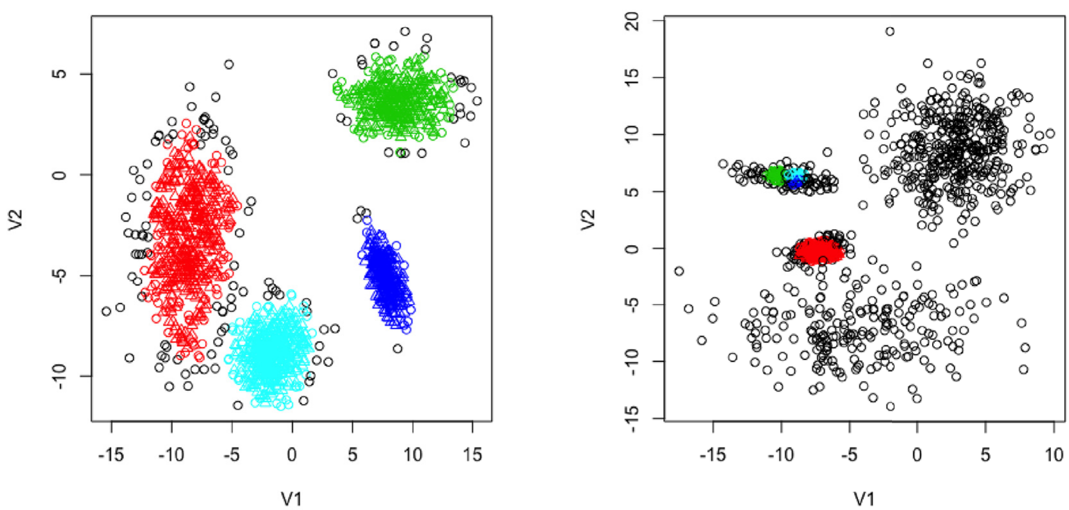
$$F_{spd} = f_{Ext} \tag{18}$$

f_{Ext} is the external clustering index function. An external index function measures the similarity between two partitions, Partition 1 and Partition 2. In this case, the set of classes represents the set of clusters in Partition 1 while Partition 2 represents some other pattern results of



(a) Dataset 07 (b) Dataset 08

Fig. 3. Clustering Pattern Results using PODCC with f_{Int} or f_{Noise} as the Fitness Function.



(a) Dataset 07 (b) Dataset 08

Fig. 4. Results Using PODCC with f_K as the Fitness Function.

which the quality to be determined. In other words, the similarity of Partition 2 compared to the "ground truth" Partition 1 indicates the accuracy of Partition 2. When considering a pair of points, α and β, in Partitions 1 and 2, there are four possibilities:

- $\alpha\alpha$: the two points belong to the same cluster in both partitions.
- $\alpha\beta$: the two points belong to the same cluster in Partition 1 but not in Partition 2.
- $\beta\alpha$: the two points belong to the same cluster in Partition 2 but not in Partition 1.
- $\beta\beta$: the two points do not belong to the same cluster in either partition.

A widely used external index is the Czekanowski-Dice index [34]. This was thus adopted in the supervised fitness function for PODCC. The CD index is defined as follows:

$$f_{CD} = \frac{2\alpha\alpha}{2\alpha\alpha + \alpha\beta + \beta\alpha} \tag{19}$$

The higher the CD index the better the pattern result. Given that PODCC is designed to minimize the fitness value by default, $f_{Ext} = -f_{CD}$ was used.

A fitness function is chosen on a case-by-case basis. Details concerning the process for choosing fitness function is discussed in Section 5. The operation of PODCC with two different fitness functions, f_{NK} and $F_{Ext} = -f_{CD}$, is illustrated in Example 2, using the same dataset in Example 1 (given in Table 1).

Example 2. The dataset of 10 data points is presented in Table 1. The swarm size (amount of particles in the swarm) is set to 4 and the maximum iteration is set to 10. Table 3 shows the unsupervised PODCC results by using the fitness function $F_{usp} = f_{NK}$ presented in Eq. (15). For example, the fitness of the pattern results produced by using the first particle within Loop 1 is computed as follows:

$$\begin{aligned} f_{NK} &= \frac{abs(\max(PR) - K)}{K} + \frac{card(\{PR_i \in PR : PR_i = 0\})}{N} \\ &= \frac{abs(3-4)}{4} + \frac{3}{10} = 0.55 \end{aligned} \tag{20}$$

In this case, convergence is reached in iteration 5 since the best fitness value 0 is reached at the 5th iteration. At the end, 3 particles (Particles 1, 3, 4) reach the best fitness value.

Table 3
Sample results of PODCC applying f_{NK}.

Iteration	Particle ID	Pattern Results	Parameters Set	Fitness
1	1	0 1 2 0 1 2 3 3 0 3	(1.508, 2)	0.55
	2	0 0 0 0 0 0 0 0 0 0	(2.054, 7)	2.00
	3	0 0 0 0 0 0 0 0 0 0	(2.726, 7)	2.00
	4	0 0 0 0 0 0 0 0 0 0	(8.505, 7)	2.00
5	1	1 1 1 1 1 1 1 1 1 1	(8.892, 4)	0.75
	2	1 2 3 4 2 3 4 4 2 4	(5.370, 0)	0.00
	3	1 2 3 4 2 3 4 4 2 4	(5.389, 0)	0.00
	4	1 1 1 1 1 1 1 1 1 1	(9.999, 2)	0.75
10	1	1 2 3 4 2 3 4 4 2 4	(2.767, 0)	0.00
	2	1 2 2 1 2 2 1 1 2 1	(7.260, 1)	0.50
	3	1 2 3 4 2 3 4 4 2 4	(5.881, 0)	0.00
	4	1 2 3 4 2 3 4 4 2 4	(6.293, 1)	0.00

Table 4
Sample results of PODCC applying $f_{Ext} = -f_{CD}$.

Iteration	Particle ID	Pattern Results	Parameters Set	Fitness
1	1	0 1 0 2 1 0 2 2 1 2	(5.034, 3)	−0.909
	2	0 1 0 2 1 0 2 2 1 2	(4.862, 3)	−0.909
	3	0 0 0 0 0 0 0 0 0 0	(2.432, 8)	−0.364
	4	0 0 0 0 0 0 0 0 0 0	(3.058, 6)	−0.364
3	1	0 0 0 0 0 0 0 0 0 0	(3.538, 6)	−0.364
	2	0 0 0 0 0 0 0 0 0 0	(8.170, 6)	−0.364
	3	1 2 3 4 2 3 4 4 2 4	(4.711, 0)	−1.000
	4	0 0 0 0 0 0 0 0 0 0	(9.472, 2)	−0.364
10	1	1 2 3 4 2 3 4 4 2 4	(4.322, 2)	−1.000
	2	1 1 1 1 1 1 1 1 1 1	(8.962, 0)	−0.364
	3	1 2 3 4 2 3 4 4 2 4	(2.733, 1)	−1.000
	4	0 1 0 2 1 0 2 2 1 2	(3.025, 3)	−0.909

Table 4 shows the supervised PODCC results by using the fitness function $F_{spd} = -f_{CD}$ presented in Eq. (19). The pairs of the 10 data points are assigned to the four possibilities as below by taking the pattern results as Partition 1 and the ground truth partition as Partition 2.

- $\alpha\alpha$: 10 pairs of points belong to the same cluster in both partitions.
- $\alpha\beta$: 0 pair of points belong to the same cluster in Partition 1 but not in Partition 2.
- $\beta\alpha$: 2 pairs of points belong to the same cluster in Partition 2 but not in Partition 1.
- $\beta\beta$: 33 pairs of points do not belong to the same cluster in either partition.

The fitness of the pattern results is computed using the above point pair values as follows:

$$f_{CD} = \frac{2\alpha\alpha}{2\alpha\alpha + \alpha\beta + \beta\alpha} = \frac{2^{*}10}{2^{*}10 + 0 + 2} = \frac{20}{22} = 0.909 \tag{21}$$

In this case, convergence is reached in iteration 3 since the best fitness value −1 is reached at the 3rd iteration by Particle 3. Half of the particles (Particle 1 and Particle 3) reach the best fitness value and the same pattern result.

5. Experiments

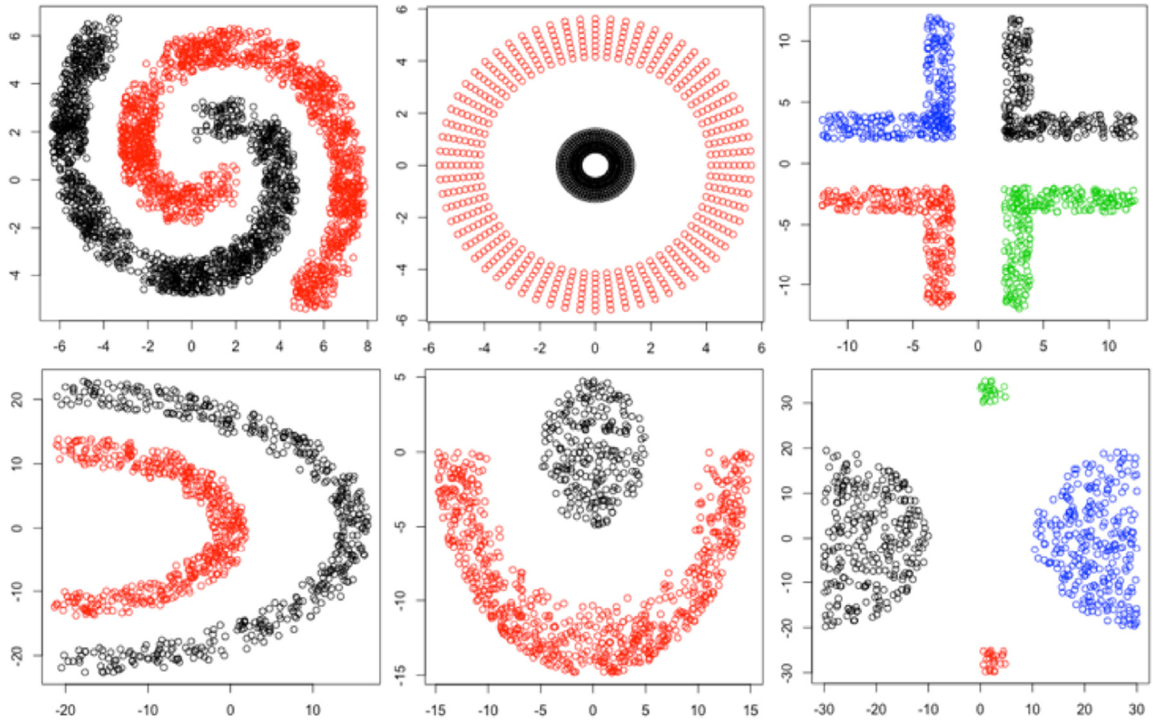
This section presents the results obtained from a sequence of experiments used to evaluate the proposed PODCC system. For the experiments 10 datasets were used. Comparisons were conducted using common clustering and classification methods. The nature of the datasets used is presented in Table 5. Six of the datasets featured challenging known arbitrary shaped clusters (Datasets 1–6): (i) Two spirals, (ii) Cluster in cluster, (iii) Corners, (iv) Half-kernel, (v) Crescent & Full Moon and (vi) Outlier. The remaining four datasets (Datasets 7–10) were synthetic datasets generated using software provided by Julia Handl [35]. The "ground truth" partitions of Datasets 1–6 are shown in Fig. 5a, and the partitions for Datasets 7–10 are shown in Fig. 5b.

Table 5
Description of 10 datasets.

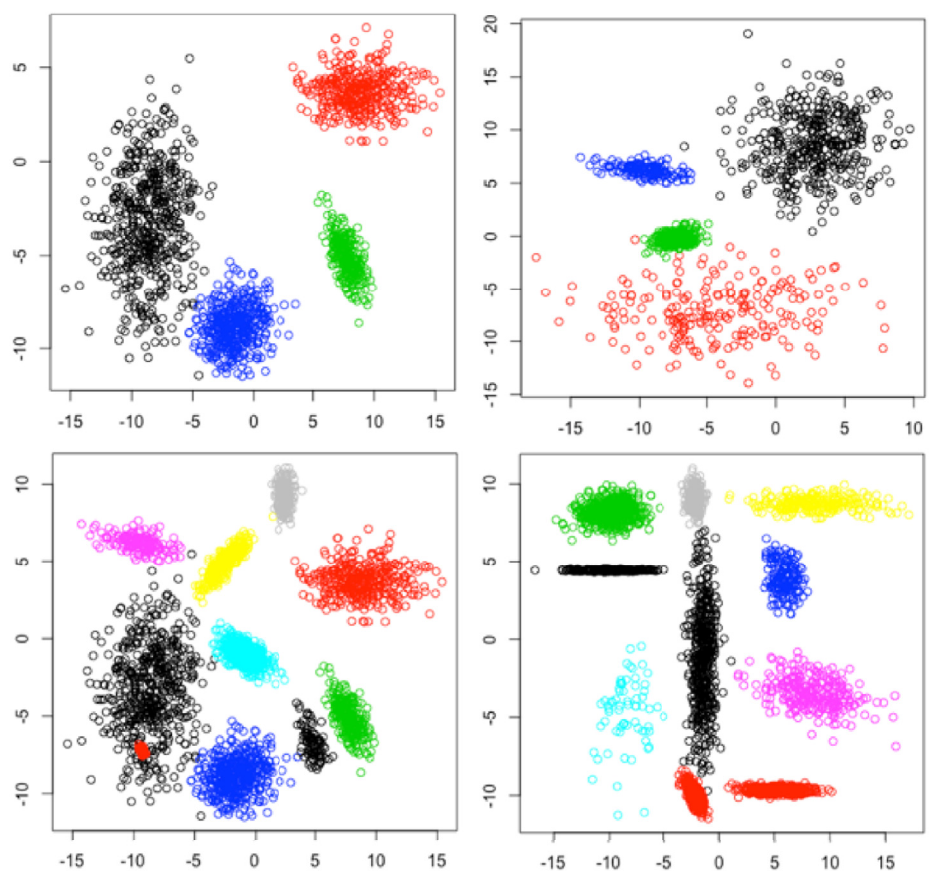
ID	Dataset Name	No. of Classes	No. of Individuals
1	Two spirals	2	3000
2	Cluster in cluster	2	1024
3	Corners	4	1000
4	Half-kernel	2	1000
5	Crescent & Full Moon	2	1000
6	Outlier	4	600
7	2d-4c-no0	4	1572
8	2d-4c-no2	4	1064
9	2d-10c-no0	10	2972
10	2d-10c-no2	10	3073

Four individual sets of experiments were conducted to evaluate the performance of PODCC. The first three were designed for evaluating PODCC in the context of unsupervised learning, for each experiment, one of the unsupervised fitness functions presented on Section 4 was used, namely: F_{NK} (Eq. (15)), F_{usp} with Davies Bouldin Index (Eqs. (10) and (11)) and F_{usp} with Silhouette Index (Eqs. (10) and (12)). For the evaluation, the performance of PODCC was compared with both DBSCAN and K-means. The fourth set of experiments was designed to evaluate the performance of supervised PODCC using the supervised fitness function F_{spd} with the Czekanowski-Dice Index (Eqs. (18) and (19)). The performance of supervised PODCC was compared with Support Vector Machine (SVM) classification [36].

For the experiments, the following PODCC settings were used: (i) swarm size of 40, (ii) maximum values of the two particles of 10 and the minimum values of 0, (iii) $c1$, $c2$ (the cognitive and social acceleration coefficients) and w (predefined inertia weight) set to 1.193, 1.193 and 0.721 respectively, and (iv) the maximum number of iterations to 50.

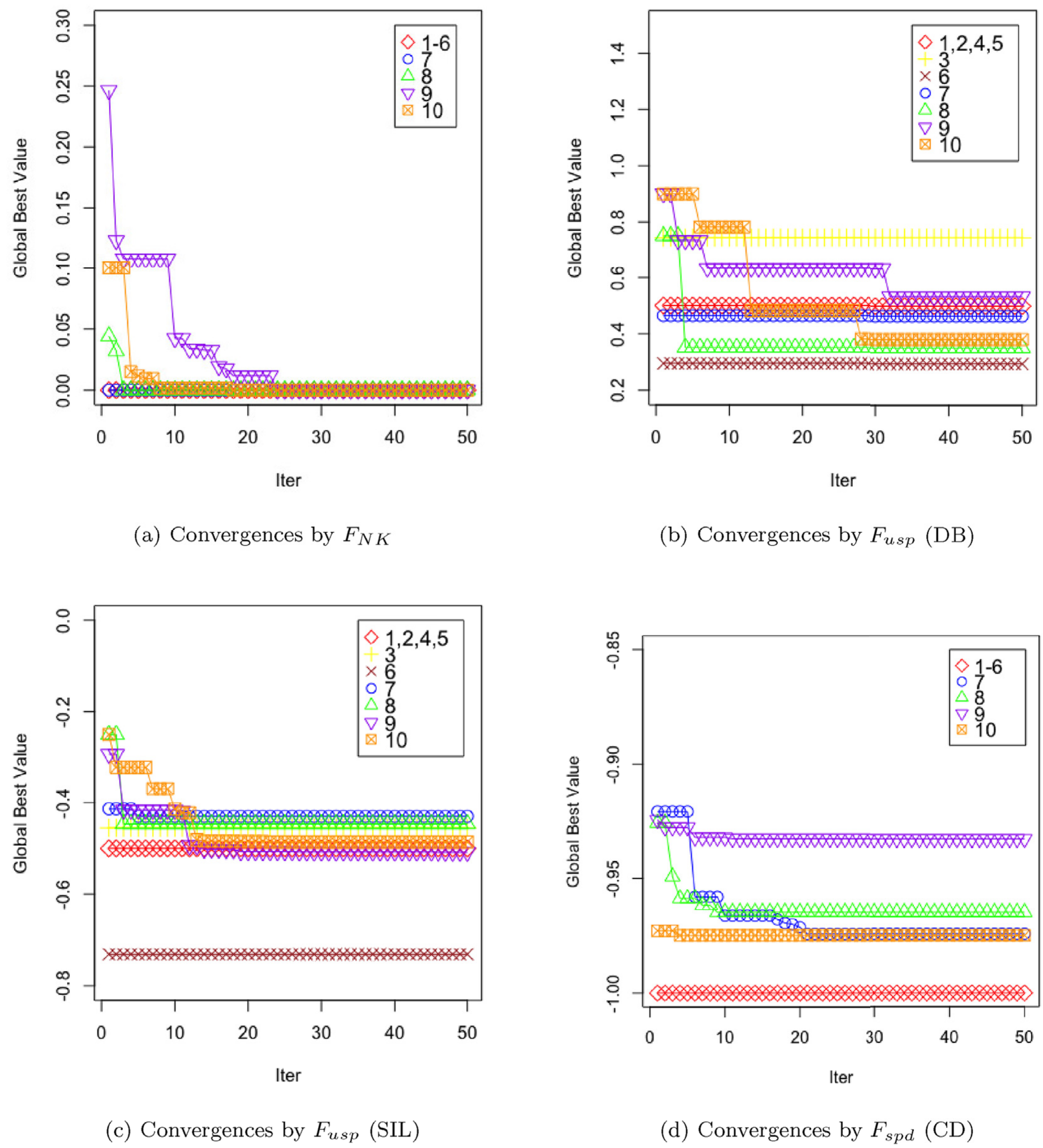


(a) Datasets 1-6



(b) Datasets 7-10

Fig. 5. Ground truth partitions of datasets.



(a) Convergences by F_{NK}

(b) Convergences by F_{usp} (DB)

(c) Convergences by F_{usp} (SIL)

(d) Convergences by F_{spd} (CD)

Fig. 6. Convergences of PODCC.

For DBSCAN, the two parameters were set to random values in the range from 0 to 10. For K-means, the *K* value was set according to the given number of clusters for each dataset. For SVM, the default settings using the e1071 package [37] were adopted. For each dataset, the number of times that DBSCAN and K-means were run was set by the product of the swam size times the number of iterations required for PODCC to reach convergence. For example, if the PODCC swarm size was set to 40, and the number of the iterations to reach the convergence point is 24, the number of times DBSCAN and K-means was run should be 40 × 24 = 960 times, which is the same as PODCC.

The convergence performance of PODCC in terms of the number of iterations required to reach a stable point is illustrated in Fig. 6. From the figure, it can be seen that PODCC converged to a stable state after about 30 iterations. In some cases, PODCC required less than 10 iterations to reach converge. The convergence speed of PODCC should be much faster than in the case of the Genetic Algorithm Density-Based Approach for Clustering (GADAC) [11] which converges at about 100 iterations.

To compare the performance of unsupervised PODCC with DBSCAN and K-means, in terms of accuracy, for each dataset, the average fitness values of the selected fitness function for all the clustering results (fit_{avg}), the fitness value for the best clustering results (fit_{best}) and the Czekanowski-Dice indices for the best clustering results (*CD*) were used. The results are presented in Tables 6–8.

Table 6 presents the results obtained using PODCC applying F_{NK} as the fitness function, in comparison to the operation of DBSCAN and K-means. For Dataset 1–6, the *CD* values show that PODCC performs better than DBSCAN and K-means. According to the clustering results shown in Fig. A1b and the convergence curve shown in Fig. 6a, PODCC applying F_{NK} can cluster Datasets 1–6 perfectly and in a relatively short time. The fitness values of all the K-means results are 0 using F_{NK}, as *K* is known and no noise is contained in the K-means results. Even though the fitness values of the K-means results are minimized, the *CD* values obtained using K-means show that the clustering results are not satisfactory with respect to the ground truth partitions. As the table and Fig. A4b shows, for Datasets 7–10, the *CD* results using PODCC applying F_{NK} are not better than K-means, as Datasets 7–10 are obviously centroid-based clustering problems. Although the K-means approach is specifically directed at centroid-based clustering, the operation of k-means is subject to the manner in which the initial cluster centroids are

Table 6
Unsupervised PODCC with F_{NK} versus DBSCAN and K-means.

ID	PODCC			DBSCAN			K-means		
	fit_{avg}	fit_{best}	CD	fit_{avg}	fit_{best}	CD	fit_{avg}	fit_{best}	CD
1	0.475	0.000	1.000	1.174	0.000	1.000	0.000	0.000	0.501
2	0.400	0.000	1.000	0.475	0.000	1.000	0.000	0.000	0.645
3	0.716	0.000	1.000	1.045	0.000	1.000	0.000	0.000	0.399
4	1.716	0.000	1.000	0.839	0.000	1.000	0.000	0.000	0.500
5	1.719	0.000	1.000	15.877	0.000	1.000	0.000	0.000	0.567
6	2.019	0.000	1.000	9.392	0.000	1.000	0.000	0.000	0.874
7	4.755	0.000	0.744	0.540	0.000	0.744	0.000	0.000	0.973
8	0.840	0.000	0.715	1.714	0.002	0.836	0.000	0.000	0.929
9	3.441	0.000	0.385	2.340	0.000	0.386	0.000	0.000	0.902
10	1.112	0.000	0.597	1.519	0.002	0.782	0.000	0.000	0.937

Table 7
Unsupervised PODCC with Davies Bouldin index versus DBSCAN and K-means.

ID	PODCC			DBSCAN			K-means		
	fit_{avg}	fit_{best}	CD	fit_{avg}	fit_{best}	CD	fit_{avg}	fit_{best}	CD
1	1.632	0.500	0.666	0.834	0.500	0.666	0.931	0.930	0.501
2	4e+15	0.500	0.666	3e+15	0.500	0.666	1.281	1.191	0.645
3	12.794	0.744	1.000	1.226	0.744	1.000	0.750	0.691	1.000
4	16.833	0.500	0.666	2.375	0.500	0.666	0.997	0.997	0.500
5	1.659	0.500	0.769	2.618	0.500	0.769	0.985	0.977	0.567
6	1.112	0.295	0.998	0.659	0.359	1.000	0.652	0.281	0.863
7	1.348	0.465	0.744	5.401	0.714	0.744	0.519	0.310	0.973
8	3.917	0.352	0.715	2.342	0.592	0.836	0.668	0.401	0.929
9	3.312	0.534	0.385	2.046	0.534	0.386	0.512	0.231	0.849
10	1.466	0.382	0.597	1.642	0.482	0.597	0.498	0.258	0.787

generated, and thus the generated cluster results may not be optimal. Examples of the cluster results obtained for Datasets 7–10 are given in Fig. A4a.

The number of clusters (K) cannot be used for DBSCAN. To address this issue, PODCC used with F_{NK} takes K as input. Figs. A6-A7 demonstrate that different user-defined K values for PODCC can lead to different pattern results. Once K is smaller than the ground truth number of clusters, 4 in the examples, some small clusters are merged to give bigger clusters, for example, Figs. A6a, A6b, A7a and A7b. Similarly, when K is larger than the ground truth number of clusters, bigger clusters are divided into some smaller clusters, for example, Figs. A6c, A6d, A7c and A7d.

Table 7 presents the results of PODCC applying fitness function F_{usp} with the Davies Bouldin clustering index. From the table, it can be seen that the performance of PODCC is better than DBSCAN for most of datasets considered. The result demonstrates that PODCC can still optimize the fitness values with respect to the chosen fitness function; however the presented CD values associated with PODCC are not satisfactory for most of the datasets. Figs. A2a and A4c show the clusters resulting from PODCC with Davies Bouldin as the fitness function. Inspection of the figures indicates that the results could be much improved. It can thus be concluded that the DB index is not appropriate in the case of unsupervised PODCC.

Table 8 presents the results of PODCC when a fitness function F_{usp} with the Silhouette Index is used. From the table it can be seen that PODCC performs better than DBSCAN for all the datasets considered. For Datasets 1–6, the fit_{best} values using PODCC are better than those associated with K-means, but the CD values are still not satisfactory. For Datasets 7–10, although the fit_{best} values of K-means are higher than PODCC, the CD values of PODCC are better than the corresponding K-means values for Datasets 9–10. Comparing the results shown in Table 7, using the Silhouette index as the basis for the fitness function achieves the better performance than using Davies Bouldin Index. It can thus be concluded that PODCC can address satisfactorily centroid-based clustering problems using a Silhouette based fitness function.

As already noted that supervised PODCC can be used for classification purposes, to evaluate this, its operation was compared to SVM in

Table 8
Unsupervised PODCC with silhouette index versus DBSCAN and K-means.

ID	PODCC			DBSCAN			K-means		
	fit_{avg}	fit_{best}	CD	fit_{avg}	fit_{best}	CD	fit_{avg}	fit_{best}	CD
1	5.637	−0.500	0.666	−0.453	−0.500	0.666	−0.431	−0.432	0.501
2	−0.435	−0.500	0.666	−0.377	−0.500	0.666	−0.321	−0.376	0.645
3	−0.105	−0.455	1.000	−0.242	−0.455	1.000	−0.419	−0.455	1.000
4	0.724	−0.500	0.666	2.402	−0.500	0.666	−0.413	−0.413	0.500
5	−0.267	−0.500	0.769	0.606	−0.500	0.769	−0.415	−0.420	0.567
6	0.295	−0.731	1.000	0.982	−0.731	1.000	−0.523	−0.594	0.850
7	0.393	−0.430	0.962	1.465	−0.415	0.742	−0.599	−0.686	0.973
8	−0.070	−0.446	0.836	0.542	−0.446	0.836	−0.494	−0.595	0.929
9	0.127	−0.507	0.926	1.125	−0.499	0.909	−0.564	−0.621	0.896
10	0.209	−0.486	0.974	0.367	−0.480	0.971	−0.577	−0.630	0.833

Table 9
Supervised PODCC with Czekanowski-dice index versus SVM.

ID	PODCC			SVM
	CD_{avg}	BP	CD_{best}	CD
1	0.694	(0.576, 5)	1.000	0.980
2	0.733	(1.456, 9)	1.000	1.000
3	0.522	(1.566, 6)	1.000	0.976
4	0.752	(2.180, 4)	1.000	1.000
5	0.846	(3.929, 8)	1.000	1.000
6	0.844	(8.098, 1)	1.000	1.000
7	0.678	(1.189, 10)	0.974	0.922
8	0.659	(1.480, 5)	0.965	0.969
9	0.457	(0.913, 6)	0.933	0.677
10	0.615	(0.628, 4)	0.975	0.542

terms of: (i) the average Czekanowski-Dice Index of all the predicted pattern results (CD_{avg}) in PODCC, (ii) the Best Parameters (BP), (iii) the corresponding CD index values of the best predicted patterns (CD_{best}) of PODCC, and (iv) the CD index values of the SVM prediction results (CD). The results are presented in Table 9. It can be seen that PODCC performs better than SVM for all datasets except for Dataset 8. However, for Dataset 8 the CD value produced by PODCC is very close to the SVM result. By comparing the pattern results of Dataset 8 given in Figs. A5a and A5b, it can be seen that the boundaries of the classes produced by PODCC are clearer than the SVM results, as PODCC inherits the character of DBCSAN which can find the presence of noises in the datasets. Such character could be either advantage or limitation subject to different situations.

The comparisons between proposed components are presented in Table 10. To summarize, PODCC when using the fitness function F_{NK} can be applied to datasets featuring arbitrary shaped clusters; whilst classical DBSCAN requires a manual generation and test process to find the appropriate parameters to produce the correct results; K-means cannot find clusters of arbitrary shape at all. PODCC when using F_{usp} with the Silhouette Index can cluster centroid-based datasets. According to the analysis of the experimental results, the combination of PSO, DBSCAN, and fitness function with SIL index leads to the best performance of the unsupervised PODCC method. Supervised PODCC can deal with all types of labelled datasets. Whilst a suitable fitness function is chosen with respect to dataset, PODCC performs better than DBSCAN and K-means for unsupervised learning and better than SVM for supervised learning.

6. Simulations

The proposed unsupervised and supervised PODCC methods with different fitness functions have been applied to analyse the open datasets with the classes of overlapped feature values. To compare PODCC with Genetic Algorithm Optimized DBSCAN for Clustering and Classification (GODCC), the SPSO part of PODCC was modified and replaced by a GA using the *GA* package in R [38,39] to implement GODCC. The performance of unsupervised PODCC was compared with the unsupervised GODCC, standard DBSCAN and K-means, whilst the performance of supervised PODCC was compared with supervised GODCC and SVM.

In this simulation, ten datasets were selected from the open sources. The details of attributes and classes in the ground truth partitions for all the datasets used are summarized in Table 11. Seven datasets were selected from UCI repository [40] (Sonar [41], Zoo [42], Ionosphere [43], Soybean [44], and Sani [45–47]) and R machine learning packages [48] [49], (Hacide [50] and Default [51]).

The other three datasets are the internet traffic datasets of three different sizes which were sampled from several big open datasets regarding TCP packet traces [52], which are the internet traffic clustering/classification cases. As the proposed method does not attempt to solve the big data problem, sampling was used. Five features of the datasets were selected to analyse: (1) mean inter-arrival time; (2) mean IP packet size; (3) the total number of packets; (4) the total number of unique bytes sent; and (5) connection duration. The examples were manually classified into different application types, including WWW, mail, p2p, services, interactive, etc.

From the class sizes and distributions shown in Table 11, eight datasets (Zoo, Ionosphere, Sani, Hacide, Default datasets and three traffic datasets) can be considered to be imbalanced datasets. Take the dataset Traffic for example; more than 80% of individuals are in one class, and the rest of individuals are in the other nine classes.

For the datasets in Table 11, the PODCC settings were as follows: (i) Swarm size was set to 50; (ii) maximum value of ϵ was the maximum distance among individuals; (iii) maximum value of *Minpts* was the value of the number of individuals divided by the number of clusters; (iv) the minimum values of ϵ and *Minpts* were 0; (v) c1, c2 (the cognitive and social acceleration coefficients) and w (predefined inertia weight) were set as 1.193, 1.193 and 0.721 respectively; and (vi) the maximum number of iterations was 50. For DBSCAN, the two parameters, radius and minpts, were set to random values in the search space

Table 10
The comparisons among k-means, SVM, DBSCAN and different combinations for PODCC.

ID	Method	Components	Clustering	Classification	Analysis Results
1	K-means	K-means	Yes	No[a]	It cannot deal with the dataset featuring arbitrary shaped clusters; The number of clusters can be controlled by the users.
2	DBSCAN	DBSCAN	Yes	No[a]	It can deal with the dataset featuring arbitrary shaped clusters; The number of clusters cannot be controlled by the users.
3	Unsupervised PODCC with f_{NK}	PSO; DBSCAN; $F = f_{NK}$	Yes	No[b]	It can deal with the dataset consisting of arbitrary shaped clusters; The number of clusters can be controlled by the users; The accuracy measured by CD Index has been improved comparing to methods 2 and 4.
4	Unsupervised PODCC with DB Index	PSO; DBSCAN; $F = f_{DB} + f_{NK}$	Yes	No[b]	It can deal with the dataset consisting of arbitrary shaped clusters; The number of clusters can be controlled by the users; The accuracy measured by CD Index has been improved comparing to method 2.
5	Unsupervised PODCC with SIL Index	PSO; DBSCAN; $F = f_{SIL} + f_{NK}$	Yes	No[b]	It can deal with the dataset consisting of arbitrary shaped clusters; The number of clusters can be controlled by the users; The accuracy measured by CD Index has been improved comparing to methods 1, 2, 3, and 4.
6	SVM	SVM	No	Yes	It may not lead to the best result.
7	Supervised PODCC with CD Index	PSO; DBSCAN; $F = f_{CD}$	No	Yes	The accuracy measured by CD Index has been improved comparing to method 6.

[a] Even the dataset has labelled variable.
[b] The dataset has no labelled variable.

Table 11
Details of the ten evaluation datasets.

Dataset	No. of Attributes	No. of Individuals	No. of Classes	Class Sizes	Class Distribution Type
Soybean	36	47	4	17/10/10/10	Balanced
Sonar	60	208	2	111/97	Balanced
Zoo	16	101	7	41/20/13/10/8/5/4	Imbalanced
Ionosphere	34	351	2	225/126	Imbalanced
Sani	55	303	2	216/87	Imbalanced
Hacide	2	1250	2	1225/25	Imbalanced
Default	2	10000	2	9667/333	Imbalanced
Traffic1K	5	1000	10	831/108/25/11/7/6/5/4/2/1	Imbalanced
Traffic2K	5	2000	9	1671/200/56/20/19/14/11/5/4	Imbalanced
Traffic5K	5	5000	10	4164/519/138/50/41/39/28/13/5/3	Imbalanced

Table 12
CD index values of clustering results of PODCC, GODCC, DBSCAN, and K-means.

Dataset	PODCC			GODCC			DBSCAN		K-Means	
	F_{NK}	F_{SINK}	F_{DBNK}	F_{NK}	F_{SINK}	F_{DBNK}	*Avg*	*Best*	*Avg*	*Best*
Soybean	1.000	1.000	0.401	1.000	1.000	0.401	0.470	1.000	0.903	1.000
Sonar	0.65	0.667	0.667	0.667	0.667	0.667	0.652	0.667	0.503	0.503
Zoo	0.951	0.951	0.378	0.951	0.761	0.378	0.422	0.956	0.755	0.936
Ionosphere	0.670	0.700	0.700	0.700	0.700	0.700	0.694	0.86	0.605	0.605
Sani	0.739	0.742	0.739	0.739	0.742	0.739	0.721	0.742	0.594	0.739
Hacide	0.980	0.980	0.980	0.980	0.980	0.980	0.975	0.991	0.661	0.664
Default	0.967	0.967	0.967	0.967	0.967	0.967	0.963	0.970	0.658	0.658
Traffic1K	0.824	0.825	0.811	0.825	0.825	0.825	0.823	0.825	0.333	0.388
Traffic2K	0.828	0.830	0.830	0.698	0.830	0.830	0.827	0.830	0.357	0.399
Traffic5K	0.827	0.827	0.827	0.827	0.827	0.827	0.826	0.827	0.374	0.403

of PODCC. For K-means, the K value was set according to the given number of groups for each dataset. For fair comparisons, DBSCAN and K-means were run for 2500 times. For SVM, the default settings using the *e*1071 package in R [37] were adopted. For GA, the default settings in the *GA* package [38,39] were adopted, but the size of the population and the maximum number of iterations were changed to 50 respectively (same number for PODCC).

Tables 12 and 13 present the simulation results of unsupervised and supervised PODCC with the four proposed fitness functions, F_{NK} (Eq (15)), F_{SINK} (Eq. (10) with Eq. (12)), F_{DBNK} (Eq. (10) with Eq. (11)), and F_{CD} (Eq. (18) with Eq. (19)). The accuracy of clustering and classification results was measured by the external CD index with respect to the ground-truth labels. Table 12 presents the results of unsupervised PODCC, unsupervised GODCC, DBSCAN and *K*-means for the ten datasets. By comparing the CD index values of the clustering results, it can be found that the accuracy of unsupervised PODCC applying F_{NK} or F_{SINK} is better than or equal to the average accuracy of DBSCAN, and the best accuracy of *K*-means.

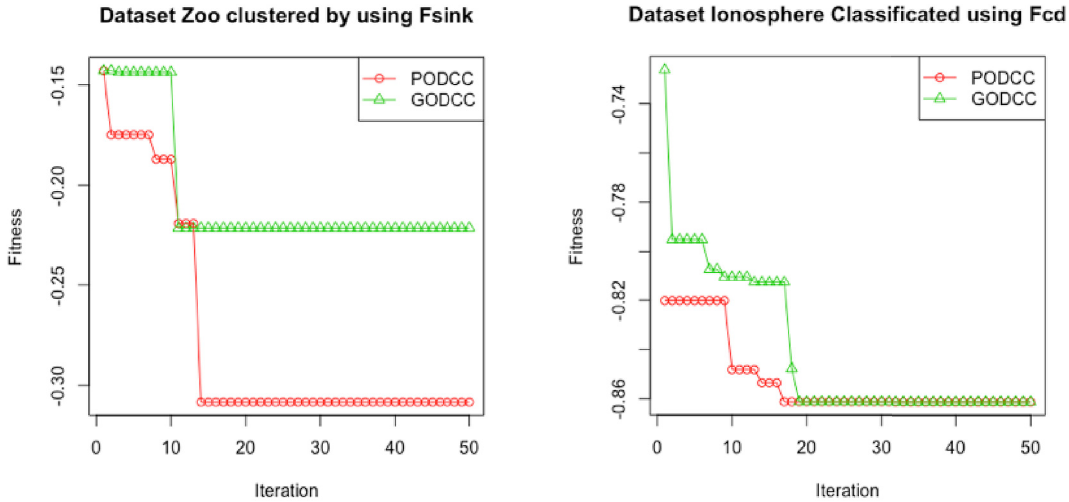
In Table 12, whilst the unsupervised PODCC achieves the similar accuracy as the GODCC for most cases, the accuracy of PODCC with F_{SINK} for the dataset Zoo and PODCC with F_{NK} for the dataset Traffic2K is significantly higher than the GODCC results. The major reason that PODCC performs better than GODCC is that PODCC adopted SPSO 2011, which performs better than GA for optimizing continuous functions [14] and more efficiently than GA [15]. Regarding continuous optimal solution, Fig. 7a demonstrates that PODCC searches the better optimal value than GODCC. Regarding computational efficiency, Fig. 7b demonstrates that PODCC converges faster than GODCC.

Table 13 presents the results of supervised PODCC with F_{CD}, supervised GODCC with F_{CD}, and SVM for the ten datasets. Both Full Train Full Prediction (FTFP) test and 90% training set and 10% prediction set (9T1P) test were conducted for each algorithm. FTFP means that all data are used for training and prediction, and 9T1P means that 90% of data was used to build a training model and the remaining 10% data was used for prediction.

Supervised PODCC and GODCC with F_{CD} achieved almost the same results for all the datasets due to sufficient searching iteration for the best results. For the datasets, Sonar, Zoo, Ionosphere, Hacide, and Default, the accuracy of SVM prediction results is higher than both PODCC and GODCC, but both Supervised PODCC and GODCC perform better than SVM for the three internet traffic datasets, whilst all of the

Table 13
CD index values of classification results of PODCC, GODCC and SVM.

Dataset	PODCC		GODCC		SVM	
	FTFP	9T1P	FTFP	9T1P	FTFP	9T1P
Soybean	1.000	1.000	1.000	1.000	1.000	1.000
Sonar	0.667	0.667	0.667	0.667	0.917	0.802
Zoo	0.955	0.956	0.955	0.956	1.000	0.944
Ionosphere	0.861	0.853	0.861	0.853	0.984	0.974
Sani	0.742	0.742	0.742	0.742	0.742	0.742
Hacide	0.991	0.991	0.991	0.991	0.993	0.992
Default	0.971	0.970	0.971	0.970	0.972	0.972
Traffic1K	0.825	0.825	0.825	0.825	0.809	0.662
Traffic2K	0.830	0.831	0.830	0.831	0.825	0.727
Traffic5K	0.827	0.827	0.827	0.827	0.827	0.811



(a) Fsink applied to Dataset Zoo

(b) Fsink applied to Dataset Ionosphere

Fig. 7. Convergences of PODCC and GODCC for two cases.

methods achieve the same prediction results for the datasets, Soybean and Sani. Although not all the supervised PODCC outperformed the SVM, a notable superiority of PODCC can be found as below. PODCC achieved better prediction results in the 9T1P test than in the FTFP. For SVM, the accuracy of FTFP results is higher or equal to the 9T1P results; the 9T1P results for datasets Sonar, Traffic1K, and Traffic2K are significantly worse than the FTFP results. For PODCC, the accuracies of FTFP and 9T1P results are similar. For datasets Traffic2K and Zoo, the 9T1P results of PODCC are slightly higher than its FTFP results.

By comparing the results of different datasets in the two tables, it can be found that both PODCC and GODCC can achieve better pattern results for the eight imbalanced datasets than the others. The accuracy of unsupervised PODCC results for the imbalanced datasets is significantly higher than the *K*-means results; and the supervised PODCC for three internet traffic dataset significantly outperforms SVM when 9T1P is applied. In PODCC, the data points in the big size class can be grouped into one class if they are in the close hyper-spheres determined by the appropriate parameters for DBSCAN, whilst the big size class can be forced to be divided into several small classes regardless of the density of data points in *K*-means.

Overall, the analysis comes to three conclusions.

- Unsupervised PODCC with F_{NK} and F_{SINK} can find better clustering results than K-means. In the experiments, the PSO applied in DBSCAN clustering method performs better than GA in some cases (Zoo and Traffic2K).
- For the selected cases in this paper, the 9T1P setting for the supervised PODCC is likely to have better prediction results than the FTFP setting, whilst 9T1P is more frequently used and practical than FTFP.
- PODCC is recommended for the imbalanced clustering and classification problems. For the simulation of some imbalanced datasets, the PODCC has better performance in clustering and classification than *K*-means and SVM respectively.

7. Conclusions

This paper proposes a novel method, Particle Swarm Optimized Density-Based Clustering and Classification (PODCC) to overcome the three drawbacks of classical Density-Based Spatial Clustering of Applications with Noise (DBSCAN). Firstly the two critical parameters for DBSCAN are difficult to set; secondly when using DBSCAN the number of desired clusters cannot be pre-specified by the user; and thirdly DBSCAN cannot be used in a supervised learning context where labelled training data can be used to drive the clustering. To address the first drawback, a Particle Swarm Optimization (PSO) based approach is proposed to search the entire parameter space for DBSCAN. The second drawback is addressed by using proposed fitness functions that take the number of desired clusters into account. The third drawback is addressed by another proposed fitness function, one that operates with labelled training data, so that PODCC can also perform in a supervised learning context.

The proposed PODCC system was evaluated using 10 datasets; comparisons were undertaken so as to analyse the operation of the proposed fitness functions, and to analyse the operation of PODCC in comparisons to DBSCAN, K-means and SVM. The experiment results show that the unsupervised PODCC performs better than DBSCAN and K-means, and that supervised PODCC can perform better than SVM when a suitable fitness function is chosen.

Ten open datasets with the classes of overlapped feature values were used to evaluated PODCC. To compare with PODCC, Genetic Algorithm Optimized DBSCAN for Clustering and Classification (GODCC) was proposed. The SPSO part of PODCC was modified and replaced by a GA to implement GODCC. The performance of unsupervised PODCC was compared with the unsupervised GODCC, standard DBSCAN and K-means, whilst the performance of supervised PODCC was compared with supervised GODCC and SVM. The results obtained indicated that unsupervised PODCC can find better clustering results than *K*-means and GODCC, when a suitable fitness function is chosen. Both unsupervised and supervised PODCC methods are found to be appropriate for both imbalanced clustering and classification problems.

For future work, the idea is to extend PODCC as a framework for ESA optimized DBSCAN clustering and classification. More comprehensive comparisons between different ESAs in optimizing the parameters of DBSCAN will be conducted. Since the advantage of DBSCAN is that it finds the arbitrary shaped clusters, the application of ESA optimized DBSCAN methods will be explored in the area of image processing, such as face recognition and medical image segmentation.

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Appendix

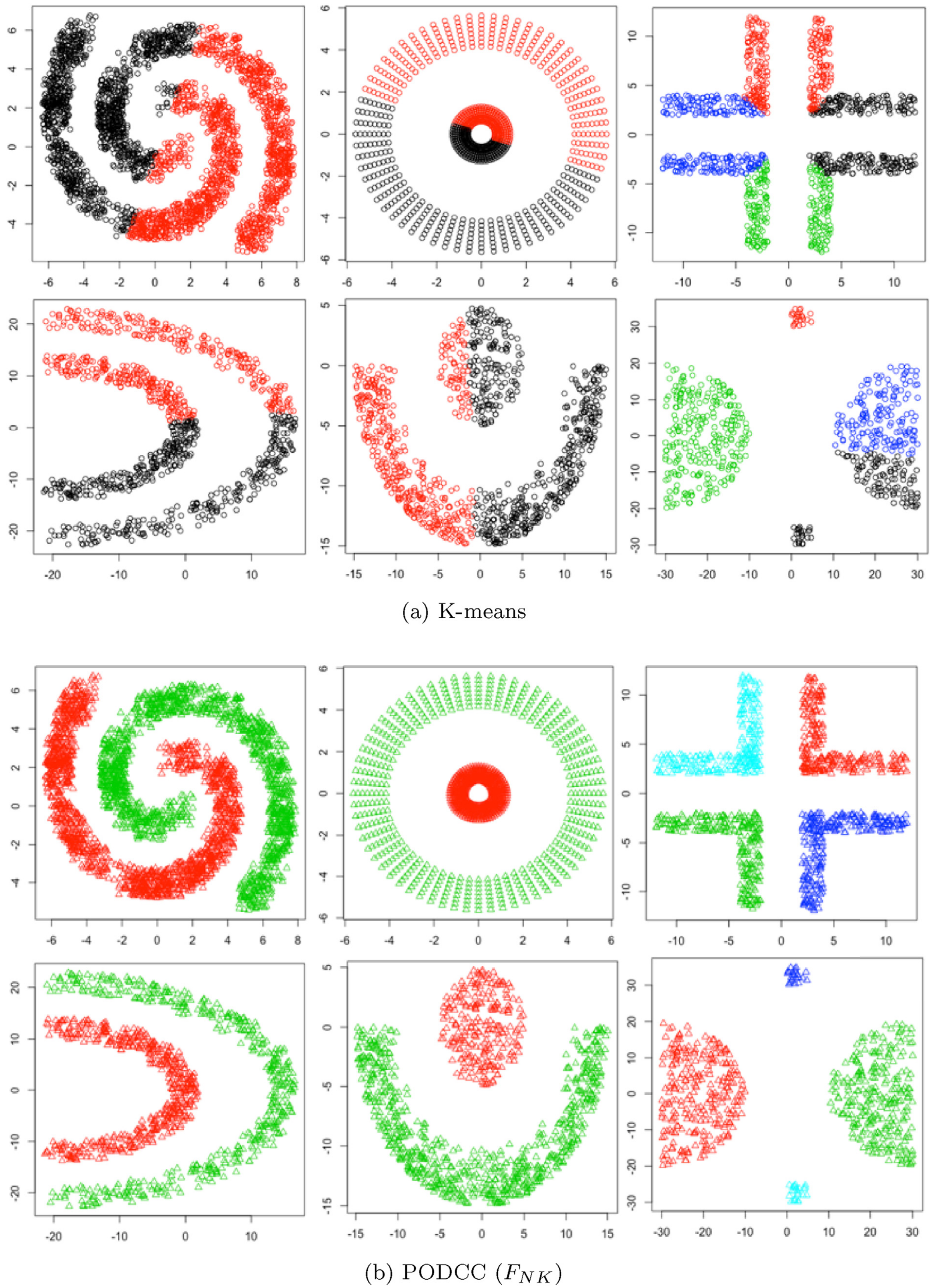
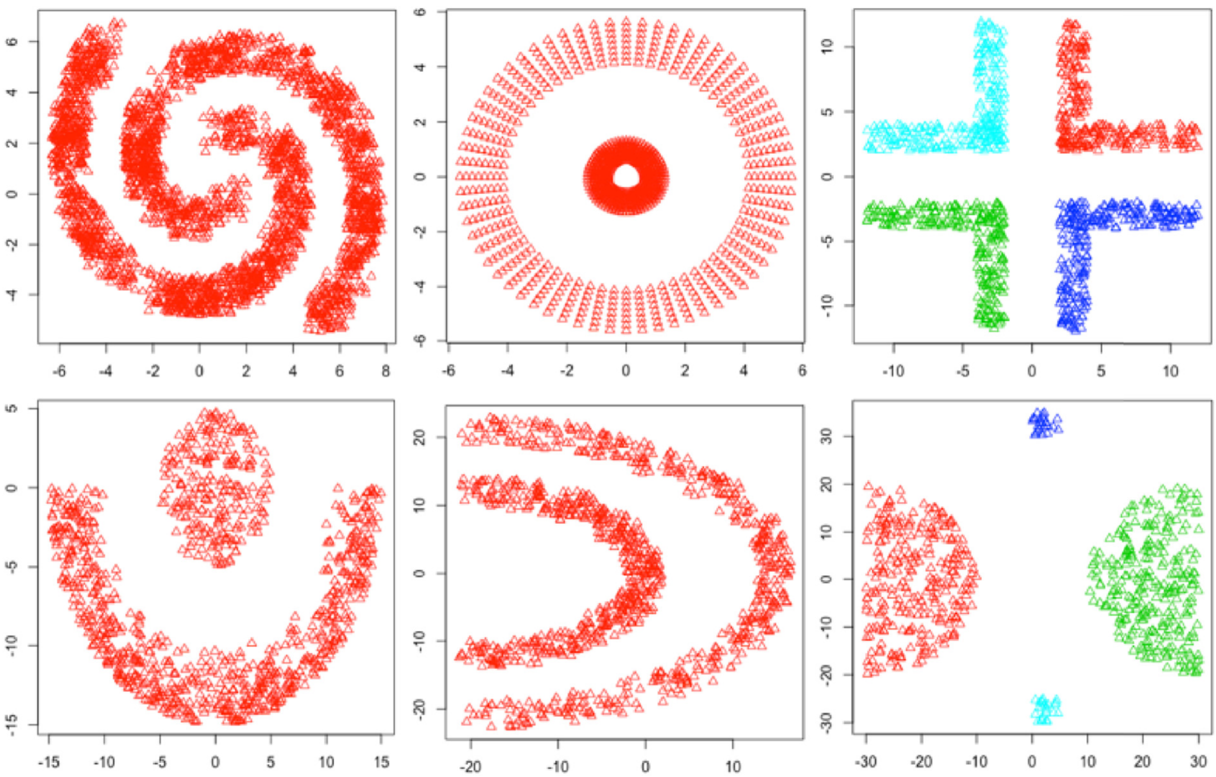
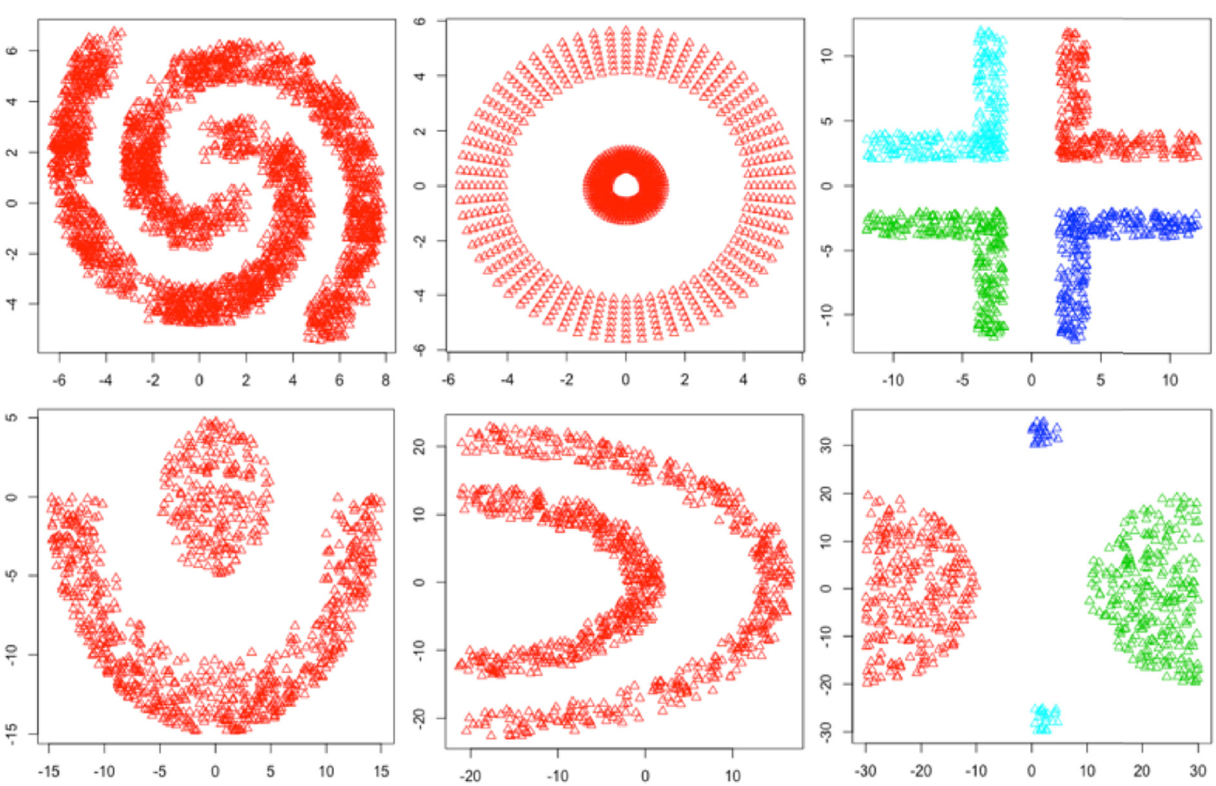


Fig. A1 Clustering Pattern Results of Datasets 1–6 Produced by K-means and Unsupervised PODCC.

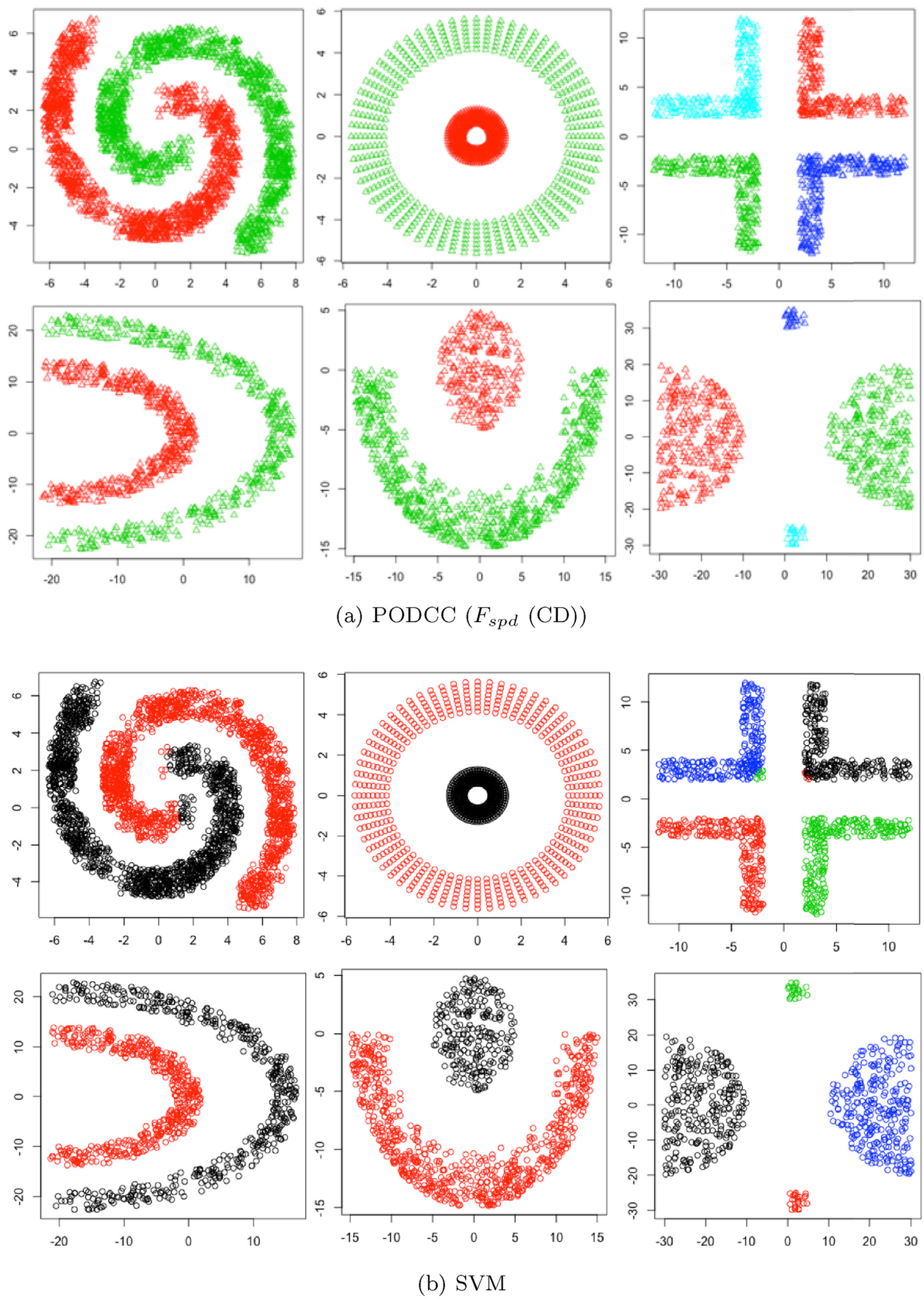


(a) PODCC (F_{usp} (DB))



(b) PODCC (F_{usp} (SIL))

Fig. A2 Pattern Results of Datasets 1–6 Produced by Unsupervised PODCC.



(a) PODCC (F_{spd} (CD))

(b) SVM

Fig. A3 Prediction Results of Datasets 1–6 Produced by Supervised PODCC and SVM.

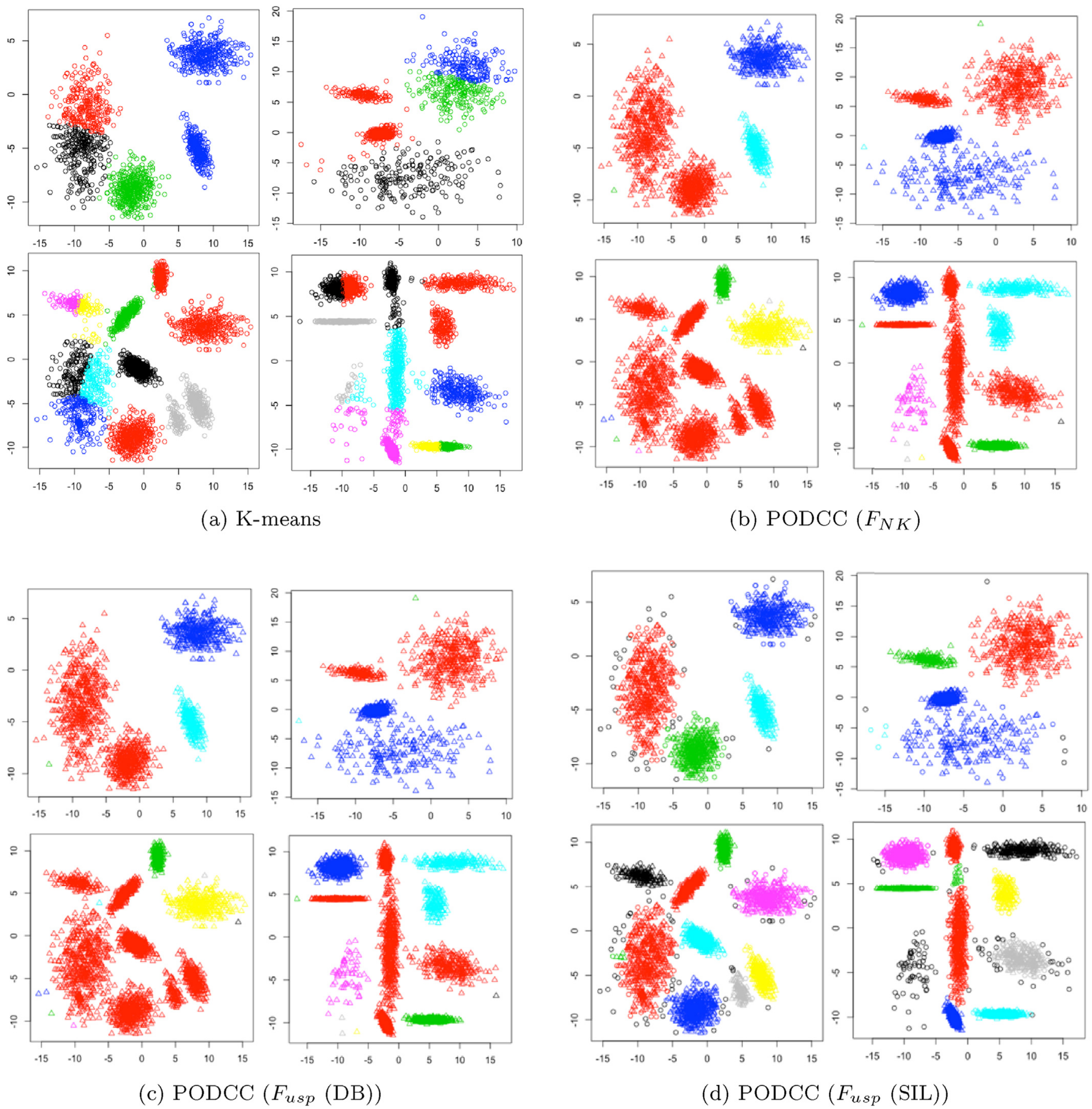
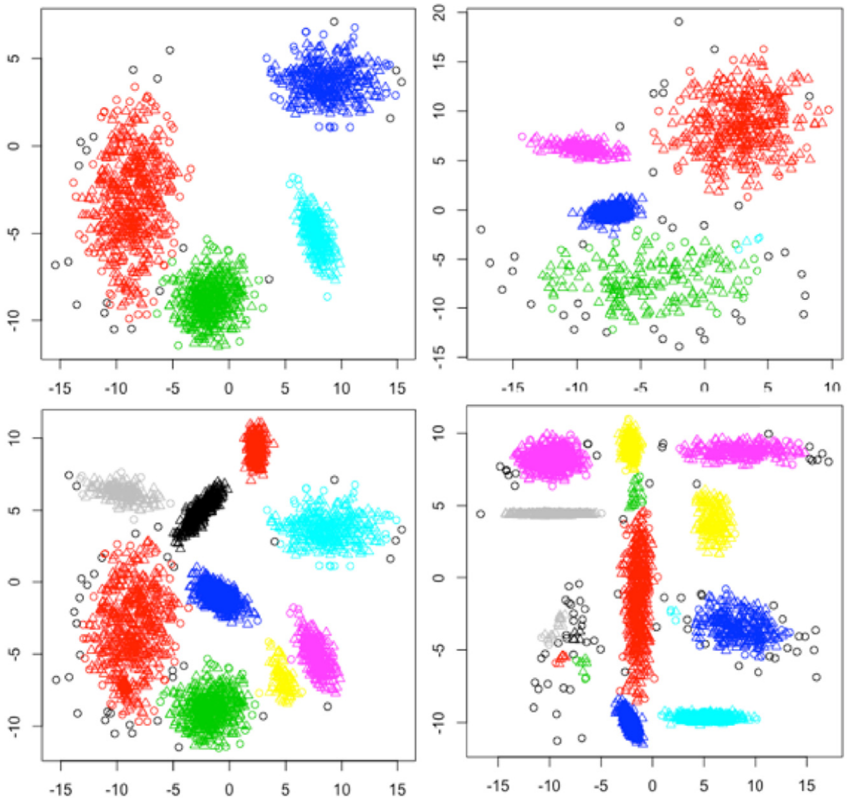
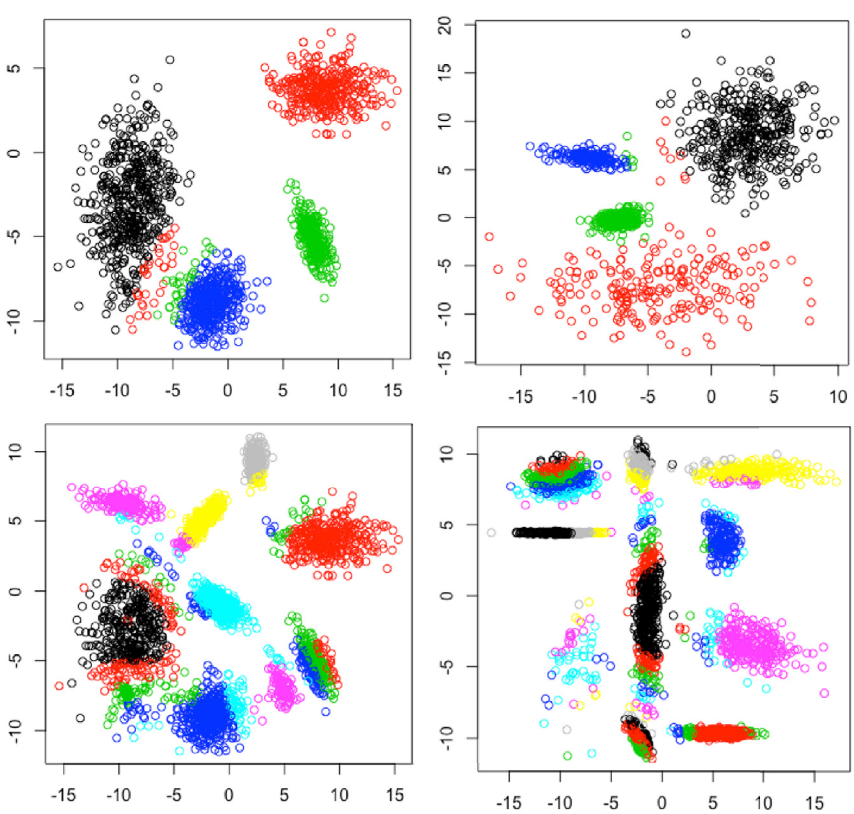


Fig. A4 Clustering Pattern Results of Datasets 7–10 Produced by Unsupervised PODCC and K-means.

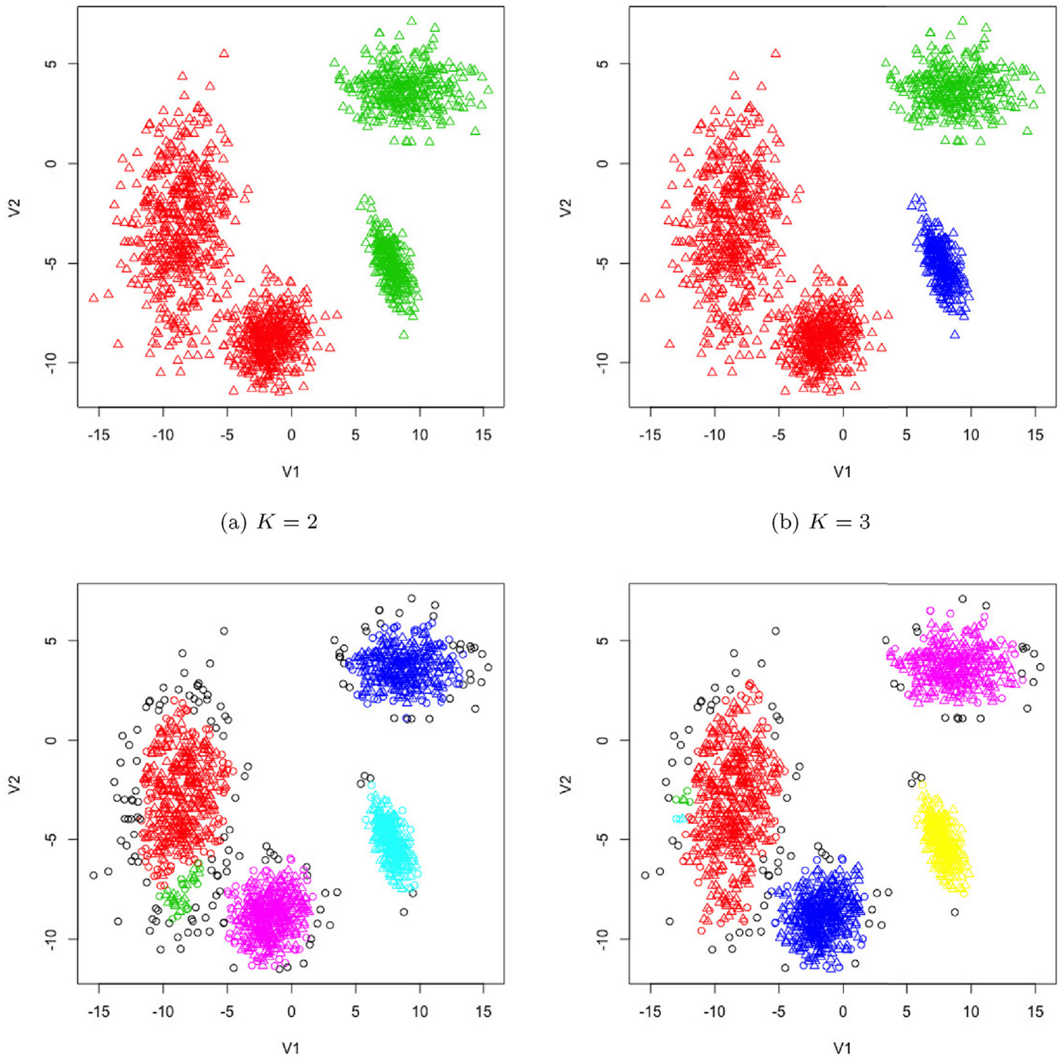


(a) PODCC (F_{spd} (CD))



(b) SVM

Fig. A5 Prediction Results of Datasets 7–10 Produced by Supervised PODCC and SVM.



(a) $K = 2$

(b) $K = 3$

(c) $K = 5$

(d) $K = 6$

Fig. A6 PODCC Results of Dataset 7 with Different Numbers of Clusters Defined by the User.

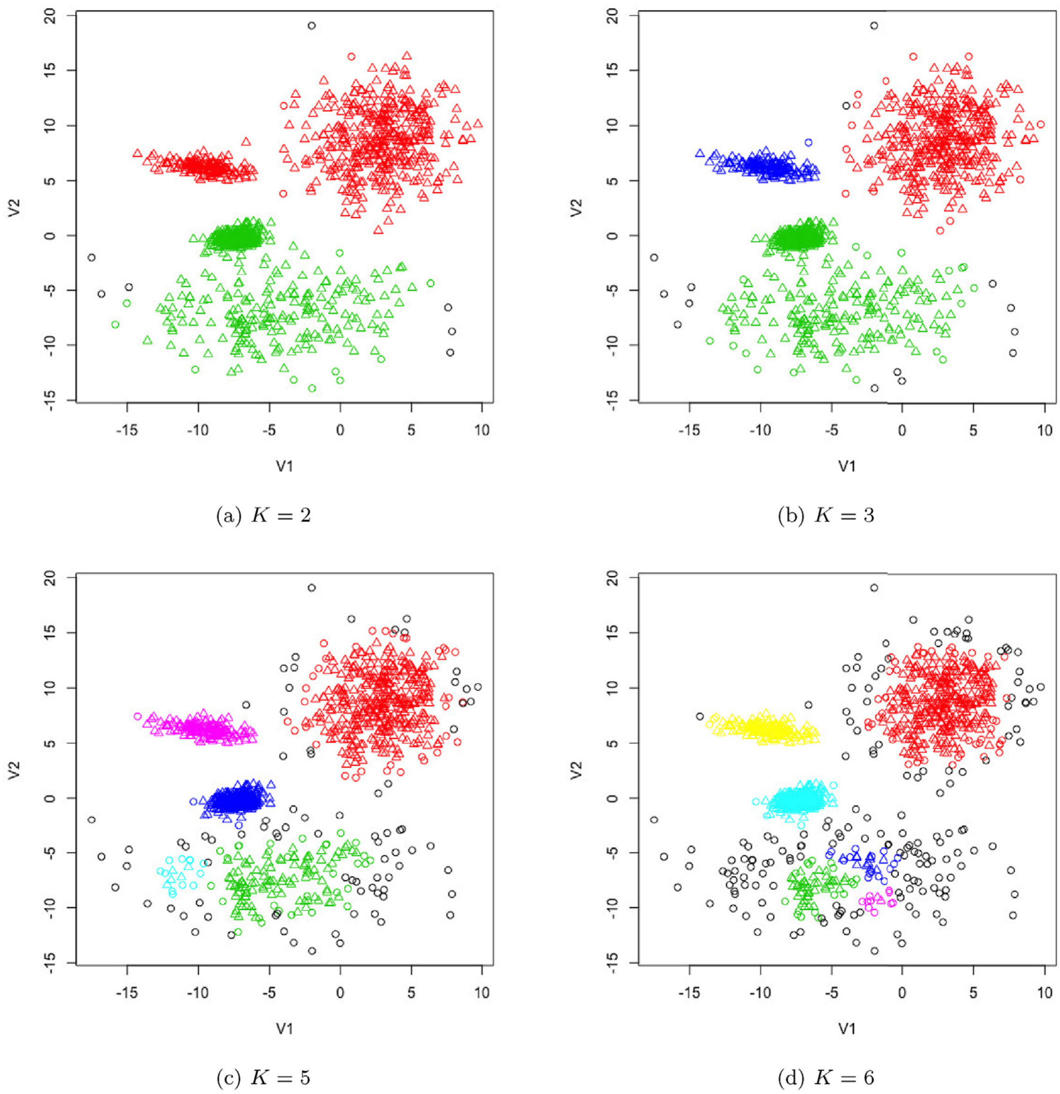


Fig. A7 PODCC Results of Dataset 8 with Different Numbers of Clusters Defined by the User.

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