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MOCF: A Multi-Objective Clustering Framework using an Improved Particle Swarm Optimization Algorithm

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Abstract— Traditional clustering algorithms, such as K-Means, perform clustering with a single goal in mind. However, in many real-world applications, multiple objective functions must be considered at the same time. Furthermore, traditional clustering algorithms have drawbacks such as centroid selection, local optimal, and convergence. Particle Swarm Optimization (PSO)-based clustering approaches were developed to address these shortcomings. Animals and their social Behaviour, particularly bird flocking and fish schooling, inspire PSO. This paper proposes the Multi-Objective Clustering Framework (MOCF), an improved PSO-based framework. As an algorithm, a Particle Swarm Optimization (PSO) based Multi-Objective Clustering (PSO-MOC) is proposed. It significantly improves clustering efficiency. The proposed framework's performance is evaluated using a variety of real-world datasets. To test the performance of the proposed algorithm, a prototype application was built using the Python data science platform. The empirical results showed that multi-objective clustering outperformed its single-objective counterparts.

Keywords- Particle Swarm Optimization(PSO), Multi-Objective Clustering(MOC),Multi-Objective Clustering Framework(MOCF)

1. INTRODUCTION

Multi-objective clustering (MOC) is aimed at dividing given data instances into similar groups while meeting multiple objective functions in parallel. MOC improves capabilities of clustering with different objectives, fitness functions and thresholds [1]. MOC promotes spatial co-location mining besides supporting various real world applications. For real world complex problems, multi-objective formulations provide realistic models. When objectives considered are in conflict, there is need for further optimization of given solution. In an MOC context, a problem needs to find a set of solutions that satisfy given objectives at an acceptable level. Most of the real world engineering problems do have many objectives such as performance, cost, and reliability and so on. These are realistic problems and difficult to solve without MOC [4].

In practice, acquiring a solution precisely and accurately is difficult. In addition to this problem, scaling among objectives is essential. Moving objectives to meet constraints with arbitrary outcomes and finally optimize a solution from a set of solutions contains trade-offs. Therefore, it is better to have multiple good solutions that satisfy all objectives to the acceptable level. However, this is the challenging problem and needs MOC support [9]. Literature has considerable coverage of MOC based on PSO technique. The work in [3] and [4] is the representative of this proposition. The framework in [3] has features of both MOPSO and MOSA. It makes use of different cluster validity indices in order to optimize solutions. Their algorithm is known as MOPSOSA. It obtains pare to optimal set with parallel optimization of objectives. In [4], an improved MOC based on PSO is defined. It has novel particle representation that helps in searching in continuous space. It also has specific leader selection strategy for improving clustering process. From the literature, it is found that most of the solutions are based on PSO as it is suitable for continuous space. However, there is need for further research on PSO based MOC to improve the state of the art. Our contributions are as follows.

1. An improved PSO based framework known as Multi-Objective Clustering Framework (MOCF) is proposed.
2. An algorithm called Particle Swarm Optimization based Multi-Objective Clustering (PSO-MOC) is proposed. It improves clustering efficiency to a greater extent.
3. A prototype application is built to evaluate the framework and underlying algorithm with many real world datasets.

The remainder of the paper is structured as follows. Section 2 reviews literature on prior works pertaining to multi-objective clustering. Section 3 provides preliminaries that help in understanding the proposed framework. Section 4 presents the proposed Multi-Objective Clustering Framework (MOCF). Section 5 presents experimental results while section 6 concludes the paper and gives suggestions for future scope of the research.

2. RELATED WORK

There is significant research, of late, on multi-objective clustering. Jiamthapthaksinet al. [1] focused on co-location mining with the help of MOC. They proposed a framework towards it in order to identity regions in which co-located Arsenic concentrations exist. Khan and Ahmad [2] explored K-modes clustering to achieve partitioned clustering of categorical data. They proposed a novel method to select most prominent attributes from given dataset. They also defined a cluster-center initialization algorithm for effectiveness of the clustering process. However, it lacks MOC.

Abubakeret al. [3] proposed MOC based on PSO [7] and Simulated Annealing (SA). Their framework is named as Multi-Objective Simulated Annealing (MOSA). Different distance measures are used to achieve MOC and its validation. Cong et al. [4] proposed an improved MOC based on PSO namely Improved Multi-Objective Clustering using PSO (IMCPSO). It could improve solution with clustering efficiency. Zhang et al. [5] used multi-objective PSO towards cost based feature selection that is used in supervised learning method.

Li and Wong [6] investigated on evolutionary multi-objective clustering and its application in patient stratification. Different clustering based indices are used for evaluation.

Dai and Sheng [8] proposed MOC algorithm with ensemble approach and with automatic k-determination. Pizzuti and Socievole [9] proposed MOC method based on genetic framework. It clusters attributed graphs with local merge and MOC optimization for high quality solutions. They intend to apply their solution to dynamic networks in future.

Godinezet al. [10] focused on optimization of MOC problems. They explored and evaluated two such algorithms known as OMOPSO and NAGA-II. He et al. [11] used MOPSO for Wireless Sensor Networks (WSNs) by defining an algorithm named Energy Efficient Trajectory Planning (EETP) in order to reduce delay in data dissemination and improve network lifetime.

Dabiriet al. [12] also used MOPSO based model for solving bi-objective inventory routing problem. Gavval and Ravi [13] used multi-objective PSO for clustering bank customer complaints. Yu et al. [14] used multi-objective models in environmental applications to save energy and reduce emissions.

Sahooet al. [15] used PSO algorithm for energy efficient clustering in WSN where sink is provided using a mobility model.

Fuchs et al. [16] proposed a methodology basedon swarm intelligence approach in order to avoid local optimal in Fuzzy C-Means (FCM) clustering. Their optimization algorithm is known as Fuzzy Self-Tuning Particle Swarm Optimization (FST-PSO).

Yu et al. [17] achievedsurrogate assisted PSO using clustering based evolution control. Guan et al. [18] used PSO based MOC solution to optimize multi-workshop facility layout.

Mousaet al. [19] studied multi-objective resource allocation problems using evolutionary algorithms based on K-Means clustering and Genetic Algorithm (GA). Feiet al. [20] investigated optimization problems with multiple objectives in WSNs. From the literature, it is found that most of the solutions are based on PSO as it is suitable for continuous space. However, there is need for further research on PSO based MOC to improve the state of the art.

3. PRELIMINARIES

This section provides basics of PSO clustering including the standard PSO algorithm used for clustering. With respect to PSO clustering a particle represents centroid vectors. Each particle denoted as x_i, in the clustering process, is created as in Eq. 1.

$$x_i=(m_i, m_{ij}, \ldots, m_{iN}) \quad (1)$$

In the cluster C_{ij}, i_{th} particle and j_{th} cluster centroid is referred to as m_{ij}. Thus, each swarm represents many clustering candidates for current data vectors. With the help of quantization error, the fitness of the particles is measured as in Eq. 2.

$$J_e = \frac{\sum_{j=1}^{N_e}[\sum \forall z_p \in C_{ij} d(z_p, m_j)/|C_{ij}|]}{N_e} \quad (2)$$

Where d refers to the centroid determination as in K-Means clustering and the number of data vectors is denoted as |Cij| which also reflects frequency of the cluster. The standard gbest PSO clustering is discussed here as it is reused in the multi-objective PSO. The algorithmic steps are as follows.

Particle initialization to represent centroids randomly chosen
For t=1 to t_{max} do
For each particle i do
For each data vector z_p do
Compute distance to all centroids
Assign z_p to cluster C_{ij}
Compute fitness using Eq. 2.
End For
Update local and global best positions
Update cluster centroids as follows

$$u_{i,k}(t+1) = wu_{i,k}(t) + c_1 r_{1,k}(t)\left(y_{i,k}(t) - x_{i,k}(t)\right) + c_2 r_{2,k}(t)\left(y_k(t) - x_{i,k}(t)\right)$$

$$x_i(t+1) = x_i(t) + v_i(t+1)$$

End For

As presented in Algorithm 1, it is the baseline PSO algorithm that performs clustering. It performs population based search and reduces the influence of initial criteria in contrast to K-Means. Multiple positions are used to start search simultaneously thus the performance is better than that of K-Means.

4. MULTI-OBJECTIVE CLUSTERING FRAMEWORK

This section describes the clustering problem considered, the proposed framework and the algorithm to achieve multi-objective clustering.

4.1 Problem Definition

Clustering is the problem that considers a dataset denoted as D with number of feature vectors. It is represented as D={p_1,p_2,...,p_n} in which p_i is a feature vector of d-dimensions such that pi=(p_{i1},p_i2,...,p_{id}). It is also known as an object where p_{ij} is considered a feature value of i^{th} object at j^{th} dimension. The variable *n* denotes number of objects in D. Clustering D does mean that grouping objects in D into k clusters denoted as {C_1,C_2,...,C_k} that satisfy properties mentioned in Eq. 3,

Eq. 4 and Eq. 5.

$$U_{i=1}^{k} C_i = D \quad (3)$$

$$C_i \cap C_j = \emptyset, i \neq j, i = 1,2,\ldots,k, j = 1,2,\ldots,k \quad (4)$$

$$C_i \neq \emptyset, i = 1,2,\ldots,k \quad (5)$$

With a single objective function, the clustering optimization is denoted as

$\underset{C \epsilon \theta}{min/max}\, f(C)$ so as to satisfy Eq. 3, Eq. 4 and Eq. 5 where the validity index function is denoted as *f*. while set of feasible solutions is denoted as x that contains different clusters of D such as C = {C_1,C_2,...,C_k} where k may be 2, 3, …, n-1. For various validity indices denoted as S, with respect to MOC problem, it is as in Eq. 6.

$$\underset{c \epsilon \Theta}{min}\, F(C) = [f_1(C), f_2(C), \ldots, f_s(C)] \quad (6)$$

where a vector associated with S is denoted as F(C). In fact, there may be no solution that is capable of minimizing all functions. Therefore, it is good to identify a set of non-dominant solutions. Thus a pair of optimal set is expected that should contain non-dominated solutions that are part of Θ.

4.2 The Framework

Based on baseline PSO [7] for clustering a Multi-Objective Clustering Framework (MOCF) is proposed as presented in Figure 1. It has different phases such as initialization that includes initialization of swarm and initialization of leaders archive that uses external storage for maintaining leader information. Afterwards, the quality of leaders is determined before starting an iterative process. There are operations that are carried out in the iterative process. They include leader selection, updating position, mutation, evaluation, updating leaders and checking leaders' quality.

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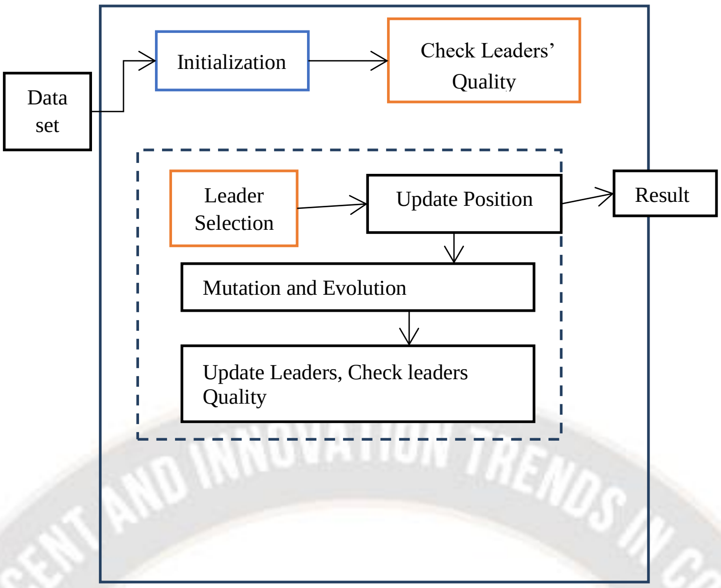

Figure 1: Overview of the proposed framework named MOCF

As presented in Figure 1, the framework considers multi-objective clustering that simultaneously focuses on clustering problem and meeting objective functions. When compared to single objective PSO, MOCF determines set of particles that are used as leaders. During the search it retains non-dominant solutions besides maintaining diversity in swarm in order to reduce possibility of convergence to a single solution.

4.3 Algorithm Design

An algorithm known as Particle Swarm Optimization based Multi-Objective Clustering (PSO-MOC) is designed and implemented.

Algorithm: Particle Swarm Optimization based Multi-Objective Clustering
Inputs: Dataset D, max generations M, number of particles N
Output: Clustering results

1. Initialize swarm vector S
2. Initialize leaders archive vector L
3. LeadersQualityCheck(L)
4. For each generation m in M
5. For each particle p in N
6. Select leader
7. Update position
8. Perform mutation
9. Perform evaluation
10. Update pbest
11. End For
12. Update L
13. LeadersQualityCheck(L)
14. End For
15. Return L

Algorithm 1: Particle Swarm Optimization based Multi-Objective Clustering

As presented in Algorithm 1, it takes dataset, number of particles and maximum number of generations as input and produces the results of clustering process that meet different objective functions.In Step 1, swarm vector S is initialized while leaders archive vector L is initialized in Step 2. In Step 3, leaders' quality check is determined. Step 4 starts an iterative process that is executed for each generation until max number of generations condition is met. In step 5, another iterative process is executed for all particles used. In Step 6 leader selection is made and Step 7 the position is updated. Mutation and evaluation are carried out in Step 8 and Step 9 respectively. At the end of the iterative process started in Step 4 is the update of pbest carried out. In Step 12, leaders archive vector is L is updated. Based on the updated leaders achieve quality of leaders is determined. Once the termination condition is met, the results are returned as in Step 15. More details of the algorithm are provided below.

4.3.1 Objective Functions

Multiple objective functions are used in the proposed PSO algorithm. The idea of choosing multiple objectives is to improve quality in clustering process. The objective functions used in the proposed clustering include overall deviation or compactness, mean distance between vectors and connectivity. The overall intra-cluster size of the data reflects compactness. It is expressed as in Eq. 7.

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$$\boldsymbol{Dev(C)} = \sum_{C_k \in C} \sum_{i \in C_k} \boldsymbol{\delta(i, \mu_k)} \qquad (7)$$

Where a set of clusters is denoted as C while Ck and μk denote a specific cluster and its centroid respectively. The Euclidean function which is used as distance function is denoted as δ(.,.). When overall deviation is minimized, it leads to higher performance. Mean distance between clusters is the other objective used. In general there should be high intra-cluster and low inter-cluster similarity in order to have better clustering solution. With respect to this fact, mean distance between clusters reflects the difference between clusters. The concept known as "minimum distance of cluster's neighbors" is used in formula this objective function. In fact, the concept of neighbor is to find the relation between two data points. This objective function is expressed as in Eq. 8.

$$Mdc(C) = \frac{1}{|C|} \sum_{C_k \in C} \left(min_{i \in C_k, j \in N_i, j \notin C_k}, \delta(i, j) \right) \qquad (8)$$

Where M_{dc} refers to mean distance between clusters and C refers to set of clusters. The neighbors set of data is denoted as N_i. When mean distance between clusters is maximized, it reflects improved quality in clustering. Connectivity is another objective function used in MOC. This objective function is expressed as in Eq. 9.

$$Conn(C) = \sum_{i=1}^{N} \left(\sum_{j=1}^{L} x_i, nn_{ij} \right) \qquad (9)$$

where $x_{r,s} = \{ \frac{\frac{1}{j}, \quad if \nexists C_k : r \in C_k \wedge S \in C_k}{0, \quad Otherwise}$

The size of data set is denoted as N while the contributing neighbors to connectedness is denoted as L. The j_{th} nearest neighbor of given item *i*is denoted as nn_{ij}. Connectivity measure reflects the degree of connectedness of the clusters which is identified by using the concept of k-nearest neighbors. In the process of multi-objective clustering, the fitness of any Pareto solution can be determined by summing up the objective functions aforementioned. The summing process is expressed as in Eq. 10.

$$fit_i = \sum_{j=1}^{m} X'_{i,j} \qquad (10)$$

where the number of objective functions is denoted as *m*. The computed fit_i determines fitness of a Pareto solution.

4.3.2 Leader Selection and Usage of External Archives

In PSO based clustering with multiple objectives in fitness function, it is essential to have leader selection process as that plays crucial role. This process is essentially different from that of traditional approaches. Choosing a non-dominated solution randomly is a straight forward approach. However, leader selection with such approach needs a quality measure that is associated with density that promotes diversity. The quality measure which is part of leader selection process also reveals the closeness of the particles in the given swarm.

While the leader selection process is indispensable, it is also important to have external archives in order to have better performance in leader selection process. The idea of having a global repository is used in this paper which is inspired by the work in [22]. When a repository is maintained, it can be used by the particles with ease to select leader. Using a single external archive that helps in retaining non-dominated solutions in relation with previous swarms is a straight forward approach. However, its drawback is that size of archive gets increased. To overcome this problem, we used three archives in order to extend PSO[23] to support multiple objectives simultaneously. Storage of global best solutions, personal best values and local best values is made with the three archives.

5. RESULTS AND DISCUSSION

The experimental results of the proposed framework are compared with the state of the art clustering algorithms such as K-Means (single objective) and GenClustMOO (Multi-Objective). Real world datasets collected from [24] such as Ecoli, Wdbc, Segment, Vehicle and Glass are used for the multi-objective clustering.

Table 1: Shows performance of different clustering algorithms in terms of F1 score

Data set	Performance (F1 Score)		
	PSO-MOC (Proposed)	**GenClustMOO**	**KM**
Ecoli	0.980036	0.955086	0.936124
Wdbc	0.919158	0.679638	0.681634
Segment	0.987022	0.679638	0.616764
Vehicle	0.979038	0.967062	0.959078
Glass	0.566864	0.493012	0.491016

As presented in Table 1, the performance is measured in terms of F1-score. The results revealed that the performance of PSO-MOC is better than its predecessors.

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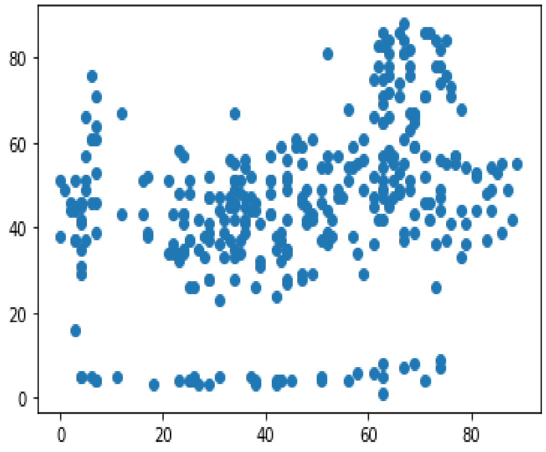

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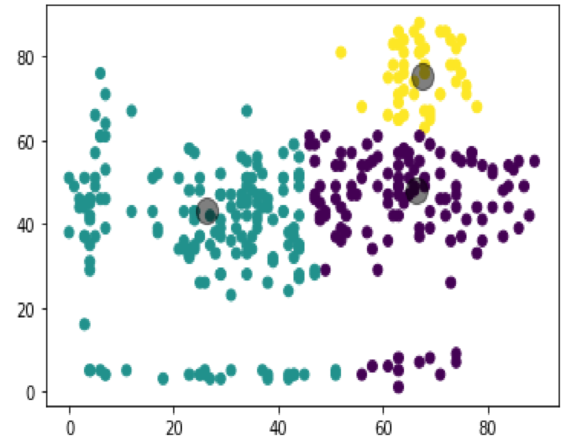

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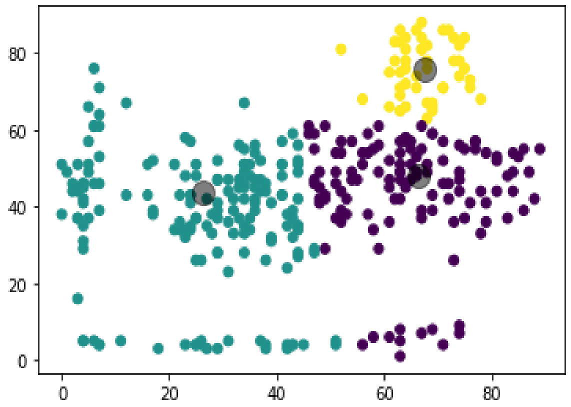

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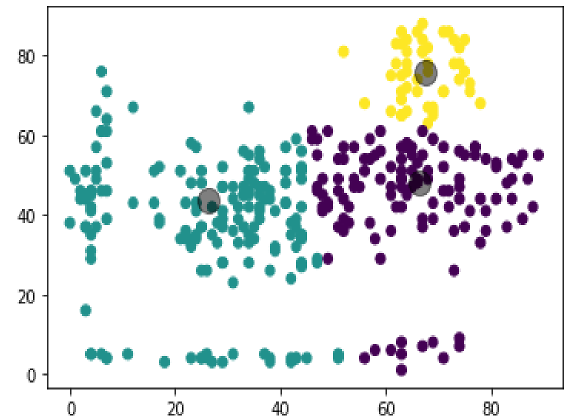
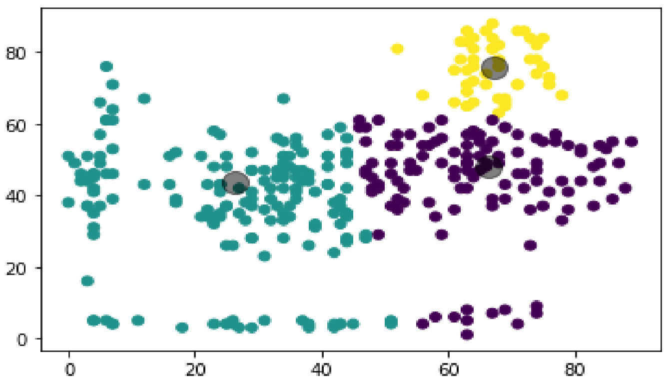


2(d)



2 (e)

Figure 2: Clustering results of Ecoli dataset

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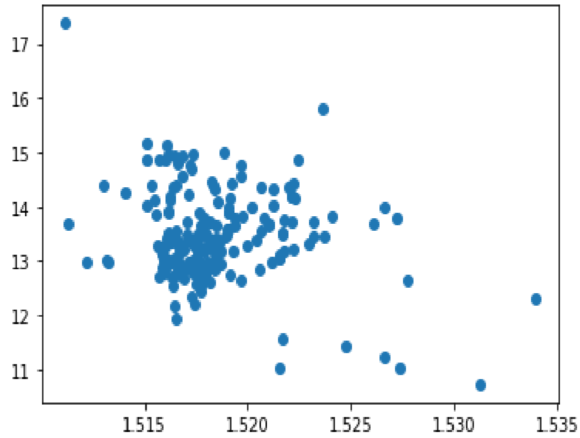

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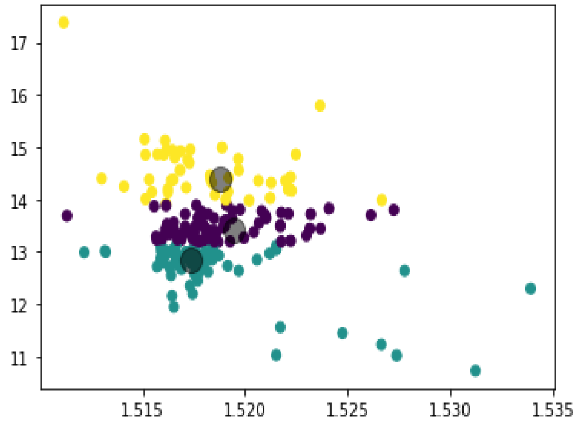

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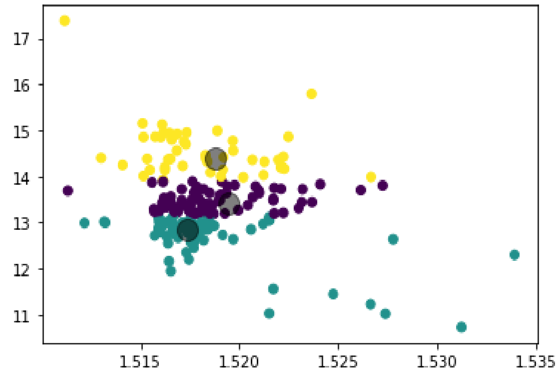

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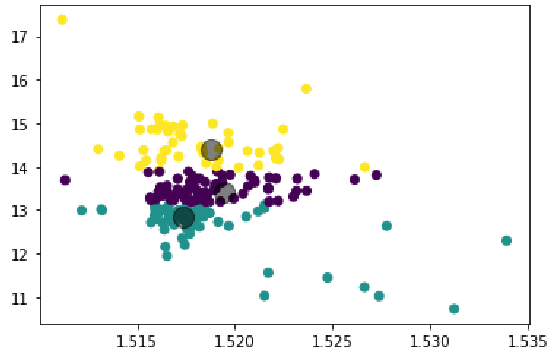

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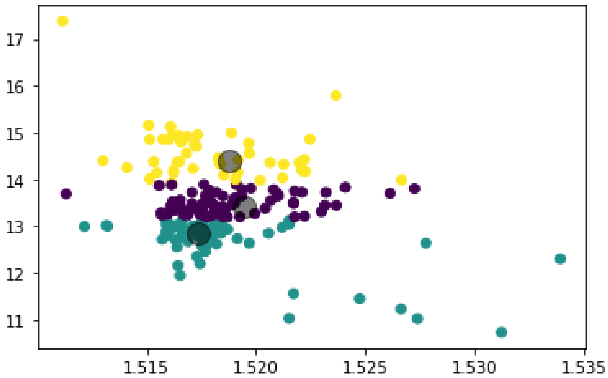

3 (e)

Figure 3: Clustering results of Glass dataset

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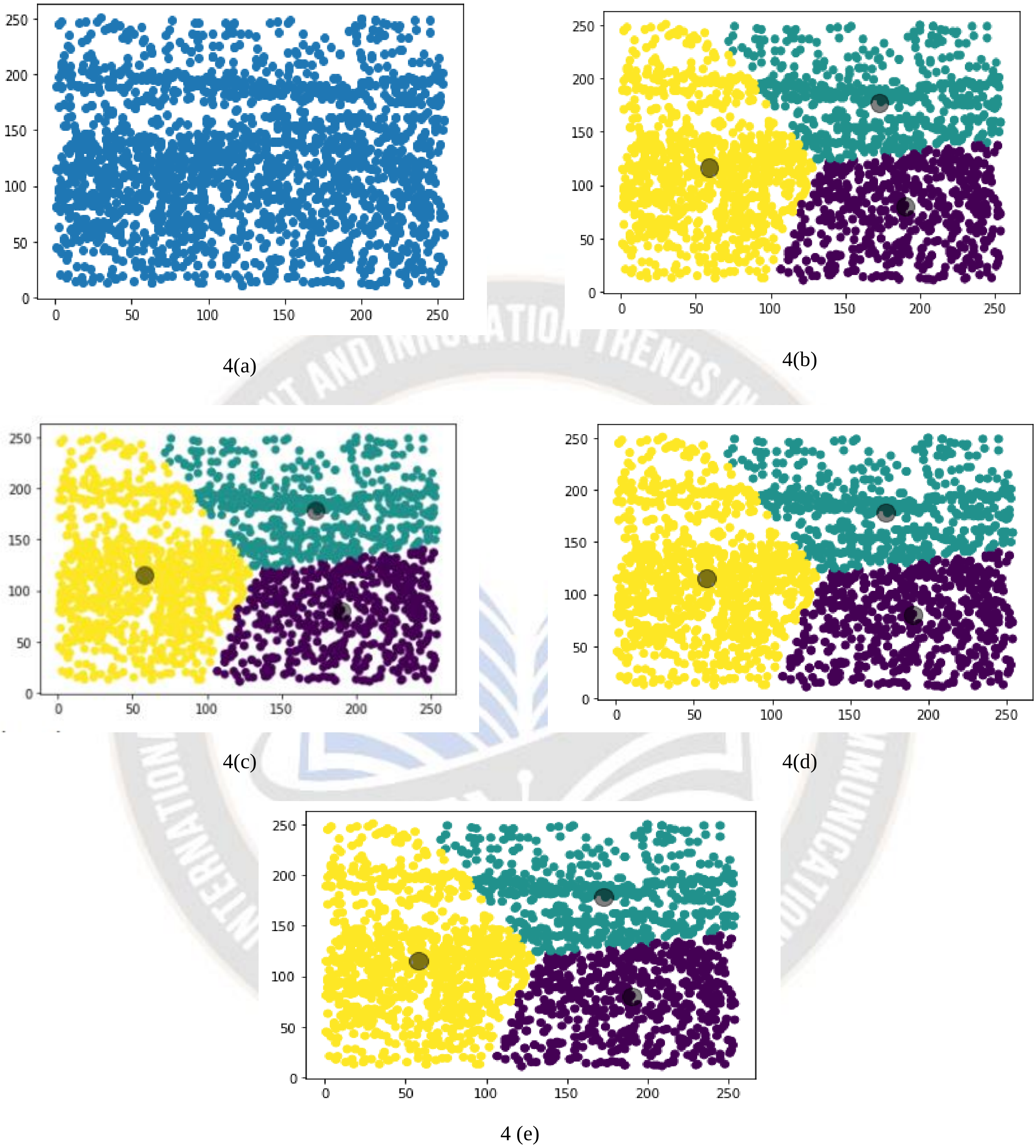

Figure 4: Clustering results of Segment dataset

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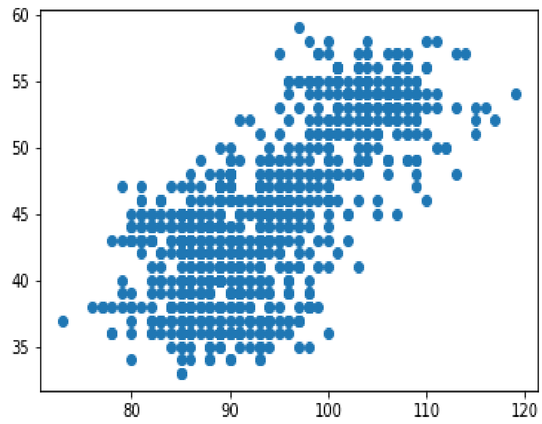
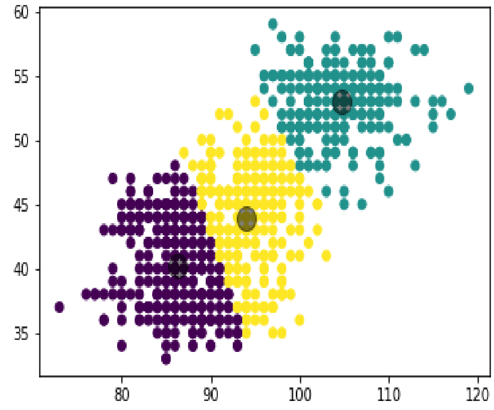


5(a)



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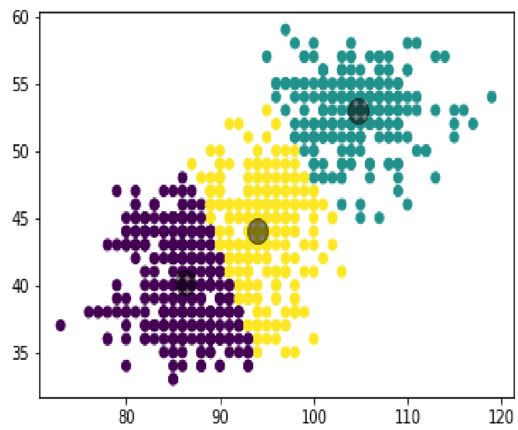

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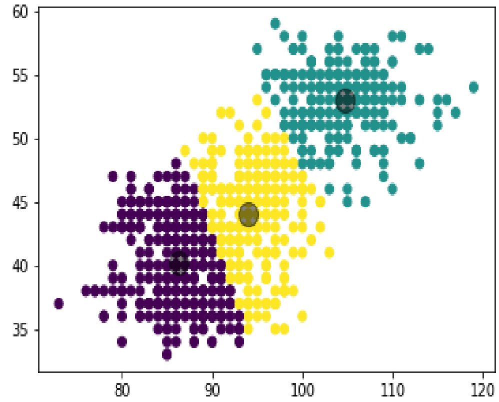

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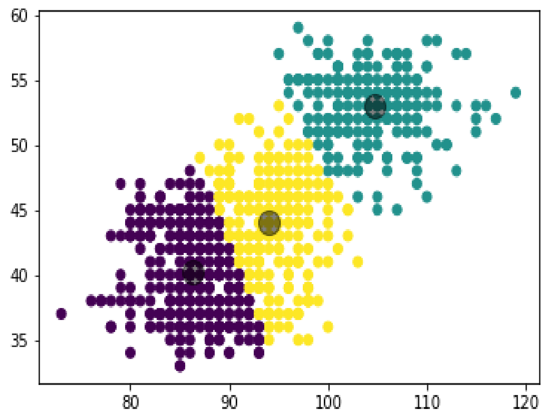

5(e)

Figure 5: Clustering results of Vehicle dataset

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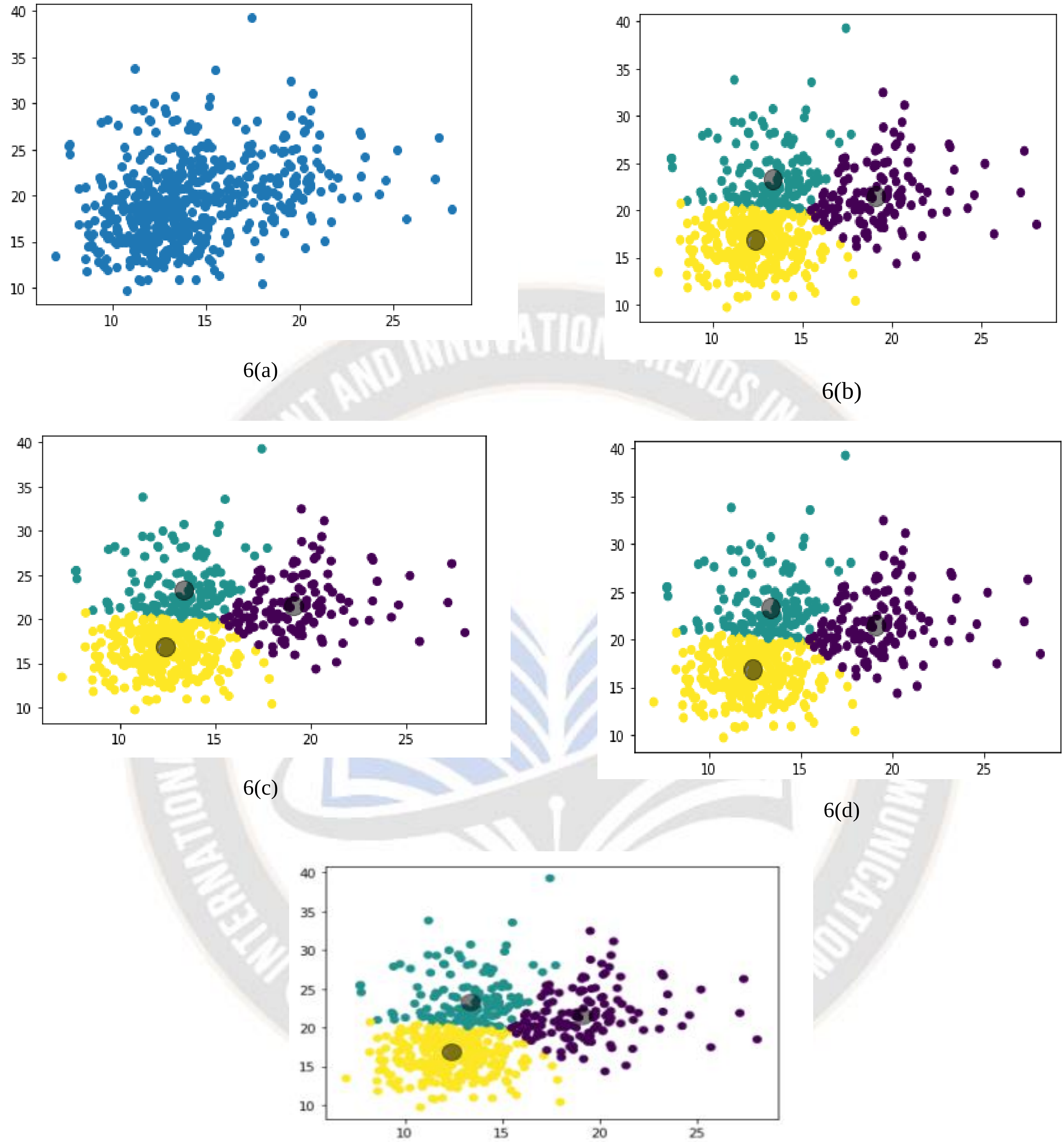

6(a) 6(b) 6(c) 6(d) 6(e)

Figure 6: Clustering results of Wdbc dataset

As presented in Figure 2 to Figure 6, the clusters generated by the proposed multi-objective clustering method are visualized. The results revealed that different solutions are provided in the process of multi-objective clustering. As many as 1000 maximum iterations are used for empirical study. Best clusters at different number of iterations are visualized. The experimental results revealed that consideration of multi-objective clustering is shown better performance over single objective clustering. Figure 2 shows set of clustering solutions pertaining to Ecoli dataset[24]. Figure 3 shows set of clustering solutions pertaining to Glass dataset. Figure 4 shows set of clustering solutions pertaining to Segment dataset. Figure 5 shows set of clustering solutions pertaining to Vehicle dataset. Figure 6 shows set of clustering solutions pertaining to Wdbc dataset. The results revealed set of clustering solutions that meet multiple objective functions.

6. CONCLUSION AND FUTURE WORK

In this paper, an improved PSO based framework known as Multi-Objective Clustering Framework (MOCF) is proposed. An algorithm called Particle Swarm Optimization based Multi-Objective Clustering (PSO-MOC) is proposed. It improves clustering efficiency to a greater extent. Multiple real world datasets are used to evaluate the performance of the proposed framework. A prototype application is built using Python data science platform to know the performance of the proposed algorithm. Real world datasets such as Ecoli, Glass, Segment, Vehicle and Wdbc are used for empirical study. The empirical results revealed that multi-objective clustering has shown better performance over its single-objective counterparts. And PSO based algorithm outperformed the existing non PSO based multi-objective clustering algorithms. In future we intend to improve our framework with optimized feature selection and particle representation to achieve clustering solutions in continuous space while improving performance of leader selection and decision maker.

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