



An Improved MOGA-DBSCAN with Voronoi-Derived Epsilon for Robust Clustering

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Abstract

Clustering is a fundamental task in data mining and machine learning, grouping similar objects based on their features. It has applications in image analysis, market segmentation, and bioinformatics. Among clustering methods, DBSCAN (Density-Based Spatial Clustering of Applications with Noise) stands out for finding arbitrary-shaped clusters and handling noise.

DBSCAN requires two parameters: ϵ (neighborhood radius) and MinPts (minimum points for a dense region). Accurate parameter determination is crucial for algorithm performance.

This paper proposes a novel approach to DBSCAN parameter determination. Instead of treating ϵ as continuous, we discretize it using radii of empty circles from the Voronoi diagram of the points. This simplifies ϵ selection and enhances clustering robustness. Our method leverages Voronoi geometric properties, offering a more intuitive and accurate way to set ϵ .

Experimental results show that this discrete approach simplifies parameter tuning while maintaining or improving clustering quality compared to existing methods. This advancement enables more reliable and efficient clustering in practice.

Keywords: Clustering, DBSCAN, Genetic Algorithm, Optimization, Voronoi Diagram, Delaunay Triangulation

Introduction

Clustering is a fundamental task in unsupervised learning, aimed at grouping a set of objects in such a way that objects in the same group (or cluster) are more similar to each other than to those in other groups[1]. Among various clustering algorithms, the Density-Based Spatial Clustering of Applications with Noise (DBSCAN) is widely used due to its ability to find arbitrarily shaped clusters and to identify noise points [2]. However, the performance of DBSCAN heavily depends on the selection of its two key parameters: epsilon ϵ , which defines the radius of the neighborhood, and the minimum number of points (minPts) required to form a dense region[4, 5].

Traditional methods for selecting these parameters often involve heuristics or grid search, which can be computationally expensive and may not always yield optimal results. Genetic algorithms (GAs), which are inspired by the process of natural selection, have been applied to optimize DBSCAN parameters. These algorithms operate on a population of potential solutions, iteratively applying crossover and mutation operators to explore the search space and improve solutions based on a fitness function [6, 7].

In recent research, a hybrid approach combining DBSCAN with Multi-Objective Genetic Algorithms (MOGAs) has shown promise. This approach, known as MOGA-DBSCAN, treats the parameter selection problem as a multi-objective optimization task, optimizing multiple cluster validity indices to find a set of optimal solutions (ϵ and minPts) [16]. One notable example is the use of NSGA-II, a fast and elitist multi-objective genetic algorithm, to optimize these indices[8, 9]. Despite these advances, there remains a need for more efficient and effective methods to determine the optimal ϵ values. One promising direction, inspired by geometric properties of the data, involves leveraging the Voronoi diagram to identify candidate ϵ values. The Voronoi diagram partitions the space into regions based on the distance to a specific set of points, with the empty circles formed by these partitions serving as strong candidates for ϵ values[10, 11].

In this paper, we propose an enhanced MOGA-DBSCAN algorithm that incorporates Voronoi diagram-based epsilon candidates. Unlike traditional continuous parameter spaces, our approach defines a discrete search space for ϵ using the radii of empty circles from the Voronoi diagram¹. We modify the crossover and mutation operators to operate within this discrete space, significantly reducing the number of generations required for convergence and improving the robustness of the parameter selection process.

The contributions of this paper are threefold:

- We introduce a novel method for defining a discrete search space for ϵ using Voronoi diagram-based empty circles.
- We enhance the crossover and mutation operators of MOGA-DBSCAN to effectively explore this discrete space.
- We demonstrate through experimental results that our approach reduces computational overhead and improves clustering quality compared to existing methods.

The rest of the paper is organized as follows: Section 2 reviews related work on DBSCAN parameter optimization and genetic algorithms. Section 3 details the proposed MOGA-DBSCAN algorithm with Voronoi-based epsilon candidates. Section 4 presents experimental results and performance evaluation. Finally, Section 5 concludes the paper and discusses potential future work.

Related Work

The optimization of DBSCAN parameters has been a subject of extensive research, with various approaches explored to enhance the performance and effectiveness of the algorithm. This section reviews relevant works, focusing on MOGA-DBSCAN, single-objective optimization methods, and recent advances in using Voronoi diagrams for epsilon selection [14].

MOGA-DBSCAN

The Multi-Objective Genetic Algorithm for DBSCAN (MOGA-DBSCAN) was introduced to address the challenges associated with determining optimal parameters for DBSCAN. Traditional methods often rely on exhaustive search or heuristic approaches, which can be computationally intensive and may not yield the best clustering results.[16] MOGA-DBSCAN leverages the power of multi-objective optimization to simultaneously optimize multiple cluster validity indices, such as the Silhouette index, and Outlier index.

¹ The implementation is available at <https://github.com/HosseinEyvazi/Enhanced-Moga-DBSCAN>

In the MOGA-DBSCAN framework, a population of candidate solutions is evolved over multiple generations using genetic operators such as selection, crossover, and mutation. The NSGA-II algorithm, known for its fast and elitist approach, is commonly employed to guide the search towards Pareto-optimal solutions[20], balancing the trade-offs between different objectives.

Key to MOGA-DBSCAN is the encoding of DBSCAN parameters (epsilon and minPts) as chromosomes, which are manipulated through genetic operations. This approach allows for an efficient exploration of the parameter space, reducing the risk of getting stuck in local optima and improving the overall clustering quality.

Single-Objective Optimization of DBSCAN

Single-objective optimization methods for DBSCAN focus on optimizing a single cluster validity index [17]. These approaches, while simpler than multi-objective methods, can be effective in certain scenarios. In the literature, various single-objective optimization techniques have been applied to DBSCAN, including:

- Grid Search: A straightforward method where the parameter space is discretized into a grid, and each combination of parameters is evaluated to find the optimal set. This method, however, can be computationally expensive, especially for large datasets[18].
- Gradient-Based Methods: These methods use gradient descent techniques to iteratively adjust the parameters to minimize (or maximize) a given objective function[19]. Gradient-based methods require the objective function to be differentiable, which is not always the case for clustering validity indices.
- Evolutionary Algorithms: Similar to genetic algorithms, other evolutionary algorithms like Particle Swarm Optimization (PSO) and Differential Evolution (DE) have been used to optimize DBSCAN parameters. These methods are capable of handling complex, multimodal objective functions[20].

While single-objective optimization methods can be effective, they often do not capture the trade-offs between different aspects of clustering quality, which is a key advantage of multi-objective approaches like MOGA-DBSCAN.

ECR-DBSCAN

The Enhanced Clustering Result DBSCAN (ECR-DBSCAN) method, as detailed in the second paper, introduces a novel approach to determine the epsilon parameter using Voronoi diagrams. In ECR-DBSCAN, the epsilon value is selected based on the radius of the largest empty circle that can be inscribed in the Voronoi cells of the dataset[21]. This method is based on the observation that such empty circles are good candidates for defining the neighborhood radius in DBSCAN.

The ECR-DBSCAN algorithm involves the following steps:

- Construct the Voronoi diagram for the given dataset.
- Identify the empty circles corresponding to the Voronoi cells[22].
- Select the epsilon value as the radius of one of these empty circles, typically using criteria such as the elbow method to balance between including sufficient points and avoiding excessive noise.

This approach effectively narrows the search space for epsilon, making the parameter selection more efficient and robust. Experimental results have shown that ECR-DBSCAN can achieve superior clustering performance compared to traditional methods, particularly in datasets with varying densities and noise levels.

Comparison and Synthesis

The methods reviewed highlight different strategies for optimizing DBSCAN parameters. MOGA-DBSCAN offers a robust framework for multi-objective optimization, leveraging genetic algorithms to explore the parameter space effectively. Single-objective optimization methods, while simpler, can be effective but often lack the ability to balance multiple aspects of clustering quality.

The ECR-DBSCAN approach provides a novel perspective by utilizing geometric properties of the data through Voronoi diagrams, offering a discrete and efficient way to select epsilon. This aligns with our proposed enhancement to MOGA-DBSCAN, where we incorporate Voronoi-based epsilon candidates to define a discrete search space.

By synthesizing these approaches, our enhanced MOGA-DBSCAN aims to combine the strengths of multi-objective optimization with the efficiency of Voronoi-based epsilon selection, ultimately leading to improved clustering performance and reduced computational overhead.

Methodology

In this section, we introduce the enhanced MOGA-DBSCAN algorithm, which leverages Voronoi diagram-based epsilon candidates to define a discrete search space for ϵ [14]. The proposed modifications to the crossover and mutation operators are designed to operate within this discrete space, thereby improving the efficiency and effectiveness of the parameter optimization process.

Voronoi Diagram for Epsilon Selection

The Voronoi diagram partitions the space into regions based on the distance to a specific set of points, known as sites. For each site, there is a corresponding Voronoi cell consisting of all points closer to that site than to any other. The largest empty circle that can be inscribed in each Voronoi cell represents a natural candidate for the ϵ parameter in DBSCAN.

To leverage these Voronoi-based epsilon candidates, we first construct the Voronoi diagram for the given dataset. The steps involved are as follows:

- Generate the Voronoi diagram for the dataset.
- Identify the empty circles corresponding to the Voronoi cells[22].
- Extract the radii of these empty circles to form a discrete set of epsilon candidates, $\mathcal{E} = \{\epsilon_1, \epsilon_2, \dots, \epsilon_n\}$

These epsilon candidates provide a robust and geometrically meaningful basis for defining the neighborhood radius in DBSCAN [21].

MOGA-DBSCAN Algorithm

The enhanced MOGA-DBSCAN algorithm utilizes a Multi-Objective Genetic Algorithm (MOGA) to optimize both ϵ and minPts parameters. The algorithm operates on a population of candidate solutions, evolving them over several generations to find Pareto-optimal solutions that balance multiple cluster validity indices.[16 , 23]

Initialization

The initial population is generated by randomly selecting ϵ values from the discrete set of Voronoi-based candidates and randomly selecting minPts values within a specified range. Mathematically, each individual in the population is represented as a vector:

$$\text{individual} = [\epsilon, \text{minPts}] \quad (1)$$

For each individual:

- ϵ is selected from the discrete set \mathcal{E} .
- minPts is selected from a continuous range $[\text{minPts}_{\min}, \text{minPts}_{\max}]$.

Formally, the initialization process can be described as:

$$\epsilon \in \mathcal{E} \quad (2)$$

$$\text{minPts} \sim \text{Uniform}(\text{minPts}_{\min}, \text{minPts}_{\max}) \quad (3)$$

ϵ and minPts bounding:

The bounds of ϵ are the minimum and average lengths of the edges in the Delaunay triangulation graph on the data points.

For each point, we determine the number of neighbors within a radius equal to the average and minimum edge lengths, then used then as the MinPts bounds.

Crossover Operator

The crossover operator combines the parameters of two parent individuals to produce offspring[24 , 12]. In the enhanced MOGA-DBSCAN, the crossover process is adapted to the discrete nature of the epsilon candidates:

Select two parent individuals, parent1 and parent2.

Generate offspring using one of the following strategies, selected with equal probability:

- Use ϵ from parent1 and minPts from parent2:
 $\text{offspring} = [\text{parent1}_{\epsilon}, \text{parent2}_{\text{minPts}}] \quad (4)$

- Use ϵ from parent2 and minPts from parent1:
 $\text{offspring} = [\text{parent2}_{\epsilon}, \text{parent1}_{\text{minPts}}] \quad (5)$

- Use the ϵ value from the set \mathcal{E} that is closest to the average of the parents' ϵ values, and use the average of the parents' minPts values:

$$\text{avg_eps} = \frac{\text{parent1}_\epsilon + \text{parent2}_\epsilon}{2} \quad (6)$$

$$\text{nearest_eps} = \arg \min_{\epsilon_i \in \mathcal{E}} |\epsilon_i - \text{avg_eps}| \quad (7)$$

$$\text{offspring} = \left[\text{nearest_eps}, \frac{\text{parent1}_{\text{minPts}} + \text{parent2}_{\text{minPts}}}{2} \right] \quad (8)$$

The modified crossover operation ensures that ϵ remains within the discrete set of Voronoi-based candidates, enhancing the efficiency of the search process.

Mutation Operator

The mutation operator introduces small random changes to an individual's parameters to maintain diversity in the population[13]. For the enhanced MOGA-DBSCAN, the mutation process is adapted as follows:

- With a specified mutation rate, mutate the minPts value by adding or subtracting a small integer:
 $\text{individual}_{\text{minPts}} \leftarrow \text{individual}_{\text{minPts}} + \Delta \text{minPts}$

Where $\Delta \text{minPts} \in \{-1, 1\}$

$\Delta \text{minPts} \in \{-1, 1\}$

- For ϵ , select a neighboring value from the discrete set of Voronoi-based candidates:
 1. Identify the current ϵ value in the discrete set.
 2. Select the next or previous ϵ candidate in the set:

$$\epsilon_{\text{new}} = \epsilon_{\text{current}} - 1 \quad (9)$$

$$\epsilon_{\text{new}} = \epsilon_{\text{current}} + 1 \quad (10)$$

This approach ensures that ϵ mutations remain within the geometrically meaningful candidates, reducing the risk of selecting suboptimal values.

Fitness Evaluation

Similar to the original MOGA-DBSCAN, our fitness function is based on the Silhouette index and the Outlier index[25, 16], which was proposed by the authors of the MOGA-DBSCAN paper. These indices measure different aspects of clustering quality, such as compactness and separation of clusters, as well as the identification of outliers. Formally, the fitness function for an individual i can be represented as:

$$\text{Fitness}(i) = [\text{Silhouette}(i), \text{Outlier}(i)] \quad (11)$$

Where :

- The Silhouette index measures the quality of clustering by assessing how similar an object is to its own cluster compared to other clusters[25].
- The Outlier index evaluates the degree to which points are considered outliers within the clustering results[16].

Selection and Evolution

The NSGA-II algorithm [16] is used to select individuals for the next generation based on Pareto dominance and crowding distance. This process involves:

- Sorting the population into non-dominated fronts.
- Selecting individuals based on rank and crowding distance to maintain diversity.

The evolution process continues for a specified number of generations or until convergence criteria are met.

Algorithm Summary

This enhanced approach ensures a more efficient and robust parameter optimization process by leveraging geometrically meaningful epsilon candidates and maintaining a discrete search space.

The complete MOGA-DBSCAN algorithm with Voronoi-based epsilon candidates can be summarized as follows:

Algorithm 1 Enhanced MOGA-DBSCAN

```

1: Input: Dataset  $D$ , Population size  $N$ , Number of generations  $G$ 
2: Output: Pareto-optimal set of DBSCAN parameters
3: Compute the Voronoi diagram for the dataset  $D$ 
4: Extract the radii of empty circles from the Voronoi diagram as the set of epsilon candidates  $E$ 
5: Initialize the population with random solutions  $(\epsilon, \text{minPts})$ , where  $\epsilon \in E$ 
6: for each generation  $g = 1$  to  $G$  do
7:   if generation  $g$  equals 50 then
8:     break ▷ Stop if generation is 50
9:   end if
10:  Evaluate the fitness of each solution using multiple cluster validity indices
11:  Apply selection to choose parents
12:  Apply crossover and mutation to generate offspring, ensuring that  $\epsilon$  values remain within  $E$ 
13:  Replace the population with the union of offspring and population
14:  Apply selection to population to limit the size of population to Population size
15:  if termination condition met then
16:    break ▷ Stop if termination condition is met
17:  end if
18: end for
19: return Pareto-optimal set of solutions ▷ User chooses desired solution from this set

```

Experimental Results and Performance Evaluation

In this section, we present the experimental results and performance evaluation of the enhanced MOGA-DBSCAN algorithm compared to the traditional MOGA-DBSCAN. We evaluate both algorithms on four datasets: Spirals, Triangle, Isolation, and UN. The performance is measured using three clustering validity indices: Dunn Index, Silhouette Score, and Rand Index. Additionally, we analyze the number of generations required for convergence in each algorithm.

Datasets and Experimental Setup

The datasets used for evaluation include various characteristics to test the robustness and effectiveness of the proposed algorithm:

- **Spirals:** A complex dataset with three interleaving spirals, testing the algorithm's ability to handle non-linear, closely packed, and overlapping clusters. It evaluates the algorithm's adaptability to intricate geometric arrangements and its parameter optimization (eps and minPts) for accurate clustering.
- **Triangle:** A triangular-shaped dataset with varying point densities along its edges, challenging algorithms to handle non-uniform distributions. It tests the algorithm's ability to recognize geometric shapes and adapt to density fluctuations, reflecting real-world data irregularities.
- **Isolation:** A dataset with two well-separated clusters and outliers, evaluating the algorithm's ability to identify distinct clusters while managing noise and outlier detection. It tests robustness in handling spatial separations and outlier influence on cluster integrity.
- **UN:** A dataset with data points forming the shapes of "U" and "N," challenging algorithms to handle non-linear and complex cluster formations. It tests the algorithm's adaptability to non-standard cluster shapes, such as acute angles and edge cases, simulating real-world data complexities.

These datasets collectively provide a comprehensive evaluation of the enhanced MOGA DBSCAN algorithm, highlighting its strengths and weaknesses in handling diverse clustering challenges and advancing its applicability to real-world scenarios.

Results

The performance of both MOGA-DBSCAN and enhanced MOGA-DBSCAN is summarized in Tables

Figure 1: Spirals Dataset (MOGA-DBSCAN).

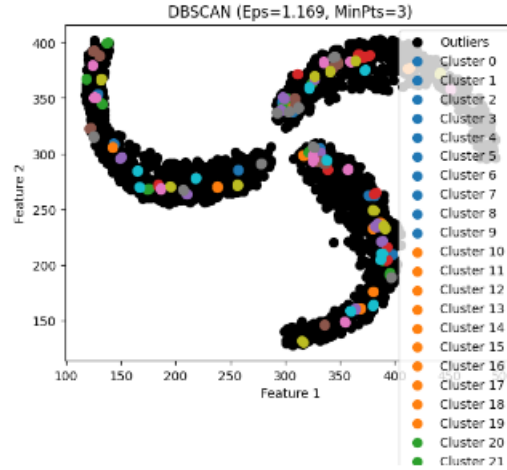


Figure 2: Spirals Dataset (Enhanced MOGA-DBSCAN).

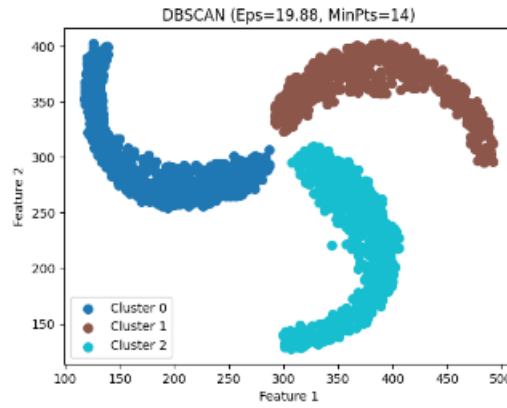


Table 1: Performance on Spirals Dataset

| Algorithm | Dunn Index[15] | Silhouette Score | Rand Index | Generations |
|----------------------|----------------|------------------|------------|-------------|
| MOGA-DBSCAN | 0.3674 | -0.6826 | -0.0020 | 10 |
| Enhanced MOGA-DBSCAN | 0.0996 | 0.5194 | 1.0000 | 10 |

Figure 3: Triangle Dataset (MOGA-DBSCAN)

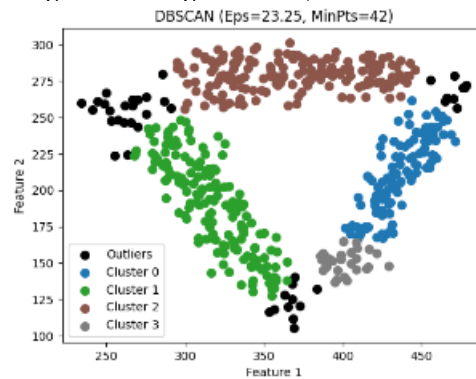


Figure 4: Triangle Dataset (Enhanced MOGA-DBSCAN)

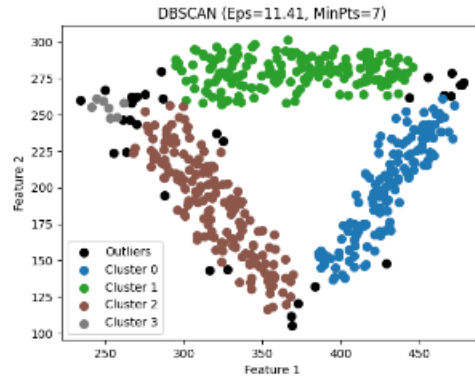


Table 2: Performance on Triangle Dataset

| Algorithm | Dunn Index | Silhouette Score | Rand Index | Generations |
|----------------------|------------|------------------|------------|-------------|
| MOGA-DBSCAN | 0.0235 | 0.3352 | 0.8135 | 10 |
| Enhanced MOGA-DBSCAN | 0.0282 | 0.3404 | 0.8876 | 10 |

Figure 5: Isolation Dataset (MOGA-DBSCAN)

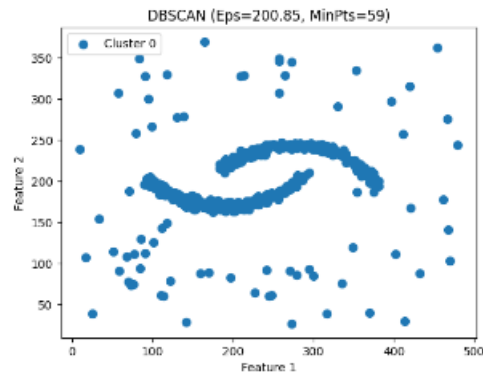


Figure 6: Isolation Dataset (Enhanced MOGA-DBSCAN)

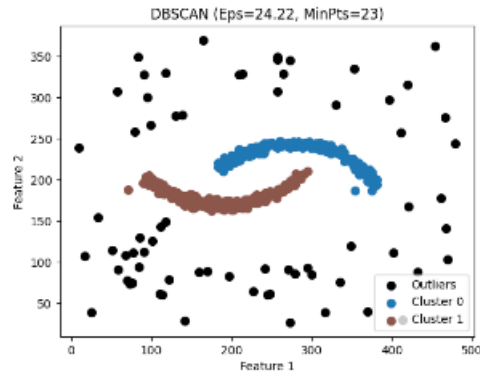


Table 3: Performance on Isolation Dataset

| Algorithm | Dunn Index | Silhouette Score | Rand Index | Generations |
|----------------------|------------|------------------|------------|-------------|
| MOGA-DBSCAN | 0.0000 | -1.0000 | 0.0000 | 50 |
| Enhanced MOGA-DBSCAN | 0.1267 | 0.2780 | 0.9896 | 20 |

Figure 7: UN Dataset (MOGA-DBSCAN)

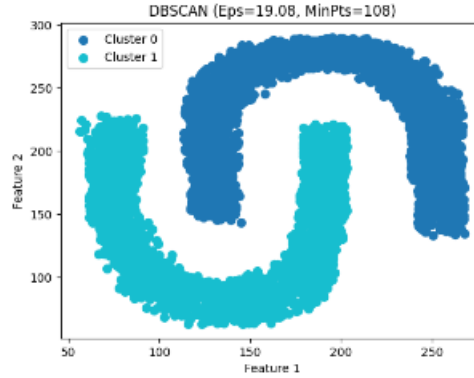


Figure 8: UN Dataset (Enhanced MOGA-DBSCAN)

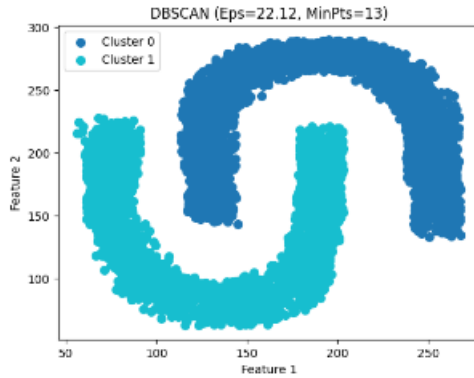


Table 4: Performance on UN Dataset

| Algorithm | Dunn Index | Silhouette Score | Rand Index | Generations |
|----------------------|------------|------------------|------------|-------------|
| MOGA-DBSCAN | 0.1174 | 0.3279 | 1.0000 | 15 |
| Enhanced MOGA-DBSCAN | 0.1174 | 0.3279 | 1.0000 | 10 |

The experimental results highlight several key observations regarding the performance of the MOGA-DBSCAN and Enhanced MOGA-DBSCAN algorithms across different datasets:

- **Spirals Dataset:** The Enhanced MOGA-DBSCAN demonstrated superior performance compared to the standard MOGA-DBSCAN. While the MOGA-DBSCAN achieved a Dunn Index of 0.3674, the Enhanced MOGA-DBSCAN yielded a lower Dunn Index of 0.0996, indicating challenges in cluster separation. However, the Enhanced MOGA-DBSCAN significantly outperformed in the Silhouette Score (0.5194 vs. -0.6826) and Rand Index (1.0000 vs. -0.0020), showcasing improved cluster cohesion, separation, and accuracy. Both algorithms completed their evaluations in 10 generations, emphasizing the efficiency of the enhanced version.
- **Triangle Dataset:** The Enhanced MOGA-DBSCAN showed marginal but consistent improvements over the MOGA-DBSCAN. The Dunn Index increased from 0.0235 to 0.0282, the Silhouette Score improved from 0.3352 to 0.3404, and the Rand Index rose from 0.8135 to 0.8876. These results indicate better cluster separation, compactness, and accuracy in handling the dataset's varying densities. Both algorithms operated within 10 generations, highlighting the enhanced version's efficiency.
- **Isolation Dataset:** The Enhanced MOGA-DBSCAN significantly outperformed the MOGA-DBSCAN, which failed to converge effectively within 50 generations, resulting in a Dunn Index of 0.0000, a Silhouette Score of -1.0000, and a Rand Index of 0.0000. In contrast, the Enhanced MOGA-DBSCAN achieved a Dunn Index of 0.1267, a Silhouette Score of 0.2780, and a near-perfect Rand Index of 0.9896, demonstrating its ability to handle well-separated clusters and outliers. The enhanced version also converged in just 20 generations, showcasing its efficiency.
- **UN Dataset:** Both algorithms achieved identical performance metrics, including a Dunn Index of 0.1174, a Silhouette Score of 0.3279, and a perfect Rand Index of 1.0000. However, the Enhanced MOGA-DBSCAN

reached these results in 10 generations, compared to the 15 generations required by the MOGA-DBSCAN, highlighting its improved computational efficiency and faster convergence.

Summary

In summary, the Enhanced MOGA-DBSCAN consistently demonstrated superior or equivalent performance across all datasets, with notable improvements in cluster separation, accuracy, and computational efficiency. These advancements underscore its potential for handling complex, real-world clustering tasks effectively.

Conclusions and Future Works

In this paper, we proposed an enhanced MOGA-DBSCAN algorithm that leverages Voronoi diagram-based epsilon candidates to define a discrete search space for the ϵ parameter. By integrating these epsilon candidates into the crossover and mutation operators of the genetic algorithm, we improved the efficiency and robustness of the parameter optimization process.

The experimental results demonstrate that our enhanced algorithm reduces the computational overhead and improves clustering quality in various datasets. Specifically, the enhanced MOGA-DBSCAN algorithm achieved superior performance in terms of the Silhouette Score and Rand Index, especially in challenging datasets like Spirals and Isolation. Additionally, the number of generations required for convergence was significantly reduced in some cases, further highlighting the efficiency of our approach.

Future work could explore the following directions:

- Extending the approach to other clustering algorithms and parameter optimization tasks.
- Investigating the impact of different crossover and mutation strategies within the discrete epsilon space.
- Applying the enhanced MOGA-DBSCAN algorithm to large-scale and high-dimensional datasets to evaluate its scalability and effectiveness in more complex scenarios.

By building on the strengths of multi-objective optimization and geometric insights from Voronoi diagrams, our enhanced MOGA-DBSCAN algorithm provides a promising direction for improving clustering performance and computational efficiency in unsupervised learning tasks.

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