

Efficient Evolutionary Unsupervised Clustering

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Abstract

Evolutionary clustering is a new trend in cluster analysis, that has the potential to provide high partitioning accuracy results. Traditional evolutionary techniques applied in clustering are typically hindered by the high cost involved in the computation of the objective function. In this paper we propose a novel objective function, that is able to provide fitness function values in sub-linear time. Next we develop an evolutionary scheme, to evolve cluster solutions. Moreover, we demonstrate how this scheme can be utilized to provide estimations for the number of clusters. Finally, by employing real world datasets, we exhibit the high quality clustering results it can provide.

1 Introduction

Clustering is a fundamental step in the procedure of transforming data to knowledge. It aims at discovering groups (clusters) in a set of objects such that similarity among the objects in the same group is higher than that of objects belonging in different clusters.

The first references to clustering date as back as the fourth century B.C. by Aristotle and Theophrastos, but it was not until 1939, that one of the first comprehensive foundations of these methods was published [29].

The application domain of clustering techniques is very wide including data mining [14], text mining [10, 13], statistical data analysis [2], compression and vector quantization [22], global optimization [6, 28] and web personalization [23].

Clustering is a hard problem, since even the simplest clustering problems are known to be NP-Hard [1]. The Euclidean k -center problem [1] in the plane is NP-Hard [19]. In fact, it is NP-Hard to approximate the two-dimensional

k -center problem even under the L_∞ -metric [19].

Clustering algorithms are traditionally categorized into three main categories, Hierarchical, Partitioning [25] and Distance-based. Hierarchical clustering algorithms construct hierarchies of clusters in a top-down (divisive) or bottom-up (agglomerative) fashion. Hierarchical clustering algorithms have proved to yield high quality results especially for applications involving clustering text collections. None the less, their high computational requirements, usually prevents their usage in real life applications, where the number of samples and their dimensionality is typically high (the cost is quadratic to the number of samples).

Partitioning clustering algorithms, start from an initial clustering (that can be randomly formed) and create partitionings by iteratively adjusting the clusters based on the distance of the data points from a representative member of the cluster. The most commonly used partitioning clustering algorithm is k -means. k -means initializes k centers and iteratively assigns each data point to the cluster whose centroid minimizes the euclidean distance from the data point. k -means type algorithms can give good clustering results at low cost, since their running time is proportional to kn . However, their results depend heavily on their initialization and it converges to arbitrary local optima.

Finally, distance based clustering algorithms create a partitioning by considering neighbors of data points. DBSCAN [24] is a distance-based clustering algorithm that has proved quite effective for spatial databases. Clusters are considered as high density neighborhoods of data points. Although the density parameter is very crucial for DBSCAN's success, recently proposed heuristics appear to give high quality results. The computational complexity of DBSCAN comes up to $O(n \log(n))$ under the assumption that the data are organized in a spatial index (R^* -tree).

Recently, many researchers investigate the

application of evolutionary clustering to cluster analysis.

The application of evolutionary clustering has been recently investigated by numerous researchers. Evolutionary clustering, motivated by natural evolution, typically encodes a solution to the clustering problem as a chromosome. Next, by employing evolutionary operators and a population of solutions the algorithm probes the search space to find a globally optimum partition of the data. The most commonly used evolutionary operators are: selection, recombination, and mutation. Each operator transforms one or more input chromosomes into one or more output chromosomes. A fitness function evaluated on a chromosome determines a chromosome's likelihood of surviving into the next generation. In early approaches [8, 17], chromosomes encoded the partition of n objects into K clusters and *Genetic Algorithms* were employed to find the best partition. However, the sensitivity of GAs to the selection of various parameters such as population size, crossover and mutation probabilities, and the difficulties of the representation scheme, have presented a major problem. Hybrid approaches [4] demonstrated that they can perform better than the simple GA.

However, it is possible to represent the clustering procedure as an optimization problem of locating the optimal centroids of clusters. Thus, any kind of evolutionary technique can be employed since a possible clustering solution has a direct representation as a real-valued vector of the centroids. Previous approaches employed *Evolutionary Strategies* [5], *Evolutionary Programming* [15], and recently *Particle Swarm Optimization* [30]. All these approaches demonstrated that it is possible to obtain high quality partitions, but at the expense of a high computational cost.

In this paper we try to tackle the high computational cost of traditional evolutionary techniques by introducing a new fitness criterion. This criterion is based on a windowing technique already used in other clustering algorithms [27, 31]. The proposed approach is independent of the evolutionary technique employed. In this paper we employ the *Differential Evolution* algorithm as recent works [20] demonstrate its superior performance on such problems.

A critical and open issue in cluster analysis, is the determination of the number of clusters present in a dataset. The evolutionary clustering techniques proposed so far, require from the user to specify the number of clusters present in the data prior to the execution of the algorithm.

The proposed approach can provide an approximation to the number of clusters present in a dataset.

The rest of the paper is organized as follows. In Section 2, we analyze the proposed fitness function. Next, in Section 3 we describe the proposed evolutionary scheme and in Section 4 we present experimental results that demonstrate the applicability of the proposed approach. The paper ends with concluding remarks and discussion in Section 5.

2 Window Density Function

Let the data set be a set $X = \{x_1, \dots, x_n\}$, where x_j is a data vector in the d dimensional euclidean space \mathbb{R}^d . A k clustering of X is a partition C of X into k disjoint groups C_i , for $i = 1, \dots, k$. The clustering problem constitutes of the determination of a partition of X which is optimal with respect to a function f that quantifies the goodness of the partition.

Different statistical functions have been proposed for f [18, 32]. But in all the previous cases at least a full scan over the dataset is necessary to compute the function value for a specific instance. Evolving a population using such a fitness criterion can be expensive in terms of computational cost, compared to k -means like approaches that typically do not require more than 10 to 20 scans of the dataset.

In the present contribution we propose the *Window Density Function* (WDF) that overcomes the aforementioned limitations:

Definition 1: Let a d -range of size $a \in \mathbb{R}$ and center $z \in \mathbb{R}^d$, be the orthogonal range $[z_1 - a, z_1 + a] \times \dots \times [z_d - a, z_d + a]$. Assume further, that the set $S_{a,z}$, with respect to the set X , is defined as:

$$S_{a,z} = \{y \in X : z_i - a \leq y_i \leq z_i + a, \forall i = 1, \dots, d\}.$$

Then the *Window Density Function* WDF for the set X , with respect to a given size $a \in \mathbb{R}$, is defined as:

$$\text{WDF}_a(z) = |S_{a,z}|. \quad (1)$$

In other words, WDF represents the number of points from the dataset X , that reside in a window of size a around z . WDF is a meaningful clustering objective function, since as the center of a d -range, z , moves to the center of the cluster the number of points around it should increase. As it is obvious the size a , is critical to whole procedure since it determines the location of the minima of the objective function.

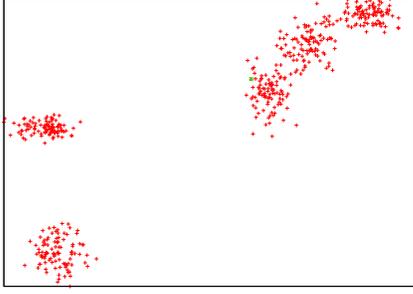


Figure 1: Dataset $DSet_1$

To illustrate this we employ the dataset $Dset_1$ exhibited in Fig. 1. This dataset is composed of 500 points organized in 5 clusters with 100 points each. Each cluster is constructed by sampling 100 points from a two dimensional Gaussian distribution. The mean of each distribution was randomly scattered in the $[0, 200]^2$ range, and the covariance matrices were randomly generated by obtaining for each element of the matrix a random number between 1 and 2.

In Fig. 2, the $3d$ -plots of WDF are provided to visualize the impact of the parameter a . As the value of a increases, the extreme points of WDF tend to merge. When $a = 1$ there exist 5 maxima, equal to the number of clusters. On the other hand, when $a = 10$, the three maxima corresponding to the 3 closest clusters previously identified merge to just one.

The most important feature of the proposed density function is that it is not necessary to scan the entire dataset to obtain a fitness for a specific object. In particular, the computation of WDF is the well studied Computational Geometry *Orthogonal Range Search Problem*. Numerous Computational Geometry techniques have been proposed to address this problem. All these techniques employ a preprocessing stage at which they construct a data structure storing the patterns. This data structure allows them to answer range queries fast. In Table 1 the computational complexity of various such approaches is summarized. In detail, for applications of very high dimensionality, data structures like the Multidimensional Binary Tree [21], and Bentley and Maurer [7] seem more suitable. On the other hand, for low dimensional data with a large number of points the approach of Alevizos [3] appears more attractive.

3 Evolutionary Clustering under the WDF

Objective Function

Evolutionary algorithms (EAs) have their roots in the stochastic search methods scientific domain, and try to mimic the natural biological evolution process. Utilizing the principle of survival of the fittest they try to evolve an initial population of potential solutions to obtain a globally optimal result. In this paper, from the broad field of EAs we employ Differential Evolution [26]. Of course our approach can be applied using any EA.

DE evolves the *population* of the potential solutions (individuals), using three operators, *mutation*, *recombination* and *selection*. An individual, in the clustering context, is expressed using a predetermined number of d -dimensional vectors that represent the centers of the d -ranges, that constitute the clustering result. The fitness of each individual is measured by the sum of WDF function over all the d -ranges, under a fixed value of the parameter a . The remaining procedure of the DE algorithm remains unchanged.

At the first step, all individuals are initialized by using a random number generator. At the mutation step, for each $i = 1, \dots, P$ (P represents the size of the population) a new mutant weight vector v_{g+1}^i is generated by combining vectors, randomly chosen from the population, and exploiting one of the mutation operators (2)–(6):

$$v_{g+1}^i = \omega_g^{best} + \mu(\omega_g^{r1} - \omega_g^{r2}), \quad (2)$$

$$v_{g+1}^i = \omega_g^{r1} + \mu(\omega_g^{r2} - \omega_g^{r3}), \quad (3)$$

$$v_{g+1}^i = \omega_g^i + \mu(\omega_g^{best} - \omega_g^i) + \mu(\omega_g^{r1} - \omega_g^{r2}), \quad (4)$$

$$v_{g+1}^i = \omega_g^{best} + \mu(\omega_g^{r1} - \omega_g^{r2}) + \mu(\omega_g^{r3} - \omega_g^{r4}), \quad (5)$$

$$v_{g+1}^i = \omega_g^{r1} + \mu(\omega_g^{r2} - \omega_g^{r3}) + \mu(\omega_g^{r4} - \omega_g^{r5}), \quad (6)$$

where $\omega_g^{r1}, \omega_g^{r2}, \omega_g^{r3}, \omega_g^{r4}$ and ω_g^{r5} are randomly selected vectors, different from ω_g^i , ω_g^{best} is the best member of the current generation. Finally, the positive mutation constant μ controls the magnification of the difference between two weight vectors. For the rest of the paper, we refer to the differential evolution algorithm that uses Eq. (2) as the mutation operator with DE_1 , DE_2 for the algorithm that uses Eq. (3), and so on.

Having constructed the mutant vectors, the

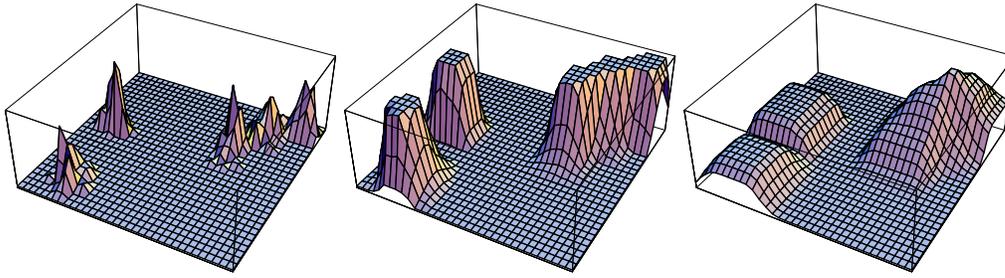


Figure 2: 3D-Plot of WDF for $Dset_1$ and $a = 1, 5, 10$ from left to right

Method	Preprocessing		Query time
	Time	Space	
Multidim. Binary Tree [21]	$\theta(dn \log n)$	$\theta(dn)$	$O(s + dn^{1-1/d})$
Range Tree [21]	$O(n \log^{d-1} n)$	$O(n \log^{d-1} n)$	$O(s + \log^d n)$
Wilard and Lueker [21]	$O(n \log^{d-1} n)$	$O(n \log^{d-1} n)$	$O(s + \log^{d-1} n)$
Chazelle [11]	$O(n \log^{d-1} n)$	$O(n \frac{\log^{d-1} n}{\log \log n})$	$O(s + \log^{d-1} n)$
Chazelle and Guibas [12]	$O(n \log^{d+1} n)$	$O(n \log^d n)$	$O(s + \log^{d-2} n)$
Alevizos [3]	$O(n \log^{d-1} n)$	$O(n \log^{d-1} n)$	$O(s + \log^{d-2} n)$
Bentley and Maurer [7]	$O(n^{2d-1})$	$O(n^{2d-1})$	$O(s + d \log n)$
Bentley and Maurer [7]	$O(n^{1+\epsilon})$	$O(n^{1+\epsilon})$	$O(s + \log n)$
Bentley and Maurer [7]	$O(n \log n)$	$O(n)$	$O(n^\epsilon)$

Table 1: Methods for orthogonal range search.

recombination step is initiated that constructs a trial vector for each individual. At the recombination step, for each component $j = 1, 2, \dots, L$ of the mutant vector a random number $r \in [0, 1]$ is generated. If r is smaller than the predefined recombination constant p , the j -th component of the mutant vector v_{g+1}^i becomes the j -th component of the trial vector. Otherwise, the j -th component of the target vector is selected as the h -th component of the trial vector. Finally, the resulting trial vector replaces the initial individual if it yields a better WDF function value. Otherwise it is discarded. This constitutes the selection step.

As it is obvious the evolutionary optimization procedure described above aims at discovering the set of d -ranges that include as many points from the dataset as possible. Thus a single execution is able to determine a clustering result. Note that in the final clustering solution empty d -ranges may appear, or even d -ranges that overlap. This, instead of becoming a problem permits the approximation of the number of clusters, by borrowing the *merge* operation of the unsupervised k -windows clustering algo-

rithm [27]. During this step, for each pair of overlapping windows, the number of patterns that lie in their intersection is computed. With respect to the proportion of this number to the total number of points contained in each window, the algorithm can decide whether to:

- Ignore one window if the proportion is very high.
- Consider the windows to contain parts of the same cluster if the proportion is relatively high.
- Consider the windows to capture different clusters, if the proportion is low.

An example of this operation is exhibited in Fig. 3.

A high level description of the proposed algorithmic scheme follows:

DE Unsupervised Clustering (DEUC)

- Construct** a data structure for the storing of the data.
- Set** the parameter a of WDF function.
- Repeat**

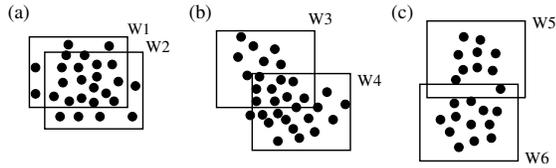


Figure 3: (a) W_1 and W_2 satisfy the similarity condition and W_1 is deleted. (b) W_3 and W_4 satisfy the merge operation and are considered to belong to the same cluster. (c) W_5 and W_6 have a small overlapment and capture two different clusters.

3. **Execute** the DE algorithm.
5. **Until** a sufficient part of the dataset is covered or a maximum number or iterations is performed.
6. **Merge** the resulting d -ranges
7. **Report** the final clusters.

4 Presentation of Experimental Results

The applicability of the proposed algorithm is evaluated using four different datasets. The first one is the two dimensional dataset $Dset_1$ demonstrated in Fig. 1. This is an easy to handle dataset, and is used to provide a visual inspection of the clustering result provided by the algorithm. Note that in all the experiments reported in this section the population was set to 20 individuals, and a maximum of 200 epochs was allowed. The parameters μ and p of DE were set to 0.6, and 0.8, respectively, in all experiments. Moreover if the d -ranges of best individual discovered contained more than 90% of the total points DE execution terminated. The application of the DEUC algorithm over the $Dset_1$ dataset with the parameter a obtaining the values 1, 2, 5, 10 is exhibited in Fig. 4. These results were obtained, by stopping the iterative executions of DE when more than 90% of the dataset was covered. Each individual encoded the center of five d -ranges. Comparing the clustering result, with the 3D-plots of the WDF function in Fig. 2, it is obvious DEUC is able to detect the extrema of WDF and form a clustering result that is on accordance with the form of WDF. The colors in the plots exhibit the different cluster label of the points that were assigned with respect to the closest d -range under the Euclidean metric. It is obvious that DEUC is able to provide visually optimal clustering results when a

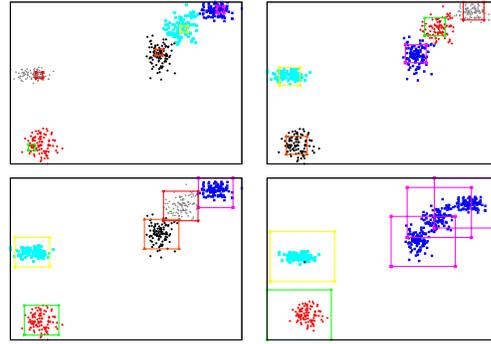


Figure 4: The clustering result of DEUC for $a = 1, 3, 5, 10$

ranges from 1 to 5. On the other hand, when a is too large the adjacent clusters are merged to a single cluster by the merging procedure.

Comparing the results of DEUC involves the usage of a clustering algorithm that can approximate the number of clusters. To compare the results of DEUC with other approaches we employ the DBSCAN clustering algorithm [24]. This choice of algorithm is motivated by the fact that DBSCAN computes the number of points ($MinPts$) that reside in a hypersphere of size Eps . Thus, the Eps parameter of DBSCAN is strongly connected with a parameter of WDF function. The execution of DBSCAN on $Dset_1$, setting $MinPts = 5$, (anything with less than 5 points in an Eps neighborhood around it is considered noise), and for Eps obtaining the values $Eps = 1, 3, 5, 10$ is exhibited in Fig. 5. Similarly in this case the colors designate different cluster labels, and the red crosses represent points recognized as noise. From the plots we can see that DBSCAN is more sensitive to the value of Eps than DEUC is on the value of a . Moreover, for the DBSCAN to be able to recognize the three different adjacent clusters a very delicate selection of Eps and $MinPts$ is needed.

Next, in Fig. 6, we investigate the ability of DEUC to approximate the number of clusters. To this end we apply DEUC using 3,5,10 and 15 windows. As illustrated, when the number of d -ranges is less than the true number of clusters, each d -range is located over a minimum of WDF, but due to the inability to cover all the minima the cluster labels are incorrect. On the other hand, as the number of d -ranges grows larger than the real number of clusters, the algorithm has no problem of detecting the five clusters, since the merging procedure assigns correctly the cluster labels.

The previous results refer to a simple dataset,

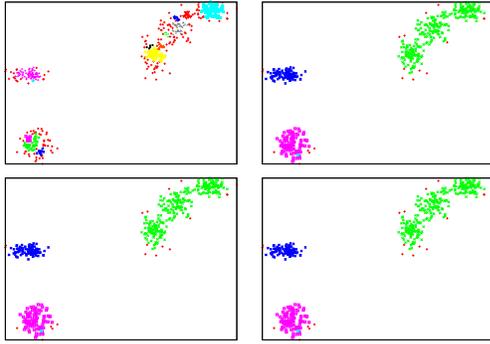


Figure 5: The clustering result of DBSCAN for $Eps = 1, 3, 5, 10$

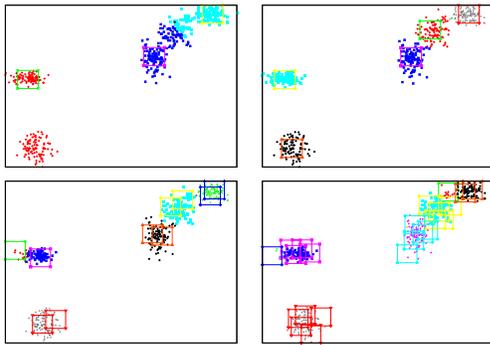


Figure 6: The impact on the clustering result of different number of d -ranges (3,5,10 and 15) when $a = 3$

and thus do not provide any evidence about the quality of the clustering result in difficult cases. To this end, to examine the quality of the partitioning results we employ two real world datasets. The first one considered is the four dimensional Iris dataset $Dset_{iris}$ from the UCI Machine Learning Repository [9]. This dataset is among the best known databases to be found in the pattern recognition literature. It contains 150 records of four features. The features are measurements of the sepal and petal length and width of three different types of the iris plant (Setosa, Versicolour and Virginica). The 150 records are equally distributed in three classes, each corresponding to a different type of the plant. To evaluate the clustering result we resolve to the correspondence they have to the true cluster labels of the patterns. Ideally, each cluster should contain patterns that belong to a single type of the Iris plant. After normalizing the data in the $[10, 100]^4$ range, DEUC was executed 100 times, using a population of 20 individuals while each individual encoded 5 d -ranges. In

most cases 3 clusters were recognized by the algorithm, but there were also cases that resulted in 4 and 5 clusters. Moreover, as a comparison measure we executed DBSCAN using all the combinations of values in $[1, 10]$ with a step of 1, for the Eps and $MinPts$ parameters, yielding 100 different clustering results. In the box-plots exhibited in Fig. 7, we summarize the results with respect to the partitioning accuracy. Each box-plot depicts the obtained values for the classification accuracy, in the 100 experiments. The box has lines at the lower quartile, median, and upper quartile values. The lines extending from each end of the box (whiskers) exhibit the range covered by the remaining data. The outliers, i.e. the values that lie beyond the ends of the whiskers, are represented with crosses. Notches represent a robust estimate of the uncertainty about the median. As it is obvious from Fig. 7, all the different DE operators are able to capture the dynamics of the dataset and result in high partitioning accuracy. Among all the operators DE_3 exhibits the most robust behavior and is able to provide the best results even with respect to outliers. On the other hand, DBSCAN is restrained from providing high accuracy results since in this dataset two of the classes are somewhat close and DBSCAN tends to merge them to a single cluster, thus destroying its classification accuracy.

The next dataset studied $Dset_L$ is the well-known and publicly available acute leukemia dataset provided by the center of genome research of the Whitehead Institute [16]. It is a well characterized dataset already used in numerous studies. This dataset contains mRNA expression profiles from 72 leukemia patients aiming at the development of an expression-based classification method for acute leukemia.

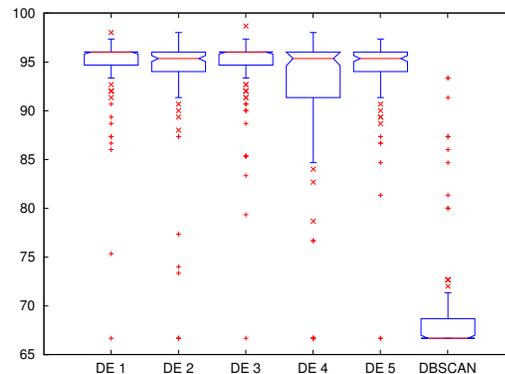


Figure 7: Box-plot of the classification accuracy for the Iris dataset

Each sample is measured over 7129 genes. The samples contain 47 acute myeloid leukemia (ALL) samples and 25 acute lymphoblastic leukemia (AML) samples. From the 7129 genes, the 50 most highly correlated genes with the ALL-AML class distinction, were selected as in [16]. Similarly, with the Iris dataset, all the values were normalized in the $[10, 100]^{50}$ range. Next 100 experiments of DEUC were performed and the partitioning accuracy of the clusters from each run with respect to the AML and ALL label of the patterns was recorded. The DBSCAN algorithm was also executed on the same dataset using all the combinations of values in $[40, 50]$ and $[1, 10]$ with a step of 1, for the *Eps* and *MinPts* parameters respectively, yielding 100 different clustering results. The box-plots in Fig. 8, exhibit the obtained results. In this case, the DEUC algorithm reported 4-6 final clusters, with the classification accuracy obtaining values over 95 a few times. In this case DE1 managed to performed better among the different variants of DE. The DBSCAN algorithm this time exhibited quite high classification results as the DEUC algorithm. It should be noted, however, that it was very difficult to establish a good range for the *Eps* parameter due to the high dimensionality of the dataset (50).

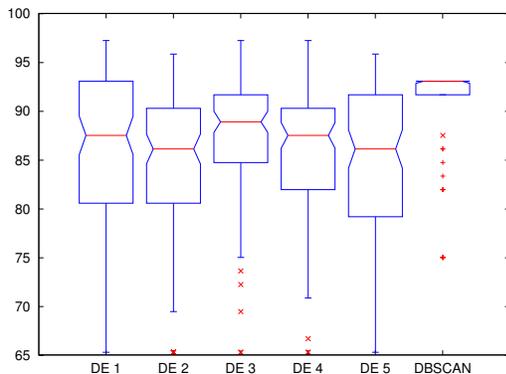


Figure 8: Box-plot of the classification accuracy for the Acute Leukemia dataset $Dset_L$

The final set of experiments aims to analyze the computational demands of the proposed algorithm. These can be analyzed by the number of function evaluations it requires to provide a clustering result. As already mentioned for each function evaluation a range search operation over the dataset is performed. Measuring the total number of range searches that are needed is a direct indication of the computational effort required. To this end, we constructed $Dset_2$ in a similar way with $Dset_1$, but with a size ranging

from 5000 to 30000 points. The mean number of range searches required over 100 executions of DEUC, for all mutation operators is depicted in Fig. 9. From this figure it is clear that all the DE operators require a steady number of range searches to converge, irrespective of the dataset size. When the dataset size is small (5000) the number of ranges searches is relatively high. It even exceeds the total number of points. DBSCAN for each dataset requires at least n range searches to finalize where n is the number of points in the dataset. Thus, for small datasets DEUC appears computationally expensive. On the other hand, as the dataset size increases, the efficiency of DEUC also increases. For example for 30000 points in the dataset DE₁ requires less than 6000 range searches, that is five times smaller than the DBSCAN requirements.

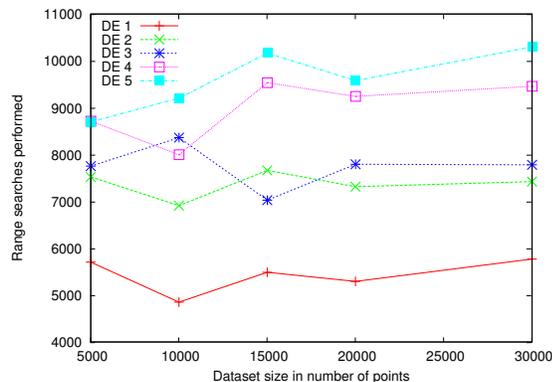


Figure 9: Mean number of range searches required for variable dataset size.

5 Concluding Remarks and Discussion

Many partitioning clustering algorithms based on evolutionary techniques have been proposed to tackle the problem of finding the optimal partition of a data set. Most of these approaches firstly encode a solution to the clustering problem as a chromosome, and then treat the clustering task as an optimization problem of locating the optimal centroids of clusters. The fitness of clustering solutions can be evaluated using various statistical functions [18, 32].

In the present contribution we present a new fitness function, that apart from being a meaningful clustering objective function, can be evaluated in sub-linear time with respect to the size of the dataset. This is achieved by utilizing Computational Geometry data structures.

Moreover, we propose an evolutionary scheme based on Differential Evolution that also has the ability to approximate the number of clusters and provide high quality partitions as it is evident from the experimental results provided. The proposed scheme can be applied using any evolutionary algorithm. In this paper we chose Differential Evolution, and aim to investigate the performance of different EAs in a future work. Furthermore, we wish to present an adaptive scheme, that will also be able to provide estimations for the parameter a of the WDF function.

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