Evolutionary Clustering Technique for finding Significant Solutions

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ABSTRACT
Evolutionary clustering technique is proposed that opts for cluster centers straight way from the data set, further making it to speed up the fitness evaluation by estimating a data table in advance. It saves the distances among pairs of data points, and by using binary instead of string representation to encode a variable number of cluster centers. The development of ECT has capability to properly cluster different data sets. The experimental results show that the ECT provides a more stable clustering performance in terms of number of clusters and clustering results. These results require less computational time as compared to other GA-based clustering algorithms.

Key Words
Clustering Technique, Evolutionary Algorithms, Reproduction, Crossover, Mutation, Fitness, Cluster Validity

1. INTRODUCTION
Cluster analysis, also known as unsupervised learning, is one of the most useful methods in the cluster analysis process for discovering groups. Clustering aims to organize a collection of data items into clusters, such that objects within the same cluster have a high degree of similarity, while objects belonging to different clusters have a high degree of dissimilarity. Cluster analysis makes it possible to look at properties of whole clusters instead of individual objects. This is a simplification that is useful when handling large amounts of data [1].

Some algorithms require certain parameters for clustering, such as the number of clusters and cluster shapes, as previous literature has stated [2]. Several non-GA-based clustering algorithms have been widely used, such as K-means, Fuzzy-c-means, EM, etc. However, the number of clusters in a data set is not known in most real-life situations. None of these non-GA-based clustering algorithms is capable of efficiently and automatically forming natural groups from all the input patterns, especially when the number of clusters included in the data set tends to be large. This is often due to a bad choice of initial cluster centers. Difficult problems such as these are referred to as unsupervised clustering or non-parametric clustering, and are often dealt with by employing an evolutionary approach. Genetic algorithms (GA) are the best-known evolutionary techniques [3]. To date, some research articles have dealt with this method [4]. Among the GA-based clustering algorithms illustrated in the current literature, the GCUK (Genetic Clustering for Unknown K)

method [5] is the most effective one. However, its cost of computational time is very high because it uses a string representation (or real-number encoding) to encode clusters that require a great deal of time for floating-point computation. In our work, the cluster centers are selected from the data set, and a binary representation is used to encode a variable number of cluster centers. In the conventional GA-based clustering

methods, the cluster mean is used as the center of a cluster, and thus the distance from every data point to its cluster center must be evaluated each time the fitness of a chromosome is evaluated.

Fitness evaluation during the conventional evolution process is quite time-consuming due to the repeated computation of the distance between every data point and its corresponding cluster center. Since our method selects cluster centers directly from the data set, it has the advantage of constructing a look-up table that saves the distances between all pairs of data points in advance. With the aid of the look-up table, the distances between all pairs of data points need to be evaluated only once throughout the entire evolution process.

The question generally asked, in relation to the cluster validity problem, is whether the underlying assumptions (cluster shapes, number of clusters, initial conditions, etc.) of the clustering technique are satisfied for all of the input data sets. In order to address this problem, several cluster validity measures such as the Dunn index, the XB index (Xie-Beni index), the BM index [6] and the DB index [7] have been proposed [8,9,10,11]. It is impossible to answer every question without prior knowledge of the data. However, we can look for measures that provide reasonable clustering results in terms of homogeneity within clusters and heterogeneity between clusters, as discussed above. Our experiments show that the Dunn index slows down the overall process although it provides good results for strip-shaped clusters, the XB index performs poorly when the number of clusters is large, and the BM index tends to form two clusters for most of the data sets. The DB index, defined as a function of the ratio of the sum of the within-cluster scatter to the between-cluster separation, is shown to provide the most reasonable measure among all indices mentioned above. Therefore, we adopt the DB index to measure cluster validity in our experiments. The superiority of the proposed algorithm, over other proposed genetic clustering algorithms, is demonstrated in the experimental results.

This paper is organized as follows: Section 2 describes how to implement a genetic algorithm. In Section 3, our proposed algorithm is introduced. Section 4 provides experimental results and comparisons with the GCUK method. Conclusions and directions for future research are given in Section 5.

2. CLUSTER ALGORITHM
Cluster analysis, also known as unsupervised learning, is one of the most useful methods in the cluster analysis process for discovering groups. Clustering aims to organize a collection of data items into clusters, such that objects within the same

cluster have a high degree of similarity, while objects belonging to different clusters have a high degree of dissimilarity. Cluster analysis makes it possible to look at properties of whole clusters instead of individual objects. This is a simplification that is useful when handling large amounts of data [7].

2.1 Clustering using Evolutionary algorithms

2.1.1 Basic principle

The searching capability of GAs has been used in this article for the purpose of appropriately determining a fixed number K of cluster centres in R^N; thereby suitably clustering the set of n unlabelled points. The clustering metric that has been adopted is the sum of the Euclidean distances of the points from their respective cluster centres. Mathematically, the clustering metric M for the K clusters C1, C2,….., CK is given by

$$\mathcal{M}(C_1, C_2, \ldots, C_K) = \sum_{i=1}^{K} \sum_{x_j \in C_i} \|\mathbf{x}_j - \mathbf{z}_i\|.$$

The task of the GA is to search for the appropriate cluster centres z1, z2,….., zK such that the clustering metric M is minimized.

2.2 GA-clustering algorithm

The basic steps of GAs, which are also followed in the

GA-clustering algorithm, are shown in Fig. 1.

```
Begin
1.  t=0
2.  initialize population P(t)
3.  compute fitness P(t)
4.  t = t+1
5.  if termination criterion achieved go to step 10
6.  select P(t) from P(t-1)
7.  crossover P(t)
8.  mutate P(t)
9.  go to step 3
10.  Output best and stop
End
```

Fig. 1. Basic steps in GAs.

These are now described in detail.

2.2.1 String representation

Each string is a sequence of real numbers representing the *K* cluster centres. For an *N*-dimensional space, the length of a chromosome is *N*K* words, where the first *N* positions (or, genes) represent the *N* dimensions of the first cluster centre, the next *N* positions represent those of the second cluster centre, and so on. As an illustration let us consider the following example.

Example 1. Let *N*"2 and *K*"3, i.e., the space is two-dimensional and the number of clusters being considered is three. Then the chromosome

51.6 72.3 18.3 15.7 29.1 32.2

represents the three cluster centres (51.6, 72.3), (18.3, 15.7) and (29.1, 32.2). Note that each real number in the chromosome is an indivisible gene.

2.2.2 Population initialization

The *K* cluster centres encoded in each chromosome are initialized to *K* randomly chosen points from the data set. This process is repeated for each of the *P* chromosomes in the population, where *P* is the size of the population.

1.2.3. Fitness computation

The fitness computation process consists of two phases. In the first phase, the clusters are formed according to the centres encoded in the chromosome under consideration. This is done by assigning each point x*i*, *i*"1, 2,2, *n*, to one of the clusters *Cj* with centre z*j* such that

$$\|\mathbf{x}_i - \mathbf{z}_j\| < \|\mathbf{x}_i - \mathbf{z}_p\|, p = 1, 2, \ldots, K, \text{ and } p \neq j.$$

All ties are resolved arbitrarily. After the clustering is done, the cluster centres encoded in the chromosome are replaced by the mean points of the respective clusters. In other words, for cluster *Ci*, the new centre z*i* is computed as

$$\mathbf{z}_i^* = \frac{1}{n_i} \sum_{\mathbf{x}_j \in C_i} \mathbf{x}_j, \quad i = 1, 2, \ldots, K.$$

These z*i* s now replace the previous z*i*s in the chromosome. As an illustration, let us consider the following example.

Example 2. The first cluster centre in the chromosome considered in Example 1 is (51.6, 72.3). With (51.6, 72.3) as centre, let the resulting cluster contain two more points, viz., (50.0, 70.0) and (52.0, 74.0) besides itself i.e., (51.6, 72.3). Hence the newly computed cluster centre becomes ((50.0+52.0+51.6)/3, (70.0+74.0+72.3)/ 3) = (51.2, 72.1). The new cluster centre (51.2, 72.1) now replaces the previous value of (51.6, 72.3).

Subsequently, the clustering metric M is computed as

follows:

$$\mathcal{M} = \sum_{i=1}^{K} \mathcal{M}_i,$$

$$\mathcal{M}_i = \sum_{\mathbf{x}_j \in C_i} \|\mathbf{x}_j - \mathbf{z}_i\|.$$

The fitness function is defined as *f*'1/M, so that maximization of the fitness function leads to minimization of M.

2.2.3 Selection

The selection process selects chromosomes from the mating pool directed by the survival of the fittest concept of natural

Evolutionary systems. In the proportional selection strategy adopted in this article, a chromosome is assigned a number of copies, which is proportional to its fitness in the population, that go into the mating pool for further Evolutionary operations. Roulette wheel selection is one common technique that implements the proportional selection strategy.

2.2.4 Crossover

Crossover is a probabilistic process that exchanges information between two parent chromosomes for generating two child chromosomes. In this article single point crossover with a fixed crossover probability of k*c* is used. For chromosomes of length *l*, a random integer, called the crossover point, is generated in the range [1, *l* — 1]. The portions of the chromosomes lying to the right of the crossover point are exchanged to produce two offspring.

2.2.5 Mutation

Each chromosome undergoes mutation with a fixed probability μ*m*. For binary representation of chromosomes, a bit position (or gene) is mutated by simply flipping its value. Since we are considering floating point representation in this article, we use the following mutation. A number d in the range [0, 1] is generated with uniform distribution. If the value at a gene position is *v*, after mutation it becomes

$$v \pm 2 * \delta * v, \quad v \neq 0,$$

$$v \pm 2 * \delta, \quad v = 0.$$

The ' + ' or ' — ' sign occurs with equal probability. Note that we could have implemented mutation as

$$v \pm \delta * v.$$

However, one problem with this form is that if the values at a particular position in all the chromosomes of a population become positive (or negative), then we will never be able to generate a new chromosome having a negative (or positive) value at that position. In order to overcome this limitation, we have incorporated a factor of 2 while implementing mutation. Other forms like

$$v \pm (\delta + \varepsilon) * v,$$

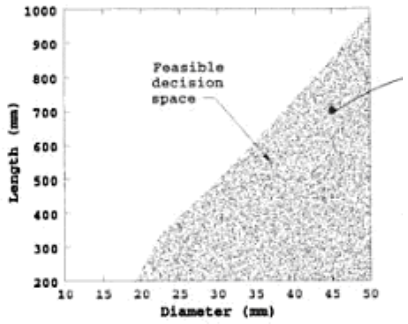
where 0‹Є‹1 would also have satisfied our purpose. One may note in this context that similar sort of mutation operators for real encoding have been used mostly in the realm of evolutionary strategies.

2.2.6 Termination criterion

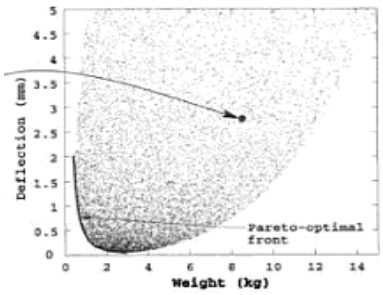
In this article the processes of fitness computation, selection, crossover, and mutation are executed for a maximum number of iterations. The best string seen up to the last generation provides the solution to the clustering problem. We have implemented elitism at each generation by preserving the best string seen up to that generation in a location outside the population. Thus on termination, this location contains the centre of the final clusters.

3. METHODOLOGY

A cantilever design problem is considered with two decision variables i.e. diameter (d) and length (l). the beam has to carry an end load P. Let us also consider two conflicting objectives of design , i.e. minimization of weight f1 and minimization of end deflection f2. the first objective will resort to an optimum solution having the smaller dimensions of d and l, so that the overall weight of the beam is minimum. Since the dimensions are small , the beam will not be adequately rigid and the end deflection of the beam will be large. On the other hand . if the beam is minimized for end deflection , the dimensions of the beam are expected to be large , thereby making the weight of the beam large .the left plot in Figure 1 marks the feasible decision variable space in the overall search space enclosed by $10 \leq d \leq 50$ mm and $200 \leq l \leq 1000$ mm. it is clear that not all solutions in the rectangular decision space are feasible . Every feasible solution in this space can be mapped to a solution in the feasible objective space shown in the right plot. The correspondence of a point in the left figure with that in the right figure is also shown.



Left Plot



Right Plot

Fig.2 The feasible decision variable space (left) and the feasible objective space (right)

This Fig 2 shows many solutions trading-off differently between the two objectives. Any two solutions can be picked from the feasible objective space and compared. For some pairs of solutions, it can be observed that one solution is better than the other in both objectives as given in Table 1.All solutions lying on this curve are special in the context of multi-objective optimization and are called Pareto-optimal solutions. The curve formed by joining these solutions is known as Pareto-optimal front.

Table 1 Five solutions for the cantilever design problem.

Solution	d (mm)	l (mm)	Weight (kg)	Deflection (mm)
A	18.94	200.00	0.44	2.04
B	21.24	200.00	0.58	1.18
C	34.19	200.00	1.43	0.19
D	50.00	200.00	3.06	0.04
E	33.02	362.49	2.42	1.31

This approach is suitable for decision-makers that do not have *a priori* knowledge of the relative importance of the conflicting objectives in Multicriteriaoptimization problem.

The developed approach is based on the following steps:

1. Obtain the entire Pareto-optimal set or sub-set of solutions by using a multiple-objective evolutionary algorithm (MOEA) or by another means.

2. Apply the GA based clustering algorithm to form clusters on the solutions contained in the Pareto set.

3. To determine the "optimal" number of clusters, *k*, in this set, silhouette plots are used. A value of the silhouette width, *s*(*i*), is obtained for several values of *k*. The clustering with the highest average silhouette width is selected as the "optimal" number of clusters in the Pareto-optimal set.

4. For each cluster, select a representative solution. To do this, the solution that is closest to its respective cluster centroid is chosen as a good representative solution.

4. ANALYZE THE RESULTS.

At this point, the decision-maker can either:

5.1 Analyze the "knee" cluster. The suggestion is to focus on the cluster that has solutions that conform to the "knee" region. The "knee" is formed by those solutions of the Pareto-optimal front where a small improvement in one objective would lead to a large deterioration in at least one other objective. Moreover, from this "knee" cluster the decision maker can select a promising solution for system implementation. This would be the solution closest to the ideal or utopian solution of the multiple objective problem, in a standardized space.

5.2 Analyze the *k* representative solutions and/or select the most promising solutions among this *k* set, selecting the solution closest to the ideal point. By applying the proposed technique, the Pareto-optimal front of a multiple objective problem can be reduced to the "knee cluster" as in 5.1, or to a set of *k* solutions as in 5.2. In both cases the decision maker can choose a good tradeoff for system implementation by selecting the closest solution to the ideal or utopian solution of the multiple objective problems, in a standardized space.

A Matlab code is developed to perform the steps of the proposed technique. From standardized data, the code will run the *clustering* algorithm and from two to a specified number of means it will calculate the average silhouette values and it will return the value of *k* suggesting the most optimal allocation. After this, it will also return the "knee cluster" of the optimal partition, the *k* representative solutions of the Pareto front, and in both cases, the solution closest to the ideal or utopian point.Fig.3 & Fig.4 shows the solution sets.

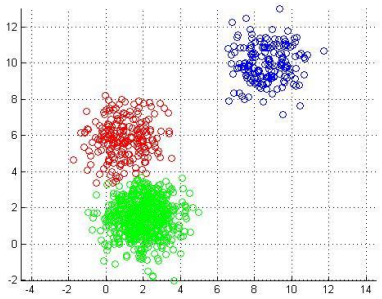


Fig.3 The Solution Set1

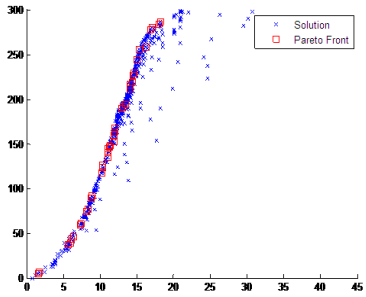


Fig.4 The Solution Set2

5. CONCLUSION

This work proposed a Evolutionary clustering technique (ECT) to determine the optimal Solution Set.

Pareto optimization methods allow the use of Multicriteria optimization models without a priori decision maker preferences. The decision makers can consider the possibilities and trade-offs between objectives before selecting a solution for implementation. These methods suffer from the shortcoming of requiring the decision makers to consider many possible solutions resulting from the optimization procedure. This paper developed and evaluated a cluster analysis methodology to address this issue.

Previous methods involved eliminating some of the Pareto optimal solutions before presenting them to the decision makers. The proposed methodology allows the entire non-dominated set to be presented to the decision makers by providing a tractable structure for the results. This methodology will continue to be applicable as computational power increases and Pareto optimization algorithms improve, leading to the generation of larger non-dominated sets.

This approach is applicable to Multicriteria problems with discrete decision variables. Multicriteria configuration optimization problems and the more general class of combinatorial Multicriteriaoptimization problems have discrete Pareto fronts. It may also be applicable to problems containing highly discontinuous Pareto fronts.

This methodology is particularly useful if similarly performing solutions based on the objective function values may be distinguishable to the decision makers based on the importance of the decision variable values or unmodeled aspects of the problem. Previous approaches to this issue would have eliminated similarly performing solutions from consideration.

Future work will revisit the issues in cluster analysis including scaling, proximity measures, selection of algorithms, and validation as well as improved visualizations. This work could be extended to consider the proximity of the solutions based on their decision variable values. It may be desirable in some applications to highlight clusters containing similarly performing solutions with very different decision variable values; these solutions could denote unmodeled aspects of the problem or possible freedom in the decision.

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