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Multi-Objective Gene Expression Programming for Clustering

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Abstract. This paper proposes a multi-objective gene expression programming for clustering (MGEPC), which could automatically determine the number of clusters and the appropriate partitioning from the data set. The clustering algebraic operations of gene expression programming are extended first. Then based on the framework of the Non-dominated Sorting Genetic Algorithm-II, two enhancements are proposed in MGEPC. First, a multi-objective k-means clustering is proposed for local search, where the total symmetrical compactness and the cluster connectivity are used as two complementary objectives and the point symmetry based distance is adopted as the distance metric. Second, the power-law distribution based selection strategy is proposed for the parent population generation. In addition, the external archive and the archive truncation are used to keep a historical record of the non-dominated solutions found along the search process. Experiments are performed on five artificial and three real-life data sets. Results show that the proposed algorithm outperforms the PESA-II based clustering method (MOCK), the archived multiobjective simulated annealing based clustering technique with point symmetry based distance (VAMOSA) and the single-objective version of gene expression programming based clustering technique (GEP-Cluster).

Keywords: Clustering; multi-objective; evolutionary algorithm; gene expression programming.

1. Introduction

Clustering is the assignment of a set of unlabeled objects into groups such that objects from the same group are more similar to each other than objects from different groups. Clustering algorithms have been widely applied into many different fields, such as image processing [6], text categorization [19], market segmentation [14], eye gaze visualizations [20], etc. Since clustering could be considered as a particular kind of optimization problem, evolutionary algorithms have been proposed for clustering [11].

Gene Expression Programming (GEP), which combines the advantages of both genetic algorithm and genetic programming, is a relatively new member in the evolutionary computation family [8]. GEP works with two entities called the chromosome and the expression tree. The separation of the chromosome and the expression tree ensures that expression trees are always syntactically correct after any genetic change of chromosomes; thus the exploration of the search space is greatly expanded. Therefore, GEP shows powerful capabilities over a large variety of domains, including regression modeling, optimization, classification tasks and time series prediction [9, 22, 12, 23].

A clustering technique based on GEP (GEP-Cluster) was first proposed in [4], and a new concept named the clustering algebra, which performs clustering as algebraic operation, is presented. GEP-Cluster could divide or merge the clusters automatically without any prior knowledge. However, like the conventional evolutionary clustering algorithms performing with just one clustering criterion, GEP-Cluster is also a single-objective clustering method. For a wide variety of real life datasets, a single clustering criterion is hardly able to judge the correctness of clustering result. Furthermore, since there would be considerable discrepancies between solutions produced by the same algorithm using different clustering criteria, an inappropriate choice of the validity measure may lead to poor clustering results [21]. Therefore, for overcoming the limitation of single-objective clustering method, the concept of multi-objective clustering has been introduced [3, 10, 13, 16, 18].

In the paper, a multi-objective gene expression programming for clustering (MGEPC) is proposed. The proposed algorithm could automatically determine the number of clusters and the appropriate partitioning from the data set. MGPEC first extends the clustering algebraic operations of GEP for

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avoiding using a huge amount of computational resources to edit those illegal chromosomes. Then based on the framework of the Non-dominated Sorting Genetic Algorithm-II (NSGA-II), two enhancements are proposed in MGEPC. First, a multi-objective k-means method is presented as a local search, which performs fine-tuning of some rough partitions obtained by the global search, to speed up the convergence. Second, the power-law distribution based selection strategy is proposed for ensuring some inferior individuals being selected into the next generation while maintaining a bias against superior solutions, which helps maintain the diversity of the population and avoids getting stuck at a local optimal or partial Pareto front. In addition, the external archive and the archive truncation are used to keep a historical record of the non-dominated solutions found along the search process.

The remainder of the paper is organized as follows: Section 2 reviews relevant previous work. In Section 3, the proposed algorithm is discussed in detail. Section 4 shows the experimental setup and comparison results on both artificial and real-life data sets. Finally, Section 5 concludes the paper.

2. Related works

MOCK is a popular multi-objective evolutionary clustering algorithm based on PESA-II (PESA-II is a multiobjective evolutionary algorithm proposed in [5]). It optimizes two complementary objectives, which are the cluster compactness and the connectedness [10]. It has been shown to outperform traditional single-objective clustering techniques across a diverse range of benchmark data sets. However, since MOCK employs a locus-based adjacency encoding scheme, namely, the length of each chromosome is equal to the number of points present in the data set; the length of each chromosome would increase with the number of points. Hence, MOCK would suffer from premature convergence for long chromosomes in large search space [15].

VAMOSA, which is an archived multiobjective simulated annealing based clustering technique with point symmetry based distance, adopts a variable-length real encoding, namely, the strings are made up of real numbers which represent the coordinates of the centers of partitions [16]. Therefore, for data sets of large cluster numbers and high dimensions, VAMOSA has the same drawback as MOCK. Moreover, since the mutation mechanism could only add or remove one cluster center at a time, the exploration of the search space would be limited to a certain extent. Thus VAMOSA suffers from a slow convergence rate and often easily falls into local optimality.

GEP-Cluster is a GEP-based clustering method without prior knowledge. It introduces a new encoding scheme based on clustering algebraic operations [4]. Although GEP-Cluster could overcome the limitation in the representation of MOCK and VAMOSA, a large number of invalid chromosomes would appear in the evolving process of GEP-Cluster and a huge amount of computational resources would be wasted. In addition, GEP-Cluster chooses the overall deviation as the objective. Since the overall deviation would increase with the number of clusters increasing, the number of clusters detected by the iteration process would always be the maximum cluster number pre-specified. Although GEP-Cluster employs an automatic merging cluster algorithm to adjust clusters after the iteration process, it is effective only when true clusters in the data set are well-separated.

In the next section, we will present a new clustering algorithm named MGEPC. In Section 4, we will use artificial and real-life datasets to compare the effectiveness of MGEPC with that of MOCK, VAMOSA and GEP-Cluster, respectively.

3. The Proposed Method

3.1. Multiobjective optimization

We consider the clustering task as a multiobjective optimization problem (MOP), which can be mathematically formulated as [24]

$$\text{Minimize } F(x) = (f_1(x), \ldots, f_m(x)^T), \text{ s.t. } x \in \Omega \quad (1)$$

where Ω is the decision space and $x \in \Omega$ is a decision vector. $F(x)$ consists of m objective functions $f_i, i = 1, \ldots, m$.

The objectives of MOP often conflict with each other. Improvement of one objective may lead to deterioration of another. Thus there no longer exists a single optimal solution but rather a set of trade-off solutions, which is called the Pareto optimal solutions. Some definitions related to the Pareto optimality are given as follows.

Definition 1 (Pareto dominance). A solution x_p is said to dominate another solution x_q (denoted by $x_p \prec x_q$), if and only if $\forall k \in 1, \ldots, m$, $f(x_p) \le f(x_q)$ and $\exists k \in 1, \ldots, m$, $f(x_p) < f(x_q)$.

Definition 2 (Pareto-optimal set). If no solution dominates x_p, then x_p is a Pareto-optimal solution. The set of all feasible Pareto-optimal solutions is called Pareto-optimal set.

Definition 3 (Pareto front). The image of Pareto-optimal set in the objective space is called the Pareto front.

Definition 4 (Non-dominated set). Among a set of solutions P, the non-dominated set of solutions P^* is composed of solutions that are not dominated by any other solution of the set P.

3.2. Representation

3.2.1. Clustering algebraic operations

Clustering operators used in GEP-Cluster are '$\cap$' and '$\cup$' [4]. Let O_x be the center of cluster C_x, and O_y be the center of cluster C_y. Then

(1) $O_x \cap O_y = \{O_{xy}\}$, where O_{xy} is the mean point of O_x and O_y.

(2) $O_x \cup O_y = \{O_x, O_y\}$.

The first operation indicates that C_x and C_y are merged into one cluster with the center O_{xy}, and the second operation indicates that C_x and C_y would not be merged together, namely, they are two separate clusters with the center O_x and O_y.

Based on the concepts of the clustering operators, we extend the clustering algebraic operations, which are presented in Theorem 1.

Theorem 1: *Let O_x, O_y and O_z be the centers of cluster C_x, C_y and C_z in the d-dimensional space, and $O_x = (x_1, x_2, ..., x_d)$, $O_y = (y_1, y_2, ..., y_d)$, $O_z = (z_1, z_2, ..., z_d)$, then*

(1) $O_x \cap O_y = O_y \cap O_x$; $O_x \cup O_y = O_y \cup O_x$

(2) $O_x \cap (O_y \cap O_z) = \{(\frac{2x_1 + y_1 + z_1}{4}, \frac{2x_2 + y_2 + z_2}{4}, ..., \frac{2x_d + y_d + z_d}{4})\}$;

$(O_x \cap O_y) \cap O_z = \{(\frac{x_1 + y_1 + 2z_1}{4}, \frac{x_2 + y_2 + 2z_2}{4}, ..., \frac{x_d + y_d + 2z_d}{4})\}$

(3) $O_x \cup (O_y \cup O_z) = (O_x \cup O_y) \cup O_z = \{(x_1, x_2, ..., x_d), (y_1, y_2, ..., y_d), (z_1, z_2, ..., z_d)\}$

(4) $O_x \cup (O_y \cap O_z) = \{(x_1, x_2, ..., x_d), (\frac{y_1 + z_1}{2}, \frac{y_2 + z_2}{2}, ..., \frac{y_d + z_d}{2})\}$

(5) $O_x \cap (O_y \cup O_z) = \{(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, ..., \frac{x_d + y_d}{2}), (\frac{x_1 + z_1}{2}, \frac{x_2 + z_2}{2}, ..., \frac{x_d + z_d}{2})\}$

▼Proof:

(1) This commutative law has been proved in [4].

(2) The operation $O_x \cap (O_y \cap O_z)$ indicates that C_y and C_z are merged into cluster C_{yz} with the center $O_{yz} = (\frac{y_1 + z_1}{2}, \frac{y_2 + z_2}{2}, ..., \frac{y_d + z_d}{2})$, and then C_{yz} and C_x are merged into cluster C_{xyz} with the center $O_{xyz} = (\frac{2x_1 + y_1 + z_1}{4}, \frac{2x_2 + y_2 + z_2}{4}, ..., \frac{2x_d + y_d + z_d}{4})$. Similarly, the operation $(O_x \cap O_y) \cap O_z$ indicates that C_x, C_y and C_z are ultimately merged into one cluster with the center $(\frac{x_1 + y_1 + 2z_1}{4}, \frac{x_2 + y_2 + 2z_2}{4}, ..., \frac{x_d + y_d + 2z_d}{4})$. Consequently, operator '$\cap$' is not always associative.

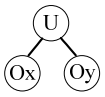
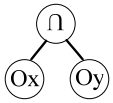
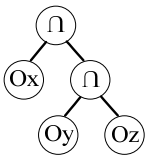
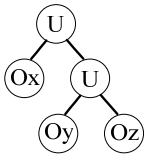
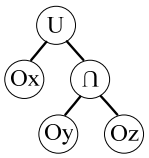
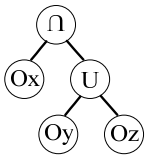
(3) The operation $O_x \cup (O_y \cup O_z)$ indicates that C_y and C_z are separate clusters, and C_x is separate from C_y and C_z. Thus C_x, C_y and C_z are three distinct clusters with the center O_x, O_y and O_z, respectively. Similarly, $(O_x \cup O_y) \cup O_z$ also indicates that C_x, C_y and C_z are three distinct clusters. Therefore, the equation $O_x \cup (O_y \cup O_z) = (O_x \cup O_y) \cup O_z$ is satisfied, and the three cluster centers are $(x_1, x_2, ..., x_d)$, $(y_1, y_2, ..., y_d)$ and $(z_1, z_2, ..., z_d)$ respectively.

(4) The formula $O_x \cup (O_y \cap O_z)$ indicates that C_y and C_z are merged into cluster C_{yz} with the center O_{yz}, and then C_{yz} and C_x are kept separate. That is to say, there are two clusters with the centers O_x and O_{yz}, namely, $(x_1, x_2, ..., x_d)$ and $(\frac{y_1 + z_1}{2}, \frac{y_2 + z_2}{2}, ..., \frac{y_d + z_d}{2})$.

(5) The operation $O_x \cap (O_y \cup O_z)$ indicates that C_x will be merged with C_y and C_z respectively. Thus the merged cluster centers are $(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, ..., \frac{x_d + y_d}{2})$ and $(\frac{x_1 + z_1}{2}, \frac{x_2 + z_2}{2}, ..., \frac{x_d + z_d}{2})$.▲

In summary, the clustering algebraic operations, the corresponding expression trees and the centers of the resultant clusters are shown in Table 1.

Table 1. The clustering algebraic operations, the corresponding expression trees and the centers of the resultant clusters

Algebraic operation	Expression tree	Centers of the resultant clusters
$O_x \cup O_y$		$(x_1, x_2, ..., x_d)$ $(y_1, y_2, ..., y_d)$
$O_x \cap O_y$		$(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, ..., \frac{x_d + y_d}{2})$
$O_x \cap (O_y \cap O_z)$		$(\frac{2x_1 + y_1 + z_1}{4}, \frac{2x_2 + y_2 + z_2}{4}, ..., \frac{2x_d + y_d + z_d}{4})$
$O_x \cup (O_y \cup O_z)$		$(x_1, x_2, ..., x_d), (y_1, y_2, ..., y_d), (z_1, z_2, ..., z_d)$
$O_x \cup (O_y \cap O_z)$		$(x_1, x_2, ..., x_d), (\frac{y_1 + z_1}{2}, \frac{y_2 + z_2}{2}, ..., \frac{y_d + z_d}{2})$
$O_x \cap (O_y \cup O_z)$		$(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, ..., \frac{x_d + y_d}{2})$, $(\frac{x_1 + z_1}{2}, \frac{x_2 + z_2}{2}, ..., \frac{x_d + z_d}{2})$.

3.2.2. Encoding

Each chromosome of MGEPC is composed of a head and a tail. The head contains symbols that represent both the functions (the elements from the function set F) and terminals (the elements from the terminal set T), whereas the tail contains only terminals. The function set F is $\{\cap, \cup\}$, and the terminal set T is $\{1, 2, \ldots, i, \ldots N\}$, $i \in [1, N]$, where N is the number of data points in the data set and i is the sequence number of the ith data point. The first position in the head should always be set as '$\cup$' in order to ensure the clustering problem meaningful. Other positions in the head are set as a randomly selected function or a randomly selected terminal based on an equal probability. Elements in the tail are chosen from the terminal set randomly. Duplicate terminals are allowed in the chromosome because the information encoded in the chromosome is cluster centers rather than link of each data item. Let h denote the length of the head and t denote the length of the tail. Since the maximum arity of the clustering operators is 2, then $t = h + 1$ [8]. It is evident from the clustering expression tree that a chromosome could express $h + 1$ clusters at most. Thus, if the maximum number of clusters is $k_{\max}$, the total length of the chromosome $m = h + t = (k_{\max} - 1) + ((k_{\max} - 1) + 1) = = 2k_{\max} - 1$. Figure 1 gives an example of the representation of a chromosome for MGEPC, where X_i (i=1,2,...,7) indicates the ith data point. Figure 1 (a) shows a chromosome of MGEPC. Figure 1 (b) and Figure 1 (c) show its corresponding expression tree and clustering algebraic operation, respectively.

3.2.3. Decoding

The translation from the chromosome to the expression tree is performed by a breadth-first traversal from left to right and from top to down [8]. The algebraic operation is obtained by a traversal in the reverse order, and the resultant cluster centers are evaluated according to Table 1.

Because the number of the nodes of an expression tree is m at most, the translation from the chromosome to the expression tree requires at most $O(m)$ time. Evaluation of expression tree also requires at most $O(m)$ time. Therefore, this decoding step requires at most $O(m)$ time.

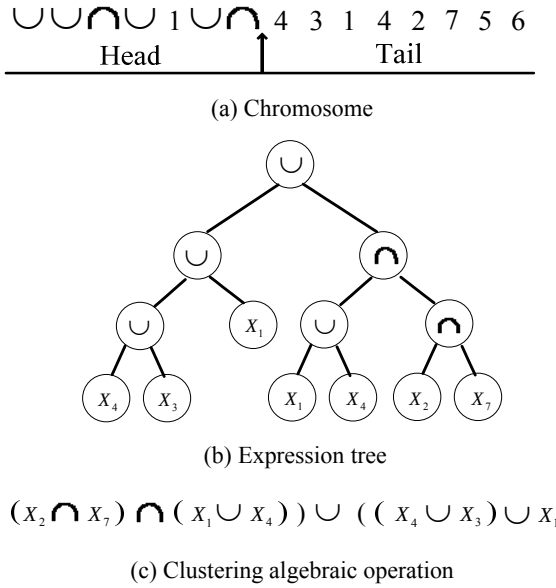


Figure 1. An example of the representation of a chromosome for MGEPC

This representation has two advantages. First, clusters could be merged or kept separate automatically by clustering operations. Thus there is no need to pre-specify the number of clusters, which is usually difficult to estimate in many applications. Second, extension of the clustering algebraic operations not only avoids using a huge amount of computational resources to edit those illegal chromosomes in the evolving process, but also allows modification of the chromosome using nearly any genetic operator without restrictions; thus the exploration of the search space is greatly enhanced.

3.3. Point symmetry based distance measure

Since symmetry is a basic feature of most shapes and objects, it can be considered as an important feature in their recognition and reconstruction. Symmetry is a natural phenomenon and clusters are not exception. Based on this observation, a point symmetry based distance (PS distance) is developed in [2]. Then assignment of points to different clusters is done based on the PS distance rather than the Euclidean distance. This enables the clustering algorithm to automatically evolve clusters of any shape, size or convexity as long as they possess some symmetry property.

The PS distance proposed in [2] is defined by

$$d_{ps}(x_i, c_k) = (d_1 + d_2) / 2 \times d_e(x_i, c_k) \qquad (2)$$

where $d_e(x_i, c_k)$ is the Euclidean distance between the point x_i and the cluster center c_k. d_1 and d_2 are distances of the two nearest neighbors of the symmetrical point (i.e. $2 \times c_k - x_i$) of x_i with respect to the center c_k. To reduce the complexity of finding d_1 and d_2, an ANN search using the Kd-tree method is used.

3.4. Objective functions

The objective functions corresponding to a state indicate the degree of goodness of the solution it represents. In this paper, two complementary objectives that reflect fundamentally different aspects of a clustering solution are selected: one is the total symmetrical compactness; the other is the cluster connectivity.

The total symmetrical compactness measures the within cluster total symmetrical distance. It is computed as the overall summed PS distance between data objects and their corresponding cluster center. It is defined as [17]

$$\delta_k = \sum_{i=1}^{k} E_i = \sum_{i=1}^{k} \sum_{i=1}^{n_i} d_{ps}(x_j^i, c_i) \qquad (3)$$

where k is the number of clusters, n_i is the total number of points present in the i th cluster, c_i is the center of the i th cluster, and x_j^i is the j th point of the i th cluster. $d_{ps}(x_j^i, c_i)$ denotes the PS distance between x_j^i and c_i. E_i is the total symmetrical deviation of a particular cluster i. Note that when the partitioning is compact and has good symmetrical structure, δ_k should be low. Thus for achieving better partitioning, the total symmetrical compactness should be minimized.

The cluster connectivity evaluates the degree to which neighboring data points have been placed in the same cluster. It is calculated as [10]

$$Conn(c) = \sum_{i=1}^{N} (\sum_{j=1}^{L} x_{i,n_{ij}}) \qquad (4)$$

where $x_{i,n_{ij}} = \begin{cases} \frac{1}{j}, & if\ \nexists C_k : x_i \in C_k \wedge n_{ij} \in C_k \\ 0, & otherwise \end{cases}$,

n_{ij} is the j th nearest neighbor of the i th datum, N is the size of the data set, and L is a parameter determining the number of neighbors that contribute to the connectedness. As an objective of clustering, the cluster connectivity should be minimized.

The objective value associated with the total symmetrical compactness necessarily improves with an increasing number of clusters, and the opposite is the case for the cluster connectivity. Thus the interaction of these two objectives allows MGEPC to automatically determine the number of clusters and generate clustering solutions corresponding to different trade-offs.

3.5. Description of the algorithm

In the subsection, MGEPC is formulated in detail. The flowchart of the MGEPC is shown in Figure.2 first, and the outline of MGEPC is presented in the following.

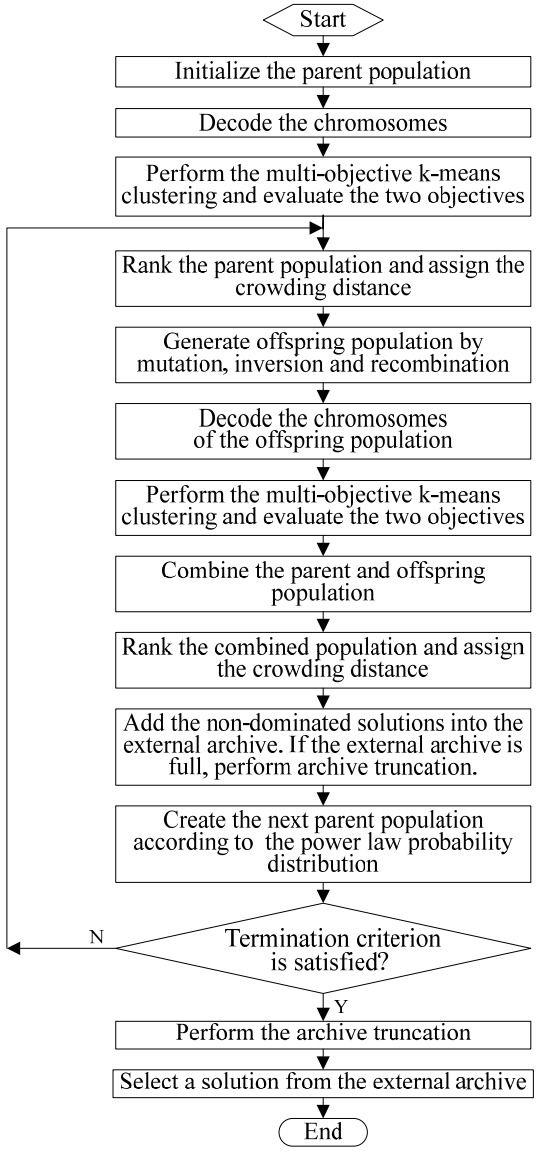


Figure 2. Flowchart of the MGEPC

Procedure MGEPC

Input: the data set D, the population size N_P, the maximum number of generations $G_{\max}$, the maximum number of clusters $k_{\max}$, the number of neighbors that contribute to the connectedness L, mutation rate p_M, inversion rate p_I, recombination rate p_R, the parameter of power law distribution τ, the maximum number of loops of multiobjective k-means clustering L_{iter} and the external archive size N_A.

Output: the cluster label of each data point.

Step 1: Initialize the parent population.

Step 2: Decode the chromosomes. Then the multi-objective k-means clustering is performed as follows: Assign each point to one of the clusters according to the point assignment method proposed in [2], which is shown in Figure 3. After the assignments are finished, two objective functions are evaluated and the cluster centers are replaced by the mean points of the respective clusters. This process is repeated until the maximum number of iterations is reached or the value of any objective function becomes larger than that computed in the last loop. Finally, output the objective values of each chromosome. Since the multi-objective k-means clustering works as a local search to refine the global search performed by the evolutionary procedure, the convergence is speeded up.

Procedure: assignment of data points

1. Let K denote the number of clusters encoded in one of the chromosomes. For all data points x_i, $1 \le i \le N$, compute

$$k^* = \arg\min_{k=1,\ldots,K} d_{ps}(x_i, c_k)$$

2. If $d_{ps}(x_i, c_{k^*}) / d_e(x_i, c_{k^*}) < \theta$, where θ is the maximum nearest neighbor distance among all the points in the data set, assign the data point x_i to the k^*th cluster.

3. Otherwise the data point x_i is assigned to the k^*th cluster, where

$$k^* = \arg\min_{k=1,\ldots,K} d_{ps}(x_i, c_k)$$

Figure 3. Data point assignment procedure

Step 3: Rank the population based on the non-dominated sorting and assign the crowding distance in each front. These two operations are proposed in [7] and are used for population selection. The non-dominated sorting is to rank each individual based on the definition of domination. Specifically, individuals not dominated by any other individuals are assigned front number 1, and individuals only dominated by individuals in front number 1 are assigned front number 2, and so on. The crowding distance is used to measure the density of individuals with the same front number. The crowding distance of a particular individual is computed as the average distance of two closest individuals on either side of this individual along each of objectives.

Step 4: Generate offspring population by using binary tournament selection (based on the front number and the crowding distance) and genetic operators. Three classes of genetic operators are adopted. (1) Mutation: the mutation operator randomly selects one element from the chromosome, except that at the root. If the element lies in the tail, then replace it with a randomly selected terminal. If the element lies in the head, two different cases should be considered: If it is a function, replace it with a different function or a randomly selected terminal based on an equal probability; if it is a terminal, replace it with a randomly selected function or a different terminal based on an equal probability. (2) Inversion: the inversion operator randomly selects a short fragment of elements in the head, except that at

the root, and inverts the element order in the fragment. Since the inversion operator is restricted to the head of the chromosome, all the new individuals created by inversion are syntactically correct. (3) Recombination: the recombination operator exchanges parts of a pair of randomly chosen chromosomes to form new offspring chromosomes. In this paper, one-point recombination is used.

Step 5: Decode the chromosomes of the offspring population and perform the multi-objective k-means clustering.

Step 6: Combine the parent and offspring population. Then rank the combined population based on non-dominated sorting and assign the crowding distance in each front.

Step 7: Add the non-dominated solutions into the external archive. We set the upper limit of the size of the external archive as N_A (N_A is a much larger number than the population size N_P) in order to prevent the elitists from growing extremely large. If the size of the external archive exceeds the upper limit, archive truncation is performed as follows: the non-dominated solutions in the external archive are identified firstly. Then the dominated solutions are discarded. If the size of non-dominated solutions is still larger than N_A, only N_A solutions with higher value of crowding distance are retained in the external archive.

Step 8: Create the next parent population from the combined population according to the power law probability distribution. This process has two substeps: a front is selected by a power law probability $P(u_1) = u_1^{-\tau}$ firstly, where u_1 is the front number sorted based on the non-domination, τ is a user specified parameter. Then a solution is chosen from the selected front by $P(u_2) = u_2^{-\tau}$, where u_2 is the sequence number of solutions sorted by decreasing the crowding distance and the solutions are selected without replacement. For $\tau = 0$, it is exactly a random selection. For $\tau \to \infty$, it approaches the elitist-preserving process as in NSGA-II. For a given value of τ, the selection ensures that no front and no crowded regions get completely excluded from further evolution while the evolution maintains a bias towards superior solutions. Hence, the power-law distribution based selection strategy for new parent population could not only keep a high convergence rate, but also maintain the diversity in the population, which would prevent the algorithm from getting stuck at a local optimal or partial Pareto front.

Step 9: Go to Step 3 if termination criterion is not satisfied, otherwise go to Step10.

Step 10: Perform the archive truncation and output solutions in the external archive. The output of the external archive contains a number of mutually non-dominated clustering solutions, which correspond to different tradeoffs between the two objectives, and also to different numbers of clusters.

Step 11: Select a solution from the external archive, where we use the model selection method proposed in MOCK to select the most promising clustering solution.

Step 12: Output the clustering result.

By the proposed algorithm, the clustering for the data set is finished and the number of clusters is determined automatically. In the next section, we will use the experimental results to verify the effectiveness of the proposed algorithm.

4. Experimental results

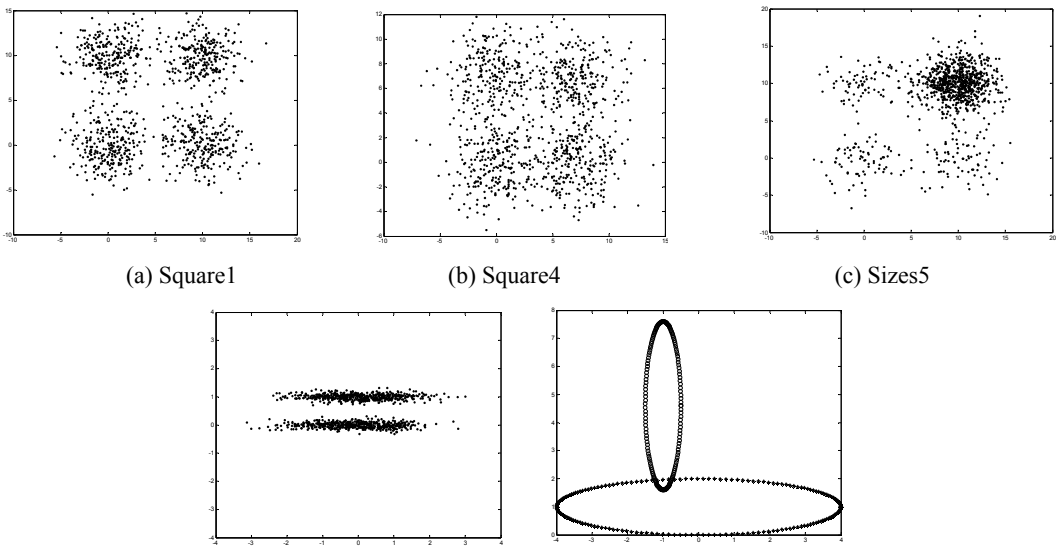
In this section, we present experiments on artificial and real-life datasets to evaluate the performance of the proposed MGEPC. The algorithm is compared with MOCK, VAMOSA and GEP-Cluster based on two widely used clustering quality evaluation measures: the adjusted rand index (ARI) [10] and the Minkowski score (MS) [16]. The higher the value of ARI and the lower the value of MS, the better the clustering quality is. Experiments are implemented in MATLAB 2009a and the running environment is an Intel (R) CPU 2.50 GHz machine with 3 GB of RAM and running Windows XP Professional.

4.1. Data sets

Five artificial data sets and three real-life data sets are used for the experiment. A short description of the data sets in terms of the number of data points, dimension and the number of clusters is provided in Table 2. The artificial data sets are displayed in Figure 4. Square1 [10] contains four well-separated squared clusters. Square4 [10] contains four overlapping squared clusters. Sizes5 [10] contains clusters of non-uniform densities. Long1 [10] contains two long-shaped clusters. Ellipse [2] contains data points distributed on two crossed ellipsoidal shells. The three real-life datasets are obtained from the UCI Machine Learning Repository [1].

Table 2. Details of the datasets used

The name of data set		The number of points	The number of dimension	The number of clusters
Artificial data sets	Square1	1000	2	4
	Square4	1000	2	4
	Sizes5	1000	2	4
	Long1	1000	2	2
	Ellipse	400	2	2
Real-life data sets	Iris	150	4	3
	Glass	214	9	6
	Wisconsin Breast Cancer Diagnosis (WBCD)	569	30	2



(a) Square1 (b) Square4 (c) Sizes5

(d) Long1 (e) Ellipse

Figure 4. Artificial data sets

4.2. Parameters of the algorithms

In this subsection, we list the specification of parameters for the four algorithms. For MGEPC, the population size $N_P = 50$, the maximum number of generations $G_{\max} = 100$, the external archive size $N_A = 1000$, the maximum number of clusters $k_{\max} = = \sqrt{N}$ (N denotes the size of the data set), the number of neighbors that contribute to the connectedness $L = 10\%N$, the recombination rate $p_R = 0.7$, the mutation rate $p_M = 0.1$, the inversion rate $p_I = 0.1$, the parameter of power law distribution $\tau = 1.4$ and the maximum number of loops of multi-objective k-means clustering $L_{iter} = 3$. These parameter values are recommended for MGEPC after performing a great number of hand-tuning experiments. For MOCK, the population size is 50, the number of generations is 100, the maximum number of clusters is $\sqrt{N}$, the number of neighbors that contribute to the connectedness L is $10\%N$, the recombination rate is 0.7 and the mutation rate is 0.1. For VAMOSA, in order to make direct comparisons possible, we set the maximum temperature $T_{\max} = 100$, the minimal temperature $T_{\min} = 2 \times 10^{-8}$, the cooling rate $\alpha = 0.8$ and the number of iterations at each temperature $iter = 50$ so that it has approximately the same number of function evaluations with the other three algorithms. For GEP-Cluster, the population size is 50, the number of generations is 100, the maximum number of clusters is $\sqrt{N}$, the recombination rate is 0.7 and the mutation rate is 0.1.

4.3. Experimental results

The mean values and standard deviations of the number of clusters, ARI and MS values for the eight data sets over 30 consecutive runs for MGEPC, MOCK, VAMOSA and GEP-Cluster are provided in Table 3. The distributions of ARI values and MS values are also visualized in Figure 5. It can be seen that MGEPC, MOCK and VAMOSA, which are the multi-objective clustering methods, consistently outperform GEP-Cluster algorithm in terms of the cluster numbers detected, ARI and MS values. For Square1, Square4 and Sizes5 which are composed of spherically-shaped clusters, MGEPC, MOCK and VAMOSA are always able to detect the appropriate number of clusters; and MGEPC performs better than MOCK and VAMOSA. The results of Square4 show that MGEPC performs well for overlapping clusters, and the results of Sizes5 show that MGEPC is also able to detect clusters of different densities and sizes. For Long1, both MGEPC and MOCK could detect the right partitions. For Ellipse, only MGEPC could detect the right number of clusters, and the mean values of ARI and MS are much better than those of MOCK and VAMOSA while their standard deviations are higher. The results of Long1 and Ellipse show that MGEPC is able to detect the appropriate partitioning from data sets with non-hyperspherical clusters as long as they possess the property of symmetry. For Iris, WDBC and Glass, MGEPC performs better than the others. Therefore, the effectiveness of MGEPC for clustering is higher.

Table 3. Mean values and standard deviations (in parentheses) of number of clusters, ARI and MS for different data sets over 30 consecutive runs of different algorithms

Data set	Real number of clusters	Algorithm	k	ARI	MS
Square1	4	MGEPC	**4 (0)**	**0.9686 (0.0076)**	**0.1995 (0.0268)**
		MOCK	**4 (0)**	0.9614 (0.0096)	0.2183 (0.0324)
		VAMOSA	**4 (0)**	0.9672 (0.0118)	0.2123 (0.0251)
		GEP-Cluster	5.42 (0.93)	0.6254 (0.1419)	0.5749 (0.2256)
Square4	4	MGEPC	**4 (0)**	**0.8305 (0.0192)**	**0.5197 (0.0146)**
		MOCK	**4 (0)**	0.7991 (0.0247)	0.5477 (0.0348)
		VAMOSA	**4 (0)**	0.8036 (0.0265)	0.5310 (0.0291)
		GEP-Cluster	3.50 (1.24)	03165 (0.2723)	0.8910 (0.2647)
Sizes5	4	MGEPC	**4 (0)**	**0.9593 (0.0176)**	**0.1821 (0.0293)**
		MOCK	**4 (0)**	0.9469 (0.0178)	0.1940 (0.0339)
		VAMOSA	**4 (0)**	0.9507 (0.0161)	0.1931 (0.0375)
		GEP-Cluster	3.48 (0.83)	0.5593 (0.1454)	0.6981 (0.1852)
Long1	2	MGEPC	**2 (0)**	**1 (0)**	**0 (0)**
		MOCK	**2 (0)**	**1 (0)**	**0 (0)**
		VAMOSA	1.58 (0.62)	0.5843 (0.0936)	0.6774 (0.1321)
		GEP-Cluster	3.72 (0.42)	0.3810 (0.1320)	0.8762 (0.1566)
Ellipse	2	MGEPC	**2 (0)**	**0.7385 (0.2472)**	**0.4433 (0.2701)**
		MOCK	7.8 (0.31)	0.2357 (0.1041)	0.7387 (02092)
		VAMOSA	4.75 (0.83)	0.2221 (0.1134)	0.7116 (0.2287)
		GEP-Cluster	6.4 (0.79)	0.1954 (0.2569)	1.9766 (0.3743)
Iris	3	MGEPC	**3 (0)**	**0.7944 (0.0529)**	**0.4831 (0.0740)**
		MOCK	3.05 (0.15)	0.7287 (0.1382)	0.5944 (0.1827)
		VAMOSA	3.87 (0.99)	0.3105 (0.1633)	0.6331 (0.0772)
		GEP-Cluster	4.83 (1.36)	0.2604 (0.1352)	0.9512 (0.1445)
Glass	6	MGEPC	**6.18 (0.20)**	**0.2138 (0.0258)**	**1.1842 (0.0304)**
		MOCK	**6.18 (0.20)**	0.1677 (0.0245)	1.3408 (0.1914)
		VAMOSA	6.7 (3.13)	0.1458 (0.0863)	1.3345 (0.1925)
		GEP-Cluster	10.2 (4.36)	0.1079 (0.1592)	1.9252 (0.2179)
WBCD	2	MGEPC	**2.18 (0.40)**	**0.6897 (0.0751)**	**0.5252 (0.0451)**
		MOCK	2.87 (0.83)	0.5358 (0.1076)	0.6505 (0.0787)
		VAMOSA	3.27 (0.99)	0.3105 (0.1633)	0.6331 (0.0772)
		GEP-Cluster	4.63 (1.36)	0.2604 (0.1352)	0.9512 (0.1445)

4.4. Runtime

In the subsection, we provide the time complexity analysis of MGEPC. The basic operations and their worst case complexities are as follows:

(1) Initialization of MGEPC needs $O(N_P \cdot m)$ $O(N_p \cdot m)$ time, where N_p and m indicate the population size and the length of each chromosome, respectively.

(2) Fitness computation is composed of three steps: (a) Decoding of the chromosome requires $O(m)$ time; (b) Assigning each point to a cluster using point symmetry based distance, updating the centers and calculating the objective functions requires $O(k_{\max} N \log N)$ time [16], where N is the size of the data set. If the maximum number of loops of multi-objective k-means clustering is L_{iter} , the time complexity of fitness evaluation is $O(L_{iter} k_{\max} N \log N)$.

(3) The time complexity of the non-dominated sorting and the crowding-distance assignment are $O(N_P{}^2)$ and $O(N_P \log(2N_P))$, respectively [7].

(4) The time complexity of creation of the new parent population is $O(N_P \log(2N_P))$. If $N_P << N$, the total time complexity of MGEPC is $O(G_{\max} \times L_{iter} \times k_{\max} \times N \times \log N)$, where $G_{\max}$ is the maximum number of generations in MGEPC.

The time taken by MGEPC for all the data sets used for experiment is also reported here. For Square1, Square4, Sizes5, Long1, Ellipse, Iris, Glass, and WDBC, MGEPC takes 10min 16 s, 11min 41 s, 11min 41s, 13min 26s, 1min 56s, 20.6s, 32.5s and 3min 1s, respectively.

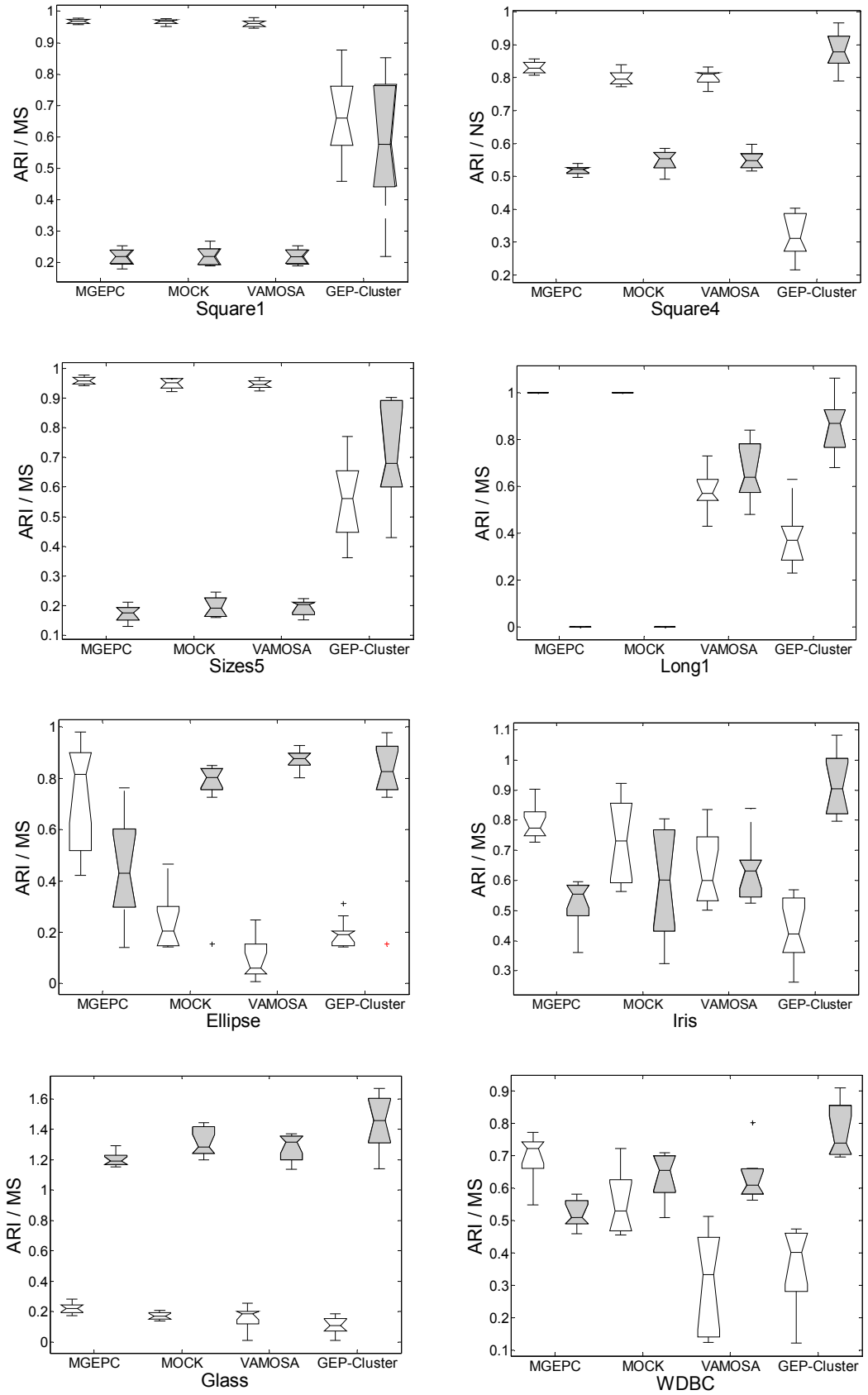


Figure 5. Boxplots showing the distribution of ARI values (with a white pattern) and MS values (with a grey pattern) for four clustering algorithms on eight data sets

5. Conclusion

In the paper, a multi-objective gene expression programming for clustering is proposed. The proposed algorithm could automatically determine the number of clusters and the appropriate partitioning from the data set. The proposed algorithm has some advantages as follows. First, the proposed algorithm extends the clustering algebraic operations used in gene expression programming to ensure all chromosomes evolved by the proposed algorithm are syntactically correct, which not only avoids using a huge amount of computational resources to edit illegal chromosomes, but also allows modification of the chromosome using nearly any genetic operator without restrictions. Second, the proposed algorithm presents a multi-objective k-means clustering as a local search, which performs fine-tuning of some rough partitions obtained by the global search, to speed up the convergence. Third, a power-law distribution based selection of new parent population is proposed, which could help maintain diversity in the population and avoid getting stuck at a local optimal or partial Pareto front. The performance of the proposed algorithm is compared with that of MOCK, VAMOSA and GEP-Cluster on five artificial and three real-life data sets. Experimental results verify the effectiveness of the proposed algorithm. In the future research work, we will investigate the effective method to select the best solution from a large number of non-dominated solutions in the final Pareto front of MGEPC.

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