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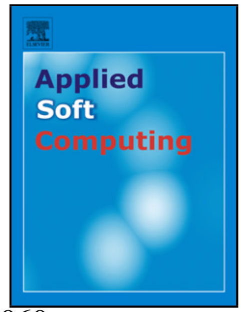

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Ant Colony Optimization based Clustering Methodology

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Highlights

- A novel ACO based methodology, ACO-C, is proposed for the spatial clustering problem with no a priori information on the number of clusters and the neighborhoods.
- ACO-C addresses several challenging issues of the clustering problem including solution evaluation, extraction of local properties, scalability and the clustering task itself.
- Two objective functions are proposed to quantify the quality of a clustering solution with arbitrary shaped clusters and different densities.
- ACO-C works in a multi-objective framework, and yields a set of non-dominated solutions.
- Experimental results show that ACO-C outperforms other competing approaches.

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Abstract

In this work we consider spatial clustering problem with no a priori information. The number of clusters is unknown, and clusters may have arbitrary shapes and density differences. The proposed clustering methodology addresses several challenges of the clustering problem including solution evaluation, neighborhood construction, and data

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set reduction. In this context, we first introduce two objective functions, namely adjusted compactness and relative separation. Each objective function evaluates the clustering solution with respect to the local characteristics of the neighborhoods. This allows us to measure the quality of a wide range of clustering solutions without a priori information. Next, using the two objective functions we present a novel clustering methodology based on Ant Colony Optimization (ACO-C). ACO-C works in a multi-objective setting and yields a set of non-dominated solutions. ACO-C has two pre-processing steps: neighborhood construction and data set reduction. The former extracts the local characteristics of data points, whereas the latter is used for scalability. We compare the proposed methodology with other clustering approaches. The experimental results indicate that ACO-C outperforms the competing approaches. The multi-objective evaluation mechanism relative to the neighborhoods enhances the extraction of the arbitrary-shaped clusters having density variations.

Keywords: Clustering, Ant Colony Optimization, Multiple objectives, Data set reduction.

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1. Introduction

Cluster analysis is the organization of a collection of data points into clusters based on similarity [1]. Clustering is usually considered as an unsupervised classification task. That is, the characteristics of the clusters and the number of clusters are not known a priori, and they are extracted during the clustering process. In this work we focus on spatial data sets in which a priori information about the data set (the number of clusters, shapes and densities of the clusters) is not available. Finding such clusters has applications in geographical information systems [2], computer graphics [3], and image segmentation [4]. In addition, clusters of spatial defect shapes provide valuable information about the potential problems in manufacturing processes of semiconductors [5, 6].

We consider spatial clustering as an optimization problem. Our aim is to obtain compact, connected and well-separated clusters. To the best of our knowledge, there is not a single objective function that works well for any kind of geometrical clustering structure. Therefore, we first introduce two solution evaluation mechanisms for measuring the quality of a clustering solution. The main idea behind both mechanisms is similar, and each mechanism is based on two objectives: adjusted compactness and relative separation. The first objective measures the compactness and connectivity of a clustering solution, and the second objective is a measure for separation. The difference between the two mechanisms is the degree of locality addressed in the calculations. The main advantage of these objectives is that the length of an edge is evaluated relatively, that is, it is scaled relative to the lengths of other edges within its neighborhood. This

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scaling permits us to evaluate the quality of the clustering solution independent of the shape and density of the clusters.

We implement the proposed solution evaluation mechanisms in a clustering framework based on Ant Colony Optimization (ACO). In order to find the target clusters, we use two complementary objective functions (adjusted compactness and relative separation) in a multiple-objective context. Hence, the output of ACO-C is a set of non-dominated solutions. Different from the literature, we are not interested in finding all non-dominated solutions or the entire Pareto efficient frontier. ACO-C has two pre-processing steps: neighborhood construction and data set reduction. Neighborhood construction extracts the local connectivity, proximity and density information inherent in the data set. Data set reduction helps reduce the storage requirements and processing time for the clustering task. Our experimental results indicate that ACO-C finds the arbitrary-shaped clusters with varying densities effectively, where the number of clusters is unknown.

Our contributions to the literature are as follows.

1. The proposed solution evaluation mechanisms allow us to quantify the quality of a clustering solution having arbitrary-shaped clusters with different densities in an optimization context. The use of these evaluation mechanisms is not restricted to ACO. They can be used in other metaheuristics and optimization-based clustering approaches.

2. The proposed ACO-based methodology introduces a general, unified framework for the spatial clustering problem without a priori information. It includes the solution evaluation mechanism, extraction of local properties, data set reduction, and the clustering task itself.

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3. ACO-C is a novel methodology for the clustering problem in which there is no a priori information, that is,

- the number of clusters is unknown,
- clusters may have arbitrary shapes,
- there may be density variations within the clusters, and
- different clusters may have density differences.

We provide the related literature in Section 2. Section 3 introduces the solution evaluation mechanisms. The details of ACO-C are explained in Section 4. Section 5 is about the empirical performance of ACO-C. First, we set the algorithm parameters using a full factorial design. Then, we compare ACO-C with some well-known algorithms. Finally, we conclude in Section 6.

2. Related Literature

The clustering algorithms can be classified into partitional, hierarchical, density-based algorithms, and metaheuristics (simulated annealing, tabu search, evolutionary algorithms, particle swarm optimization, ACO, and so on). [1], [7] and [8] provide comprehensive reviews of clustering approaches.

In this section, we present the related literature on the solution evaluation mechanisms and ant-based clustering algorithms.

2.1. Solution Evaluation Mechanisms

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A good clustering solution has compact and connected clusters that are well-separated from each other. However, quantifying and measuring the clustering objectives (compactness, connectivity and separation) for a data set is not a trivial task. We review the solution evaluation mechanisms in the literature under four categories: partitional approaches, graph-based approaches, clustering validity indices, and multi-objective approaches.

Partitional approaches consider objective functions such as minimization of total variance/distance between all pairs of data points, or minimization of total variance/distance between data points and a cluster representative such as *k*-means [9, 10] or *k*-medoids [11]. In these approaches, the number of clusters needs to be given as input, and the resulting clusters have spherical or ellipsoid shapes in general.

In order to handle the data sets with arbitrary-shaped clusters and density variations, graph-based approaches are proposed. Objective functions used are minimization of the maximum edge length in a cluster, maximization of the minimum/maximum/average distance between two clusters, and so on [12, 13]. A typical complication for such objective functions is illustrated in Figure 1(a). In Figure 1(a) the maximum edge length within the spiral clusters is larger than the distance between these two clusters. In this case elimination of the longest edge causes division of the spiral clusters.

Another research stream in solution evaluation makes use of cluster validity indices. Validity indices are used to quantify the quality of a clustering solution and to determine the number of clusters in a data set [14, 15]. In an effort to find the target clusters, some researchers use validity indices as objective functions in genetic algorithms [16, 17, 18, 19, 20, 21]. However, most of the validity indices assume a

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certain geometrical structure in the cluster shapes. When a data set includes several different cluster structures, such as arbitrary shapes and density differences, these indices may fail. An example is provided in Figure 1(b). The clustering solutions generated by DBSCAN [22] are evaluated using Dunn index [23] with different *MinPts* settings (within a range of 1 to 15). The number of clusters found with each setting is shown, e.g. 30 clusters are found when *MinPts* is set to two. Dunn index measures the minimum separation to maximum compactness ratio, so a higher Dunn index implies better clustering. Although the highest Dunn index (0.31) is achieved for the solutions with two and four clusters, the target solution has three clusters with a Dunn index of 0.09. Hence, Dunn index is not a proper objective function for such a data set.

[24] evaluates the performance of three clustering algorithms, namely *k*-means, single-linkage, and simulated annealing (SA) by using four cluster validity indices, namely Davies-Bouldin index, Dunn index, Calinski-Harabasz index, and index I. Compared to other validity indices, index I is found to be more consistent and reliable in finding the correct number of clusters. However, the four cluster validity indices are limited to extracting spherical clusters only. To handle different geometrical shapes, [25] uses a point symmetry-based distance measure in a genetic algorithm. The algorithm has difficulty in handling asymmetric clusters and density differences within a cluster.

- Insert Figure 1 here. -

Since a single objective is often unsuitable to extract target clusters, multi-objective (MO) approaches are considered to optimize several objectives simultaneously. To the best of our knowledge, VIENNA [26] is the first multi-objective

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clustering algorithm, which is based on PESA [27]. It optimizes two objective functions, total intra-cluster variance and connectedness. However, the algorithm requires the target number of clusters. One of the well-known MO clustering algorithms is the multi-objective clustering with automatic *k*-determination (MOCK) [28]. MOCK is based on evolutionary algorithms, and uses compactness and connectedness as two complementary objective functions. It can detect the number of clusters in the data set. The output of the algorithm is a set of non-dominated clustering solutions. However, it is capable of finding well-separated clusters having hyperspherical shapes. Improvements in this algorithm and its applications have been investigated [29, 30]. [31] also considers the clustering problem in a multi-objective framework. They optimize Xie-Beni (XB) index [32] and *Sym*-index [21] simultaneously, and introduce a multi-objective SA algorithm. This work is also limited to finding symmetric clusters. [33] proposes several connectivity-based validity indices based on the relative neighborhood graph. In addition to *Sym*-index and index I, [34] uses one of the connectivity-based validity indices in [33] as the third objective. Adding this connectivity measure helps extraction of arbitrary shapes and asymmetric clusters.

There are additional solution approaches proposed for MO clustering such as differential evolution [35, 36], immune-inspired method [37], and particle swarm optimization [38]. In these studies clustering objectives are either cluster validity indices such as XB index, *Sym*-index and FCM index, or compactness-connectivity objectives as in [28].

To the best of our knowledge, [39] is the only study that applies ACO to MO clustering problem. In this algorithm, there are two ant colonies working in parallel. Each colony optimizes a single objective function, either compactness or connectedness.

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The number of clusters is required as input. In addition, they test the proposed algorithm using the Iris data set only.

2.2. ACO and Ant-based Clustering Algorithms

ACO was introduced by [40, 41, 42]. It is inspired from the behaviors of real ants. As ants search for food on the ground, they deposit a substance called pheromone on their paths. The concentration of the pheromone on the paths helps direct the colony to the food sources. Ant colony finds the food sources effectively by interacting with the environment. Solution representation, solution construction and pheromone update mechanisms are the main design choices of ACO.

In the clustering literature, several ant-based clustering algorithms have been proposed. For a comprehensive review about ant-based and swarm-based clustering one can refer to [43]. In this study, we categorize the related studies into three: ACO-based approaches, approaches that mimic ants' gathering/sorting activities, and other ant-based approaches.

ACO-based approaches [44, 45, 46, 47, 48, 49, 50, 51, 52] are built upon the work of [42]. In these studies the total intra-cluster variance/distance is considered as the objective function, and the number of clusters is required a priori. An ant constructs a solution by assigning a data point to a cluster. The desirability of assigning a data point to a cluster is represented by the amount of pheromone. Ants update the pheromone in an amount proportional to the objective function value of the solution they generate. The proposed algorithms are capable of finding the clusters with spherical and compact shapes. There are also hybrid algorithms using ACO [53, 54, 55]. For instance, [53]

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modifies the *k*-means algorithm by adding a probabilistic centroid assignment procedure. [54] introduces a hybridization of ACO and particle swarm optimization (PSO). In this approach, PSO helps optimize continuous variables, whereas ACO directs the search to promising regions using the pheromone values. Another hybrid algorithm that combines *k*-means, ACO and PSO is [55]. In [55] the cluster centers obtained by ACO and PSO are used to initialize *k*-means. In these hybrid studies the number of clusters is required as input, and the resulting clusters are compact and spherical.

The approaches that mimic ants' gathering/sorting activities [56] form another research stream. ACO uses an explicit objective function whereas these approaches have an implicit objective function, and clusters emerge as the result of the gathering/sorting activities. An ant picks up a point in the space and drops it off near the points that are similar to it. These picking up and dropping off operations are performed using the probabilities that are calculated based on the similarity of the points in the neighborhood. Hence, ants work as if they are forming a topographic map. After forming this pseudo-topographic map, a cluster retrieval operation is applied to find the final clusters. [57] generalizes this method for exploratory data analysis. [58, 59, 60, 61, 62, 63, 64, 65] are the extensions and modifications of the algorithms proposed by [55, 56]. For instance, [60] uses parallel and independent ant colonies aggregated by a hypergraph model. In [65] the local similarity of a point is measured by entropy rather than distance.

Other ant-based approaches use the emergent behavior of the ants. [66] introduces a hierarchical ant-based algorithm to build a decision tree. Ants move a data point close to the similar points and away from the dissimilar ones on the decision tree. In [67, 68] ants generate tours by inserting edges between data points. Pheromone is

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updated for each edge connecting a pair of points. The closer the distance between two points, the larger the amount of pheromone released. In the first phase of the algorithm, the edges between similar points become denser in terms of pheromone concentration. The next phase is the cluster retrieval process by using a hierarchical clustering algorithm. [69] introduces a clustering approach based on aggregation pheromone. Aggregation pheromone leads the data points to accumulate around the points with higher pheromone density. In order to obtain the desired number of clusters, merging operations are performed using the average-linkage agglomerative hierarchical clustering algorithm. Another ant-based clustering algorithm is the chaotic ant swarm optimization proposed by [70]. It combines the chaotic behavior of a single ant and self-organizing behavior of the ant colony. Given the number of clusters, the proposed approach optimizes the total intra-cluster variation. Although it provides some improvement over PSO and *k*-means, the resulting clusters are still spherical.

3. How to Evaluate a Clustering Solution?

Our aim is to obtain compact, connected and well-separated clusters. For this purpose, we introduce two solution evaluation mechanisms: Clustering Evaluation Relative to Neighborhood (CERN) and Weighted Clustering Evaluation Relative to Neighborhood (WCERN).

3.1. Clustering Evaluation Relative to Neighborhood (CERN)

Adjusted Compactness: This objective is built upon the trade-off between the connectivity and relative compactness.

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a) Connectivity: Basically, connectivity is the degree to which neighboring data points are placed in the same cluster [26, 28]. Then, we first need to define the neighborhood of a point. There are several neighborhood construction algorithms such as k-nearest neighbors (KNN), ε-neighborhood [22], NC algorithm [71], and so on. When there are arbitrary-shaped clusters with density differences, NC outperforms KNN and ε-neighborhood. It provides a unique neighborhood for each data point. NC also generates subclusters (closures), which are formed by merging the data points having common neighbors. These closures can be used as the basis of a clustering solution. For these reasons, we use the NC algorithm to determine the neighborhoods of individual data points.

Let C_m and Cl_p be the sets of points in cluster *m* and closure *p*, respectively. Connectivity of cluster *m* with respect to closure *p* is $connect_{mp} = \left|C_m \cap Cl_p\right| / \left|Cl_p\right|$ if $C_m \cap Cl_p \neq \varnothing$. In the ideal case, connectivity takes a value of one, which means that cluster *m* and closure *p* fully overlap. The connectivity of cluster *m* is calculated as $connect_m = \prod_{p=1}^{nc} connect_{mp}$, where *nc* is the total number of closures. In this calculation, if $C_m \cap Cl_p = \varnothing$, then closure *p* is part of a cluster other than *m*, and, in this case, we take $connect_{mp} = 1$ so that the value of $connect_m$ is not affected by such unrelated closure and cluster pairs. Merging multiple closures that are in the same cluster results in a connectivity value of one, whereas it is less than one when there are divided clusters.

b) Relative compactness: We define the relative compactness of cluster *m* as the most inconsistent edge within its neighborhood. In relative compactness calculation we consider the edges in the minimum spanning tree (MST) of a cluster. MST is a graph in

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which the sum of the edge lengths is the minimum, and the graph is connected with no cycles. These two properties together allow us to define compactness of a cluster in an efficient way. Then, we compare each edge in the MST with the edges in the neighborhood. More formally, relative compactness of cluster m is

$$r\_comp\_c_m = \max_{(i,j)\in \mathrm{MST}_m} \left\{ \frac{d_{ij}}{\max\limits_{\substack{(k,l)\in \mathrm{MST}_{m(i)} \\ \text{or} \\ (k,l)\in \mathrm{MST}_{m(j)}}} \{d_{kl}\}} \right\}$$

where (i,j) is the edge between points i and j, d_{ij} is the Euclidean distance between points i and j, MST_m and $\mathrm{MST}_{m(i)}$ are the sets of edges in the MST of the points in cluster m and in the neighborhood of point i in cluster m, respectively.

When the number of clusters increases, relative compactness improves (decreases) whereas the connectivity deteriorates (decreases). Combining connectivity and compactness, adjusted compactness of cluster m is obtained as $comp_m = \frac{r\_comp\_c_m}{connect_m}$. The overall compactness of a clustering solution is found as $\max_m \{comp_m\}$.

Relative Separation: A good clustering solution must have well-separated clusters. We define the relative separation based on the local properties of clusters. Let the nearest cluster to cluster m be n such that $(m(i^*), n(j^*)) = \mathrm{argmin}\{d_{ij} : i \in \mathrm{C}_m, j \in \mathrm{C}_n, m \neq n\}$. The relative separation of cluster m is

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$$r\_sep\_c_m = \begin{cases} \min\left\{ \dfrac{d_{m(i^*),n(j^*)}}{\max\limits_{\substack{(k,l)\in \mathrm{MST}_{m(i^*)} \text{ if } |C_m|>1 \\ \text{or} \\ (k,l)\in \mathrm{MST}_{n(j^*)} \text{ if } |C_n|>1}} \{d_{kl}\}} \right\}, & \text{if } |C_m|>1 \text{ or } |C_n|>1 \\ 1, & \text{otherwise.} \end{cases}$$

The overall separation of a clustering solution is $\min\limits_{m} \{r\_sep\_c_m\}$. CERN minimizes the adjusted compactness and maximizes the relative separation.

3.2. Weighted Clustering Evaluation Relative to Neighborhood (WCERN)

WCERN is similar to CERN; both compactness and separation are calculated relative to the neighborhoods. The only difference between CERN and WCERN is that the edge lengths are used as a weight factor in compactness and separation calculations in WCERN. Hence, relative compactness and relative separation of cluster *m* are calculated as $r\_comp\_w_m = \max\limits_{(i,j)\in \mathrm{MST}_m} \left\{ \dfrac{d_{ij}^2}{\max\limits_{\substack{(k,l)\in \mathrm{MST}_{m(i)} \\ \text{or} \\ (k,l)\in \mathrm{MST}_{m(j)}}} \{d_{kl}\}} \right\}$ and

$$r\_sep\_w_m = \begin{cases} \min\left\{ \dfrac{d^2_{m(i^*),n(j^*)}}{\max\limits_{\substack{(k,l)\in \mathrm{MST}_{m(i^*)} \text{ if } |C_m|>1 \\ \text{or} \\ (k,l)\in \mathrm{MST}_{n(j^*)} \text{ if } |C_n|>1}} \{d_{kl}\}} \right\}, & \text{if } |C_m|>1 \text{ or } |C_n|>1 \\ d_{m(i^*),n(j^*)}, & \text{otherwise.} \end{cases}$$

Similar to CERN, WCERN minimizes the adjusted compactness, and maximizes the relative separation.

4. The ACO-based Clustering (ACO-C) Methodology

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ACO-C is a clustering methodology in a multi-objective framework. It has two pre-processing steps: neighborhood construction and data set reduction. Neighborhood construction helps extract the local information inherent in the data set. This local information is used in the solution evaluation. Data set reduction ensures the scalability of the approach.

In ACO-C an ant is a search agent. Ants construct tours by inserting edges between pairs of data points. Connected points in a tour form a cluster. During edge insertion each point is connected to exactly two points. This makes it easier to extract arbitrary-shaped clusters and reduces computational requirements.

The outline of the ACO-C methodology is presented in Figure 2 where *max_iter* and *no_ants* denote the maximum number of iterations and the number of ants, respectively.

- Insert Figure 2 here. -

Step 0. Pre-processing

Neighborhood Construction

We construct the neighborhood of each data point and obtain closures (subclusters) using the NC algorithm [71]. NC closures have two properties: 1) A closure is either a cluster itself or a subset of a cluster (divided cluster). 2) There may be an outlier mix on the boundary of a closure. Hence, we focus on the merging operations and outlier detection in the clustering. In order to allow outlier detection and closure merging, we extend NC neighborhoods with *distant neighbors* and *nowhere*. *Distant neighbors* are the nearest pair of data points between two adjacent closures. *Nowhere* is

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a dummy point used for outlier detection. If a data point is connected to nowhere twice, then it is classified as an outlier. If a data point is connected to nowhere once, then it is the start/end point of a cluster. An example for neighborhood definition is provided in Figure 3. Points *j*, *k*, *l*, *m* and *n* are neighbors of point *i* generated by NC, and point *p* is the distant neighbor of point *i*. Neighborhood of point *i* is extended by point *p* and nowhere. Note that not every point has a distant neighbor.

- Insert Figure 3 here. -

Data Set Reduction via Boundary Formation

The interior points of a closure are already connected, hence it is sufficient to consider only the points on the boundaries of the closures for merging and outlier detection. Exclusion of interior points in a closure decreases the number of points in a data set and contributes to the scalability of ACO-C. We use the boundary extraction algorithm in [72].

Step 1. Initialization of parameters

The parameters of ACO-C, including the number of ants (*no_ants*), the number of maximum iterations (*max_iter*), and the evaporation rate (ρ) are initialized. We conduct a factorial design in Section 5 to determine the values of these parameters.

Step 2. Solution construction

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When an ant starts clustering, the set of unvisited points, D_o, is initialized as the entire data set, D. For each point in the data set, the set of currently available neighbors, NCS_i, is initialized as the set of its neighbors, NS_i. The current number of clusters (m) is set to one. There are two substeps in solution construction: point selection and edge insertion.

Point selection: Every time an ant starts a new tour, a new cluster is formed. When a new cluster, C_m, is initialized, a point, say point i, is selected at random from the set of unvisited points, D_o. Then, the related sets are updated as $C_m = C_m \cup \{i\}$, $D_o = D_o / \{i\}$, and $NCS_k = NCS_k / \{i\}$ for $\forall k \in D_o$. If NCS_i is non-empty or point i is not nowhere, we continue with edge insertion. Otherwise, the construction of the current cluster is finished, and a new cluster is initialized by incrementing the cluster index, m, by 1.

Edge insertion: An ant inserts an edge between point i and a point selected from NCS_i. The pheromone concentration on edge (i,j), τ_{ij}, represents the tendency of edge (i,j) to occur in a cluster. Hence, the probability of selecting edge (i,j) is calculated as $p_{ij} = \frac{\tau_{ij}}{\sum_{k \in NCS_i} \tau_{ik}}$ for $\forall j \in NCS_i$. Then, the ant continues edge insertion starting from point j. The initial pheromone concentration is inversely proportional to the evaporation rate, $\tau_{ij} = \frac{1}{\rho}$ for $\forall i \in D$, $j \in NS_i$.

Point selection and edge insertion substeps are repeated until D_o is empty. The details of Step 2 are presented in Figure 4.

- Insert Figure 4 here. -

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Step 3. Solution evaluation

The performance of a clustering solution is evaluated using CERN and WCERN as described in Section 3.

Step 4. Local search

In order to strengthen the exploitation property of ACO-C we apply local search to each clustering solution constructed. Conditional merging operations are performed in the local search. Let clusters *m* and *n* are adjacent clusters considered for merging, and let *comp* and *sep* be the adjusted compactness and relative separation of the current clustering solution, respectively. The adjusted compactness and relative separation after merging are *comp'* and *sep'*, respectively. If *comp'* ≤ *comp* and *sep'* ≥ *sep*, clusters *m* and *n* are merged. The clustering solutions at the end of the local search form the set of solutions constructed by the ants (SC) in the current iteration.

Step 5. Pheromone update

Pheromone update is performed for each solution component (edge) so that the effect of the solution component is well-reflected in the pheromone concentration.

There are two important properties about our clustering problem: 1) We are interested in arbitrary-shaped clusters with different densities, so reflecting the local density, connectivity and proximity relations are crucial in finding the target clusters. 2) We use adjusted compactness and relative separation as two complementary objective functions. Hence, we use the following pheromone update mechanism. For each data point *i*, the incumbent (minimum) adjusted compactness obtained so far for point *i*,

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inc_comp$_i$, and the incumbent (maximum) relative separation obtained so far for point *i*, *inc_sep*$_i$, are kept in the memory. We check whether or not the adjusted compactness and relative separation of the cluster to which edge (*i*,*j*) belongs are better than the corresponding incumbent values. More pheromone is released if an incumbent improves.

For all the edges in the clustering solution, E, the amount of pheromone released is proportional to the amount of improvement in the incumbents. The initial incumbent adjusted compactness and relative separation for each point are taken from the closures of the NC algorithm. Formally, the pheromone values are updated as

$$\tau_{ij} = (1-\rho)\tau_{ij} + \rho w_{ij}\tau_{ij} \quad \forall i \in \mathrm{D}, j \in \mathrm{NS}_i,$$

where

$$w_{ij} = \begin{cases} \dfrac{\min\{inc\_comp_i, inc\_comp_j\}}{comp_{(i,j)}} + \dfrac{sep_{(i,j)}}{\max\{inc\_sep_i, inc\_sep_j\}}, & \text{if } (i,j) \in \mathrm{E} \\ 0, & \text{otherwise.} \end{cases}$$

Step 6. Non-dominated set update

Let $s1$ and $s2$ be two clustering solutions generated by the ants. The aim is to minimize the maximum adjusted compactness and to maximize the minimum relative separation.

Definition 1: Solution $s1$ *dominates* solution $s2$ if

i) $comp_{s1} < comp_{s2}$ and $sep_{s1} \geq sep_{s2}$, or

ii) $comp_{s1} \leq comp_{s2}$ and $sep_{s1} > sep_{s2}$.

Definition 2: If there does not exist any other clustering solutions dominating solution $s1$, then solution $s1$ is called a *non-dominated* solution.

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We update the current set of non-dominated solutions (SN) at the end of each iteration using Definitions 1 and 2. We also update the incumbent compactness and separation (inc_comp_i and inc_sep_i) for the data set.

If the maximum number of iterations is not exceeded, Steps 2-6 are repeated. Otherwise, ACO-C terminates with the non-dominated solutions in set SN.

5. Experimental Results for the ACO-C Methodology

In this section, we test the performance of ACO-C empirically. First, we present the test data sets and the performance evaluation criteria. Second, using some pilot data sets, we conduct a full factorial experiment in order to set the ACO-C parameters. Third, we elaborate on the impact of data set reduction. Finally, we compare the performance of ACO-C with other clustering algorithms.

The algorithm was coded in Matlab 7.9 and run on a PC with Intel Core2 Duo 2.33 GHz processor and 2 GB RAM.

5.1. Data Sets and Performance Evaluation Criteria

We tested ACO-C using 32 data sets compiled from several sources [73, 74, 75]. These include 2- and higher dimensional data sets with various shapes of clusters (circular, elongated, spiral, etc.), intra-cluster and inter-cluster density variations, and outliers. Some example data sets are presented in Figure 5.

We evaluated the accuracy of the clustering solution using Jaccard index (JI) and Rand index (RI). We define these measures as follows.

a: the number of point pairs that belong to the same target cluster and are assigned to the same cluster in the solution.

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b: the number of point pairs that belong to the same target cluster but are assigned to different clusters in the solution.

c: the number of point pairs that belong to different target clusters but are assigned to the same cluster in the solution.

d: the number of point pairs that belong to different target clusters and are assigned to different clusters in the solution.

- Insert Figure 5 here. -

$$\mathrm{JI} = \frac{a}{a+b+c} \tag{1}$$

$$\mathrm{RI} = \frac{a+d}{a+b+c+d} \tag{2}$$

JI is one of the well-known external clustering validity indices. It takes values between zero and one, one indicating the target clustering is achieved. RI is also known as the simple matching coefficient. While JI focuses on point pairs correctly assigned to the same cluster, RI also takes into account the point pairs correctly assigned to different clusters. Both indices penalize the division of clusters as well as mixing them. We report the maximum JI and RI values in the set of non-dominated solutions.

5.2. Parameter Settings for ACO-C

The three parameters of ACO-C are *no_ants*, *max_iter*, and ρ. We set *max_iter* to twice the number of points in the data set, and recorded the iteration number in which the target clustering was found. We used a full factorial experimental design in order to

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determine the best settings for *no_ants* and ρ. We also studied the impact of the solution evaluation function (EF) on the performance of ACO-C. The three factors used in the experimental design and their levels are presented in Table 1. We conducted the full factorial experiment using a subset of 15 data sets. These 15 data sets were selected to represent different properties of all data sets.

- Insert Table 1 here. –

Before discussing the full factorial design results, we present the ACO-C results for the example data set given in Figure 5(d). The three non-dominated clustering solutions found by ACO-C are presented in Figure 6. These solutions include the target clustering with a JI value of one. The resulting non-dominated solutions can be interpreted as clustering of points in different resolutions.

We also checked the convergence of ACO-C in the example data set. In Figure 7 the set of non-dominated solutions stays the same after iteration number 70. This implies that convergence is achieved.

The main effect plots for the maximum RI and execution time are presented in Figure 8. The low setting of the evaporation rate slows the convergence down and prevents ACO-C from missing the target solutions. However, the time spent in ACO-C increases three times with this setting. Increasing the number of ants used in ACO-C provides a slight improvement in the maximum RI in return for increase in the time. Considering the trade-offs between the performance and time, the experiments are performed with the parameter settings $\rho = 0.01$ and *no_ants* = 5.

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In Figures 8(a) and 8(b) WCERN performs better than CERN in terms of the maximum RI and time. On the other hand, only CERN finds the target clustering in some data sets, i.e. data sets in Figures 5(d) and 5(e). Hence, CERN ensures finding the target clustering that is visible in low resolution. WCERN is more powerful in extracting clusters that are visible in higher resolution such as data sets in Figures 5(f) and 5(h). CERN and WCERN complement each other in finding the target clusters, so we run ACO-C using both evaluation mechanisms. We consider the union of the non-dominated solutions obtained by both as the final solution set.

Note that there is no significant interaction among the factors.

- Insert Figure 6 here. -

- Insert Figure 7 here. -

- Insert Figure 8 here. -

5.3. Data Set Reduction

We tested the impact of data set reduction using 32 data sets. The boundary extraction algorithms in [72] were used for data set reduction. The number of points in the original data set was compared with the number of points after reduction.

Table 2 shows the data set reduction percentages for 2- and higher dimensional data sets. The reduction percentages vary depending on the shape of the clusters. The highest data set reduction percentages are achieved when clusters are convex, as in

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Figures 5(f) and 5(h). When there are non-convex clusters as in Figure 5(g), the reduction percentages are lower.

In Section 5.4 clustering is performed on the data sets after the reduction.

- Insert Table 2 here. -

5.4. Comparison of the ACO-C Methodology with Others

The performance of ACO-C is compared with the results of *k*-means, single-linkage, DBSCAN, NC closures, and NOM [76]. In our comparisons *k*-means represents the partitional clustering algorithms, and single-linkage the hierarchical clustering algorithms. DBSCAN is selected as a representative of the density-based clustering algorithms. The number of clusters is an input for *k*-means and single-linkage, therefore we run *k*-means and single-linkage for several values of the number of clusters. This number varies between 2-10% of the number of points in the data set with increments of 1, and the one with the best JI value is selected for each algorithm. In the same manner, for DBSCAN, among several *MinPts* settings the one with the best JI value is selected for comparison. NOM is a graph theoretical clustering algorithm. It also uses the neighborhoods constructed by the NC algorithm, hence we can elaborate on the impact of ACO-C better. For ACO-C, we consider the union of the non-dominated solutions obtained with CERN and WCERN settings, and the sum of the execution times with CERN and WCERN is considered as the execution time of ACO-C.

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The results for 32 data sets are summarized in Table 3. ACO-C finds the target clusters in 29 data sets out of 32. Single-linkage and NOM follow ACO-C with 24 and 18 data sets, respectively. ACO-C has the best average JI and RI values, followed by NOM, NC, DBSCAN and single-linkage. This indicates that ACO-C is able to form clusters that are close to the target clusters on the average. Moreover, the standard deviations of JI and RI are the smallest, and the minimum values of JI and RI are the highest for ACO-C. This indicates that even in the worst case ACO-C performs better than the competing approaches.

Typically, ACO-C has difficulty in detecting target clusters when there is noise, as for the data set in Figure 5(g). The relative solution evaluation mechanisms of both CERN and WCERN are sensitive to density and distance changes, so these points are labeled as separate clusters. Although ACO-C yields the general structure of the target clusters in such data sets, it forms clusters by enclosing the noise as well.

- Insert Table 3 here. -

The number of non-dominated solutions generated by CERN and WCERN varies between 1 to 6 for different data sets. Hence, the size of the non-dominated sets is reasonable for practical use.

The main limitation of ACO-C is the longer execution times compared to *k*-means, single-linkage and DBSCAN, partly due to the Matlab implementation. In this respect, improvements are required.

6. Conclusion

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In this work we consider the spatial clustering problem with no a priori information on the data set. The clusters may include arbitrary shapes, and there may be density differences within and between the clusters. Moreover, the number of clusters is unknown. We present a novel ACO-based clustering methodology, namely ACO-C. In ACO-C we combine the connectivity, proximity, density and distance information with the exploration and exploitation capabilities of ACO in a multi-objective framework. The proposed clustering methodology is capable of handling several challenging issues of the clustering problem including solution evaluation, extraction of local properties, scalability and the clustering task itself. The performance of ACO-C is tested using a variety of data sets. The experimental results indicate that ACO-C outperforms other competing approaches in terms of the validity indices JI and RI. In particular, the multi-objective framework and the solution evaluation relative to the neighborhoods enhance the algorithm in extracting arbitrary-shaped clusters, handling density variations, and finding the correct number of clusters. ACO-C achieves a reasonable number of non-dominated solutions for practical use.

The proposed methodology can generate non-dominated clustering solutions, which include the target clustering most of the time. These solutions represent alternative clustering patterns having different levels of resolution. Solutions with different resolutions allow the decision maker to analyze the trade-offs between the merging and division operations. A future research direction can be to find all the non-dominated clustering solutions in different resolutions, i.e. the Pareto efficient frontier.

ACO-C typically has problems with detection of the noise. Also, its execution times are relatively longer. The proposed approach can be improved in both areas.

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References

[1] Jain, A.K., Murty, M.N., and Flynn, P.J., 1999. Data clustering: A review. ACM Computing Surveys. 31 (3), 264–323.

[2] Alani, H., Jones, C.B., and Tudhope, D., 2001. Voronoi-based region approximation for geographical information retrieval with gazetteers. International Journal of Geographical Information Science, 15 (4), 287-306.

[3] Pfister, H., and Gross, M., 2004. Point-based computer graphics. IEEE Computer Graphics and Applications, 24 (4), 22-23.

[4] Freixenet, J., Muñoz, X., Raba, D., Martí, J., and Cufí, X., 2002. Yet another survey on image segmentation: Region and boundary information integration. Lecture Notes in Computer Science, 2352/2002, 21-25, DOI: 10.1007/3-540-47977-5_27.

[5] Yuan, T., and Kuo, W., 2007. A model-based clustering approach to the recognition of the spatial defect patterns produced semiconductor fabrication. IIE Transactions, 40 (2), 93-101.

[6] Wang, C.H., Kuo, W., and Bensmail, H., 2006. Detection and classification of defect patterns on semiconductor wafers. IIE Transactions, 39, 1059-1068.

[7] Xu, R., and Wunsch, D., 2005. Survey of clustering algorithms. IEEE Transactions on Neural Networks. 16 (3), 645-678.

[8] Berkhin, P., 2006. A survey of clustering data mining techniques. In Kogan, J., Nicholas, C., and Teboulle M., editors, Grouping Multidimensional Data: Recent Advances in Clustering, 25-71. Springer, Berlin.

[9] MacQueen, J.B., 1967. Some methods for classification and analysis of multivariate observations. In: Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability. Berkeley, 281-297.

Accepted Manuscript

ACCEPTED MANUSCRIPT

[10] Hartigan, J.A., and Wong, M.A., 1979. Algorithm AS 136: A *k*-means clustering algorithm. Journal of the Royal Statistical Society. Series C (Applied Statistics). 28 (1), 100-108.

[11] Kaufman, L., and Rousseeuw, P.J., 1990. Finding groups in data: An introduction to cluster analysis. John Wiley & Sons.

[12] Zahn, C.T., 1971. Graph-theoretical methods for detecting and describing gestalt clusters. IEEE Transactions on Computers. C-20 (1), 68-86.

[13] Jain, A.K., and Dubes, R.C., 1988. Algorithms for clustering data. Prentice-Hall advanced reference series. Prentice-Hall Inc., Upper Saddle River, NJ.

[14] Halkidi, M., Batistakis, Y., and Vazirgiannis, M., 2002. Cluster validity methods: Part I. ACM SIGMOD Record. 31 (2), 40-45.

[15] Halkidi, M., Batistakis, Y., and Vazirgiannis, M., 2002. Cluster validity methods: Part II. ACM SIGMOD Record. 31 (3), 19-27.

[16] Bandyopadhyay, S., and Maulik, U., 2001. Nonparametric genetic clustering: Comparison of validity indices. IEEE Transactions on Systems, Man, and Cybernetics – Part C: Applications and Reviews. 31 (1), 120-125.

[17] Bandyopadhyay, S., and Maulik, U., 2002. Genetic clustering for automatic evolution of clusters and application to image classification. Pattern Recognition. 35, 1197–1208.

[18] Hruschka, E.R., and Ebecken, N.F.F., 2003. A genetic algorithm for cluster analysis. Intelligent Data Analysis. 7, 15–25.

[19] Sheng, W., Swift, S., Zhang, L., and Liu, X., 2005. A weighted sum validity function for clustering with a hybrid niching genetic algorithm. IEEE Transactions on Systems, Man, and Cybernetics – Part B: Cybernetics. 35 (6), 1156-1167.

Accepted Manuscript

ACCEPTED MANUSCRIPT

[20] Bandyopadhyay, S., and Saha, S., 2007. GAPS: A clustering method using a new point symmetry-based distance measure. Pattern Recognition. 40, 3430-3451.

[21] Bandyopadhyay, S., and Saha, S., 2008. A point symmetry-based clustering technique for automatic evolution of clusters. IEEE Transactions on Knowledge and Data Engineering. 20 (11), 1441-1457.

[22] Ester, M., Kriegel, K.P., Sander, J., and Xu, X., 1996. A density-based algorithm for discovering clusters in large spatial databases with noise. In: Proceedings of the Second International Conference on Knowledge Discovery and Data Mining, Portland, Oregon, 226-231.

[23] Dunn, J.C., 1974. Well-separated clusters and optimal fuzzy partitions. Journal of Cybernetics. 4 (1), 95-104.

[24] Maulik, U., and Bandyopadhyay, S., 2002. Performance evaluation of some clustering algorithms and validity indices. IEEE Transactions on Pattern Analysis and Machine Intelligence, 24 (12), 1650-1654.

[25] Bandyopadhyay, S., Maulik, U., and Mukhopadhyay, A., 2007. Multi-objective genetic clustering for pixel classification in remote sensing imagery. IEEE Transactions on Geoscience and Remote Sensing, 45 (5), 1506-1511.

[26] Handl, J., and Knowles, J., 2004. Evolutionary multi-objective clustering. In: Proceedings of 8th International Conference on Parallel Problem Solving From Nature. 1081–1091.

[27] Corne, D.W., Jerram, N.R., Knowles, J.D., and Oates, M.J., 2001. PESA-II: Region-based selection in evolutionary multi-objective optimization. In: Proceedings of Genetic Evolutionary Computation Conference, 283–290.

[28] Handl, J., and Knowles, J., 2007. An evolutionary approach to multi-objective

Accepted Manuscript

ACCEPTED MANUSCRIPT

clustering. IEEE Transactions on Evolutionary Computation. 11 (1), 56-76.

[29] Matake, N., Hiroyasu, T., Miki, M., and Senda, T., 2007. Multi-objective clustering with automatic k-determination for large-scale data. In: Proceedings of Genetic and Evolutionary Computation Conference, London, England, 2007.

[30] Tsai, C.-W., Chen W.-L., and Chiang, M.-G., 2012. A modified multi-objective EA-based clustering algorithm with automatic determination of the number of clusters. In: Proceedings of IEEE International Conference on Systems, Man, and Cybernetics. Doi: 10.1109/ICSMC.2012.6378178.

[31] Saha, S., and Bandyopadhyay, S., 2010. A symmetry-based multi-objective clustering technique for automatic evolution of clusters. Pattern Recognition. 43, 738-751.

[32] Xie, X.L., and Beni, G., 1991. A validity measure for fuzzy clustering. IEEE Transactions on Pattern Analysis and Machine Intelligence. 13, 841-847.

[33] Saha, S., and Bandyopadhyay, S., 2012. Some connectivity-based cluster validity indices. Applied Soft Computing. 12, 1555–1565.

[34] Saha, S., and Bandyopadhyay, S., 2013. A generalized automatic clustering algorithm in a multi-objective framework. Applied Soft Computing. 13, 89-108.

[35] Das, S., Abraham, A., and Konar, A., 2009. Clustering using multi-objective differential evolution algorithms. Metaheuristic Clustering, Springer, 213–238.

[36] Suresh, K., Kundu, D., Ghosh, S., Das, S., and Abraham, A., 2009. Data clustering using multi-objective differential evolution algorithms. Fundamenta Informaticae. 97 (4), 381-403.

Accepted Manuscript

ACCEPTED MANUSCRIPT

[37] Gong, M., Zhang, L., Jiao, L., and Gou, S., 2007. Solving multi-objective clustering using an immune-inspired algorithm. In: Proceedings of IEEE Congress on Evolutionary Computation. Doi: 10.1109/CEC.2007.4424449.

[38] Paoli, A., Melgani, F., and Pasolli, E., 2009. Clustering of hyperspectral images based on multi-objective Particle Swarm Optimization. IEEE Transactions on Geoscience and Remote Sensing. 47 (12), 4175-4188.

[39] Santos, D.S., Oliveira, D.D., and Bazzan, A.L.C., 2009. A multiagent multi-objective clustering algorithm. Data Mining and Multi-agent Integration. Springer, 239-249.

[40] Dorigo, M., Maniezzo, V., and Colorni, A., 1991. Positive feedback as a search strategy. Technical report, 91-016, Politecnico di Milano, Dip. Elettronica.

[41] Dorigo, M., Maniezzo, V., and Colorni, A., 1996. Ant system: Optimization by a colony of cooperating agents. IEEE Transactions on Systems, Man, and Cybernetics - Part B. 26 (1), 29–41.

[42] Dorigo, M., Caro, G.D., and Gambardella, L.M., 1999. Ant algorithms for discrete optimization. Artificial Life. 5 (2), 137–172.

[43] Handl, J., and Meyer, B., 2007. Ant-based and swarm-based clustering. Swarm Intelligence. 1, 95–113.

[44] Liu, X., and Hu, F., 2010. An effective clustering algorithm with ant colony. Journal of Computers, 5(4), 598-605.

[45] Yong, W., and Peng-Cheng, W., 2009. Data clustering method based on ant swarm intelligence. In: Proceedings of IEEE International Conference on Computer Science and Information Technology. 358-361.

Accepted Manuscript

ACCEPTED MANUSCRIPT

[46] Chen, A.-P., and Chen, C.-C., 2006. A new efficient approach for data clustering in electronic library using ant colony clustering algorithm. The Electronic Library. 24 (4), 548-559.

[47] He, Y., Hui, S., and Sim, Y., 2006. A novel ant-based clustering approach for document clustering. Ng, H., Leong, M.-K., Kan, M.-Y., and Ji, D. (Eds.), Asia Information Retrieval Symposium, Springer, Singapore, 537–544.

[48] Kao, Y., and Fu, S.C., 2006. An ant-based clustering algorithm for manufacturing cell design. International Journal of Advanced Manufacturing Technology. 28, 1182–1189.

[49] Ho, C.K., and Ewe, H.T., 2005. A hybrid ant colony optimization approach (hACO) for constructing load-balanced clusters. In: Proceedings of the 2005 IEEE Congress on Evolutionary Computation. Doi: 10.1109/CEC.2005.1554942.

[50] Runkler, T.A., 2005. Ant colony optimization of clustering models. International Journal of Intelligent Systems. 20 (12), 1233-1251.

[51] Saatchi, S., and Hung, C.C., 2005. Hybridization of the ant colony optimization with the *k*-means algorithm for clustering. Lecture notes in computer science: Vol. 3540. Image analysis. Berlin: Springer. 511-520.

[52] Shelokar, P.S., Jayaraman, V.K., and Kulkarni, B.D., 2004. An ant colony approach for clustering. Analytica Chimica Acta. 509, 187–195.

[53] Kuo, R.J., Wang, H.S., Hu, T.-L., and Chou, S.H., 2005. Application of ant *k*-means on clustering analysis. Computers and Mathematics with Applications. 50, 1709-1724.

[54] Huang, C.L., Huang, W.-C., Chang, H.Y., Yeh, Y.-C., and Tsai, C.-Y., 2013. Hybridization strategies for continuous ant colony optimization and particle swarm optimization applied to data clustering. Applied Soft Computing. 13, 3864–3872.

Accepted Manuscript

ACCEPTED MANUSCRIPT

[55] Niknam, T., and Amiri, B., 2010. An efficient hybrid approach based on PSO, ACO and *k*-means for cluster analysis. Applied Soft Computing. 10 (1), 183-197.

[56] Deneubourg, J.-L., Goss, S., Franks, N., Sendova-Franks, A., and Detrain, C., 1991. The dynamics of collective sorting: robot-like ant and ant-like robot. In: Proceedings of the First Conference on Simulation of Adaptive Behavior: From Animals to Animats, MIT Press. 356–365.

[57] Lumer, E., and Faieta, B., 1994. Diversity and adaptation in populations of clustering ants. In: Proceedings of the Third International Conference on Simulation of Adaptive Behavior, Cambridge: MIT Press. 501–508.

[58] Boryczka, U., 2009. Finding groups in data: Cluster analysis with ants. Applied Soft Computing. 9, 61–70.

[59] Kao, Y., and Fu, S.C., 2006. An ant-based clustering algorithm for manufacturing cell design. International Journal of Advanced Manufacturing Technology. 28, 1182–1189.

[60] Yang, Y., and Kamel, M.S., 2006. An aggregated clustering approach using multi-ant colonies algorithms. Pattern Recognition. 39, 1278 – 1289.

[61] Handl, J., Knowles, J., and Dorigo, M., 2006. Ant-based clustering and topographic mapping. Artificial Life. 12, 35–61.

[62] Martin, M., Chopard, B., and Albuquerque, P., 2002. Formation of an ant cemetery: Swarm intelligence or statistical accident? Future Generation Computer Systems. 18, 951–959.

[63] Handl, J., and Meyer, B., 2002. Improved ant-based clustering and sorting in a document retrieval interface. Lecture notes in computer science. Vol: 2439. Parallel problem solving from nature, Berlin: Springer. 913–923.

Accepted Manuscript

ACCEPTED MANUSCRIPT

[64] Monmarché, N., Slimane, M., and Venturini, G., 1999. On improving clustering in numerical databases with artificial ants. Lecture notes in artificial intelligence: Vol. 1674. Advances in artificial life. Berlin: Springer. 626–635.

[65] Zhang, L., Cao, Q., and Lee, J., 2013. A novel ant-based clustering algorithm using Renyi entropy. Applied Soft Computing. 13 (5), 2643-2657.

[66] Azzag, H., Venturini, G., Oliver, A., and Guinot, C., 2007. A hierarchical ant-based clustering algorithm and its use in three real-world applications. European Journal of Operational Research. 179 (3), 906-922.

[67] Sinha, A.N., Das, N., and Sahoo, G., 2007. Ant colony based hybrid optimization for data clustering. Kybernetes. 36 (1/2), 175-191.

[68] Tsai, C.F., Tsai, C.W., Wu, H.C., and Yang, T., 2004. ACODF: A novel data clustering approach for data mining in large databases. Journal of Systems and Software. 73 (1), 133-145.

[69] Ghosh, A., Halder, A., Kothari, M., and Ghosh, S., 2008. Aggregation pheromone density-based data clustering. Information Sciences. 178, 2816–2831.

[70] Wan, M., Wang, C., Li, L., and Yang, Y., 2012. Chaotic ant swarm approach for data clustering. Applied Soft Computing. 12 (8), 2387-2393.

[71] İnkaya, T., Kayalıgil, S., and Özdemirel, N.E., 2013a. A neighborhood construction algorithm for the clustering problem. Technical Report. Middle East Technical University, Ankara, Turkey.

[72] İnkaya, T., Kayalıgil, S., and Özdemirel, N.E., 2013b. Extracting the non-convex boundary of a data set via Delaunay Triangulation. Technical Report. Middle East Technical University, Ankara, Turkey.

[73] Bache, K., and Lichman, M., 2013. UCI Machine Learning Repository

Accepted Manuscript

ACCEPTED MANUSCRIPT

[http://archive.ics.uci.edu/ml]. Irvine, CA: University of California, School of Information and Computer Science.

[74] Sourina, O., 2013. Current projects in the homepage of Olga Sourina. (http://www.ntu.edu.sg/home/eosourina/projects.html, last accessed on November 21, 2013).

[75] Iyigün, C., 2008. Probabilistic distance clustering. Ph.D. Dissertation. Rutgers University, New Brunswick, New Jersey.

[76] İnkaya, T., Kayalıgil, S., and Özdemirel, N.E., 2010. A new density-based clustering approach in graph theoretic context. IADIS International Journal on Computer Science and Information Systems. 5 (2), 117-135.

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Figure Captions

Figure 1. (a) Example data set. (b) Dunn index values for the clustering solutions generated by DBSCAN with different *MinPts* settings.

Figure 2. The outline of the ACO-C methodology.

Figure 3. An example for neighbors of point *i*.

Figure 4. The details of Step 2.

Figure 5. Example data sets: (a) train2, (b) data-c-cc-nu-n, (c) data-uc-cc-nu-n, (d) data-c-cv-nu-n, (e) data-uc-cv-nu-n, (f) data_circle, (g) train3, (h) data_circle_1_20_1_1, (i) iris (projected to 3-dimensional space), (j) letters.

Figure 6. Non-dominated clustering solutions for data-c-cv-nu-n, (a) Solution with six clusters (JI=1), (b) Solution with three clusters (JI=0.57), (c) Solution with two clusters (JI=0.54).

Figure 7. Convergence analysis for the example data set, data-c-cv-nu-n.

Figure 8. (a) Main effect plots for maximum RI, (b) Main effect plots for time.

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Table Captions

Table 1. Experimental factors in ACO-C.

Table 2. The percentages of data set reduction.

Table 3. Comparison of ACO-C with *k*-means, single-linkage, NC closures and NOM (32 data sets).

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Factors	Level 0	Level 1
evaluation function, EF	CERN	WCERN
evaporation rate, ρ	0.01	0.05
number of ants, *no_ants*	5	10

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	2-dimensional data sets	Higher dimensional data sets
average (%)	42.79	19.11
std. dev. (%)	20.42	12.41
min. (%)	1.52	4.90
max. (%)	74.29	53.84

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		k-means	Single-linkage	DBSCAN	NC	NOM	ACO-C
# of data sets TC is found		6	24	13	13	18	29
JI	average	0.71	0.91	0.91	0.93	0.96	0.99
	std.dev.	0.24	0.19	0.17	0.12	0.08	0.02
	min.	0.28	0.45	0.50	0.56	0.59	0.89
RI	average	0.84	0.94	0.95	0.96	0.98	0.99
	std.dev.	0.13	0.14	0.11	0.02	0.08	0.01
	min.	0.62	0.53	0.53	0.91	0.59	0.96
Time	average	0.44	4.76	1.29	27.34	235.31	1089.41
	std.dev.	0.60	8.47	2.01	71.29	511.85	823.81
	min.	0.05	0.38	0.03	0.05	0.07	2.09
	max.	2.19	32.60	7.45	318.46	1721.47	2916.20

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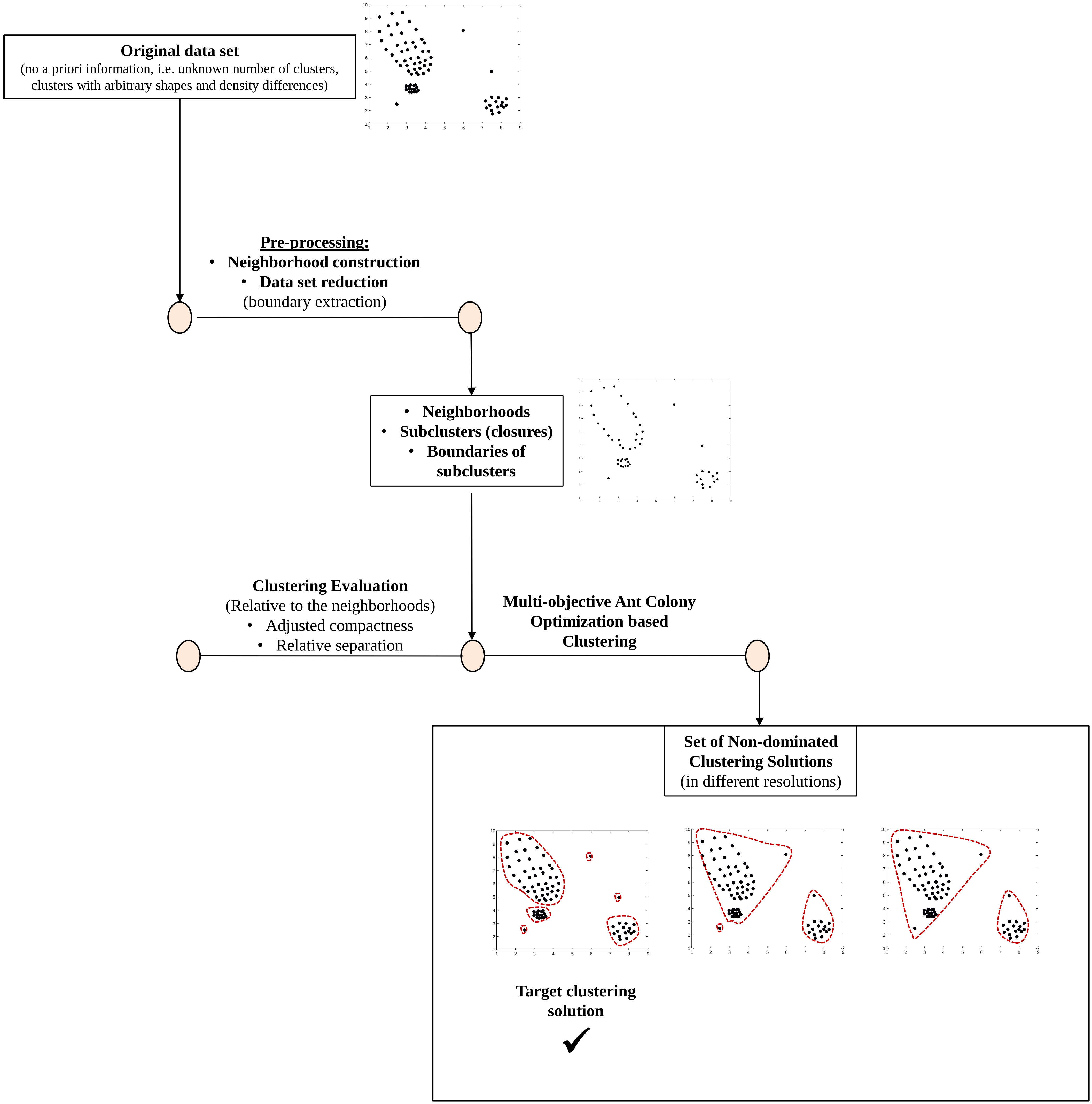
Graphical abstract (for review)



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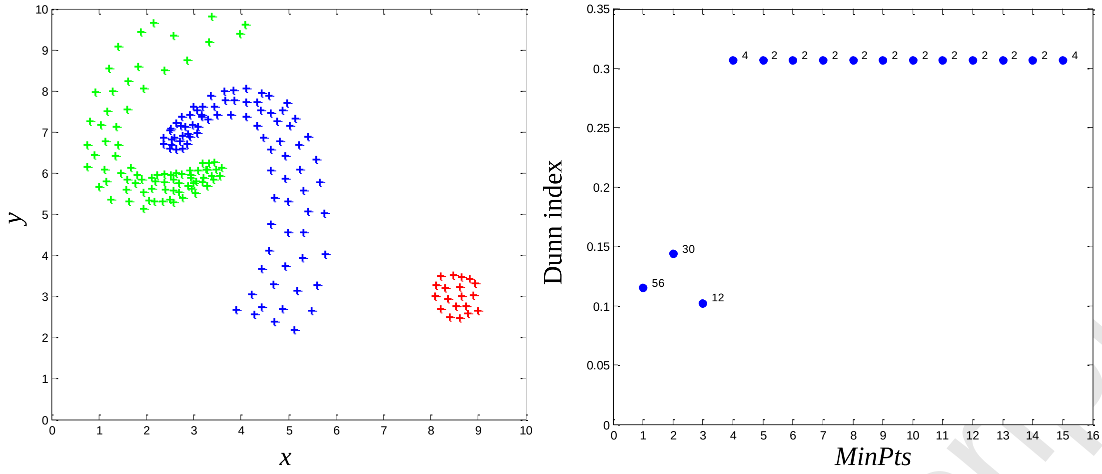

(a) (b)

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The ACO-C Methodology

Step 0. Pre-processing (neighborhood construction and data set reduction)

Step 1. Initialization of parameters

For *t* = 1,.., *max_iter*

    For *s* = 1,.., *no_ants*

        Step 2. Solution construction

        Step 3. Solution evaluation

        Step 4. Local search

    End for

    Step 5. Pheromone update

    Step 6. Non-dominated set update

End for

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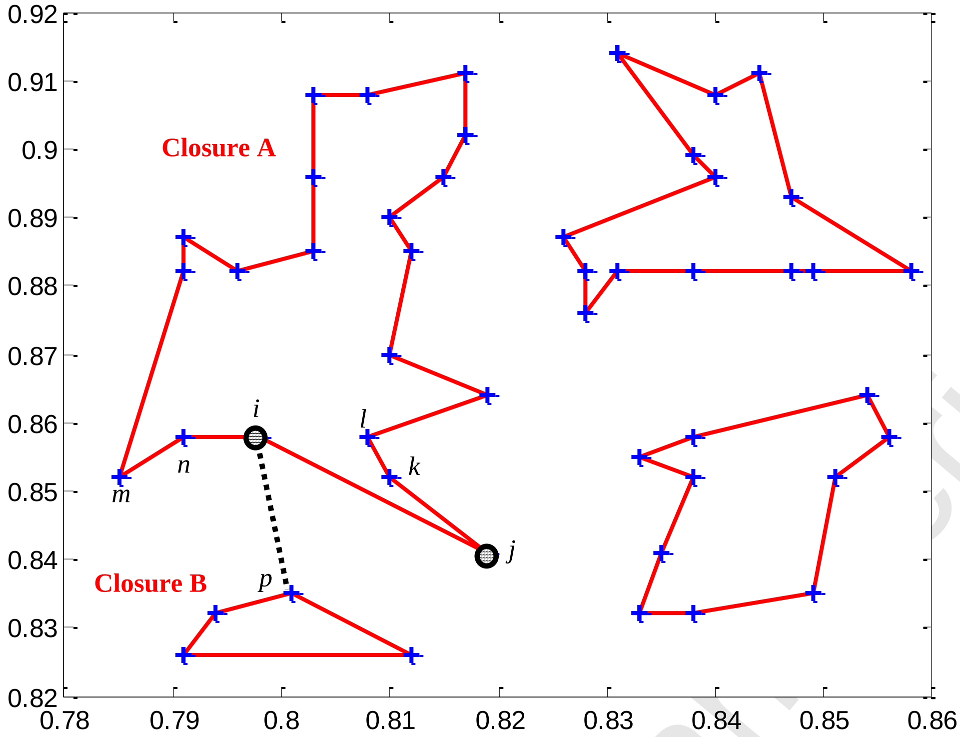

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Step 2. Solution construction

Set m = 1, D_o = D and $NCS_i = NS_i$, $\forall i \in D$.

While $D_o \neq \varnothing$

2.1. Point selection

Select point i from D_o at random.

Set $C_m = C_m \cup \{i\}$, $D_o = D_o / \{i\}$, and $NCS_k = NCS_k / \{i\}$ for $\forall k \in D_o$.

While $NCS_i \neq \varnothing$ and $i \neq$ "*nowhere*"

2.2. Edge insertion

Select edge (i,j) where $j \in NCS_i$ using probabilities based on τ_{ij}, and insert edge (i,j).

Set $C_m = C_m \cup \{j\}$, $D_o = D_o / \{j\}$, and $NCS_k = NCS_k / \{j\}$ for $\forall k \in D_o$.

Then, set $i = j$.

End while

Set $m = m + 1$, and start a new cluster.

End while

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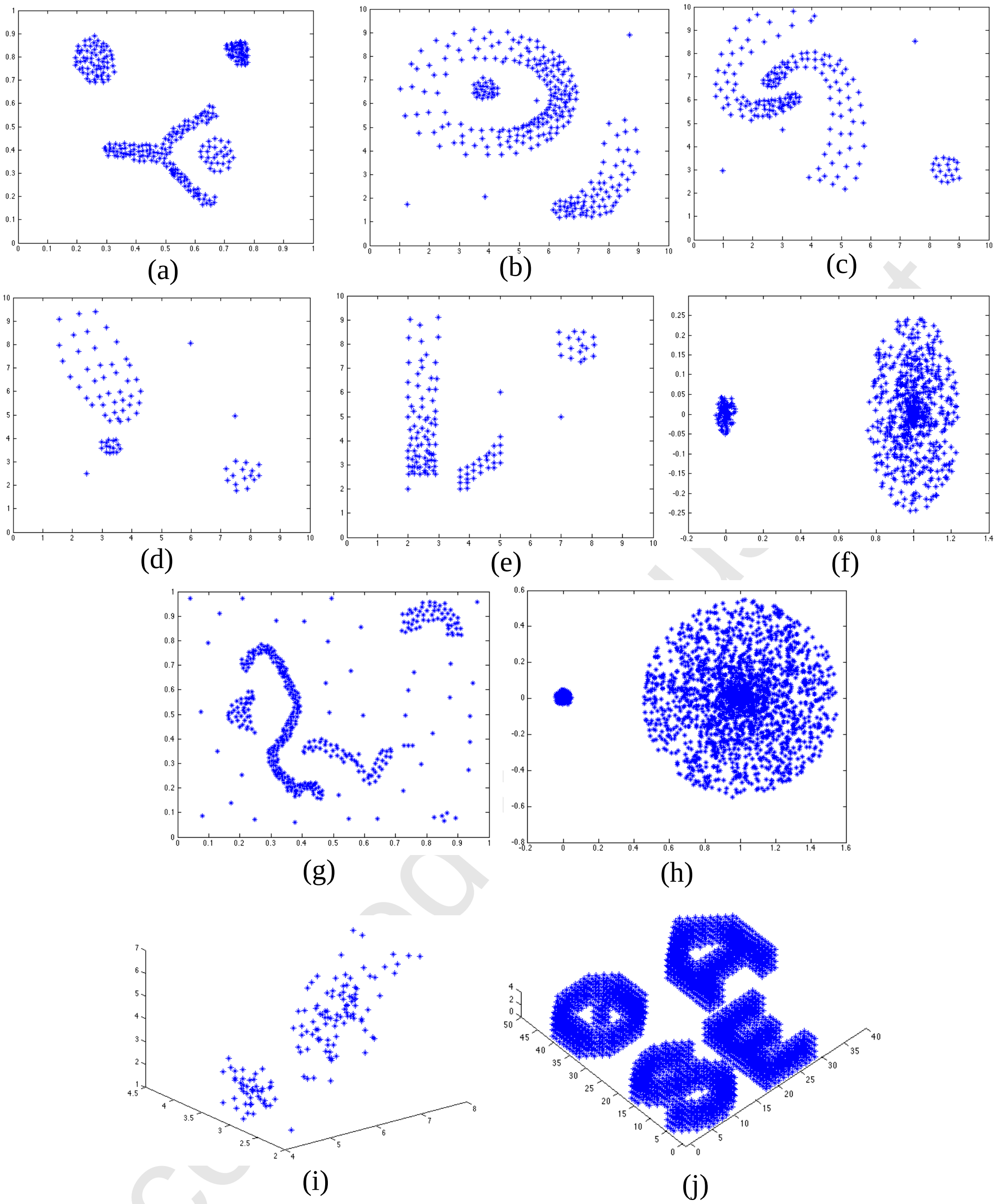
Figure 5



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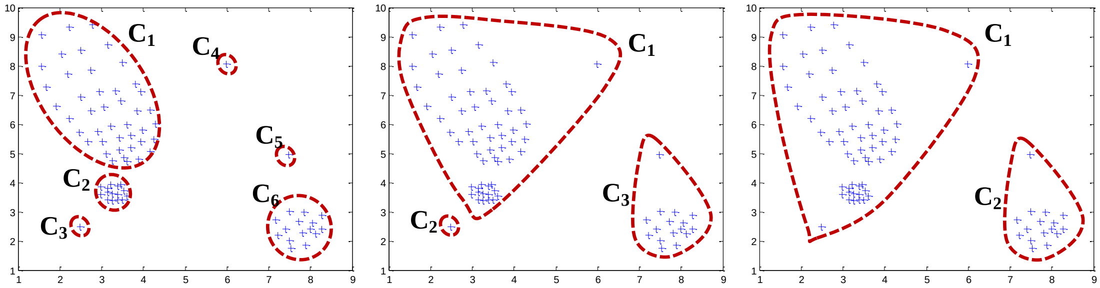

(a) (b) (c)

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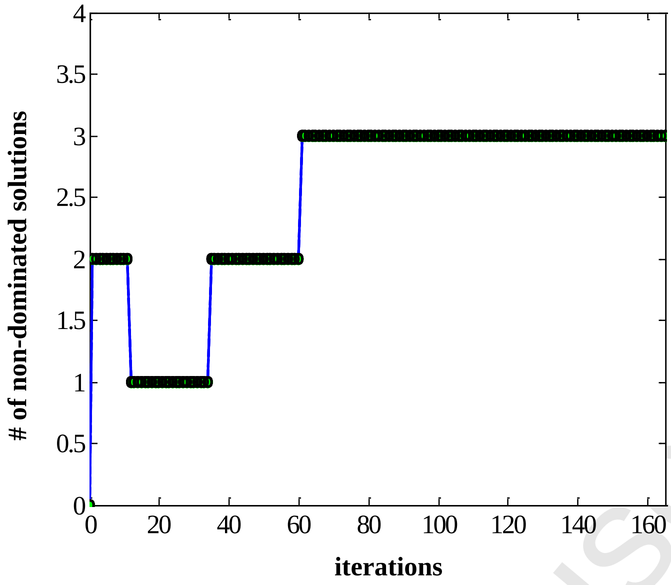

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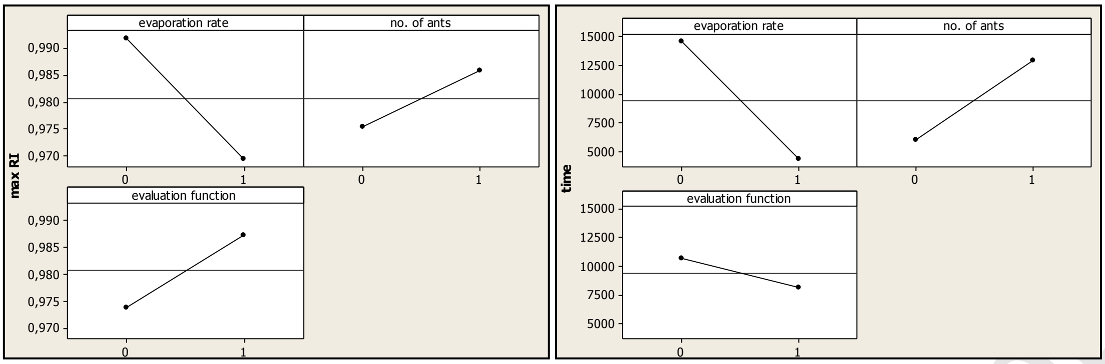

(a) (b)

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