Survey of Multiobjective Evolutionary Algorithms for Data Mining: Part II

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Abstract—This paper is the second part of a two-part paper, which is a survey of multiobjective evolutionary algorithms for data mining problems. In Part I [1], multiobjective evolutionary algorithms used for feature selection and classification have been reviewed. In this part, different multiobjective evolutionary algorithms used for clustering, association rule mining, and other data mining tasks are surveyed. Moreover, a general discussion is provided along with scopes for future research in the domain of multiobjective evolutionary algorithms for data mining.

Index Terms—Association rule mining, biclustering, clustering, ensemble learning, multiobjective evolutionary algorithms.

I. Introduction

AS MENTIONED in Part I of this paper [1], multiobjective evolutionary algorithms (MOEAs) [2] have become increasingly popular in the domain of data mining. In this two-part paper, we survey several MOEAs for different data mining tasks. In [1], we introduced the basic concepts of multiobjective optimization and data mining and reviewed different MOEAs designed for addressing two important data mining tasks, namely feature selection and classification.

Here, MOEAs used for two other major data mining tasks such as clustering [3] and association rule mining [4] are surveyed. Both of these data mining tasks are unsupervised in nature and can be easily posed as multiobjective optimization problems. In recent years, several MOEAs have been proposed in the literature to accomplish these tasks. We review many of these approaches with a focus on chromosome representation, objective functions, evolutionary operators, and methods for obtaining the final solution from the non-dominated set. Besides this, here we also review MOEAs employed for several other data mining tasks such as, ensemble learning, biclustering, feature extraction, sub-group discovery, and so

on. Fig. 1 shows the different MOEAs-based data mining tasks reviewed in this part of the paper along with the corresponding references. A general discussion on the future scope of research in this area of multiobjective data mining is also provided.

II. MOEAs for Clustering

Clustering techniques aim to find a suitable grouping of the input dataset so that some criteria are optimized. A straightforward way to pose clustering as an optimization problem is to optimize some cluster validity index [5] that reflects the goodness of the clustering solutions. All possible partitionings of the dataset and the corresponding values of the validity index define the complete search space. Under this context, genetic and other evolutionary algorithms have been widely used to reach the global optimum value of the chosen validity measure. Conventional evolutionary clustering techniques [6] use some validity measure as the fitness value. However, no single validity measure works equally well for different kinds of datasets. Thus, it is natural to simultaneously optimize multiple of such measures for capturing different characteristics of the data. Hence, it is useful to utilize MOEAs for clustering. Multiobjective clustering techniques optimize more than one cluster validity index simultaneously, leading to high-quality results. The resultant set of near-Pareto-optimal solutions contains a number of non-dominated solutions, from which the user has to select the most appropriate one based on his/her own preferences. A number of multiobjective evolutionary clustering algorithms are available in the literature. They vary in different aspects, including the type of MOEA, the chromosome encoding, the objective functions optimized, the evolutionary operators adopted and the mechanism used to select the final solution from the non-dominated front.

A. Underlying MOEAs

There are mainly four MOEAs that have been used as the underlying optimization tool for multiobjective clustering. Pareto envelope-based selection algorithm-II (PESA-II) [7] has been used in the algorithms Voronoi initialized evolutionary nearest-neighbor algorithm (VIENNA) [8], multiobjective clustering with automatic k determination around medoids (MOCK-AM) [9], MOCK [10], and multiobjective evolutionary clustering ensemble algorithm (MECEA) [11]. Non-dominated sorting genetic algorithm-II (NSGA-II) [12] has
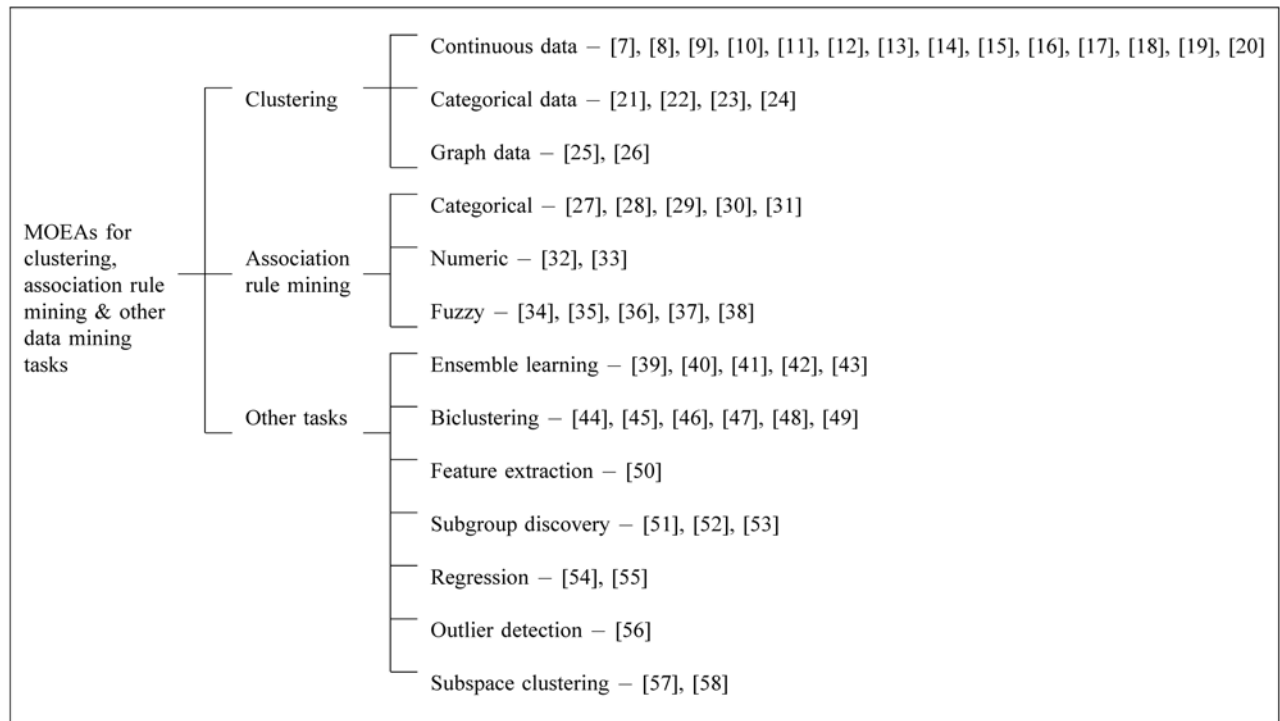
Fig. 1.   MOEAs for clustering, association rule mining, and other data mining tasks surveyed in Part II.

been employed in many multiobjective clustering approaches such as MOEA (dynamic) [13], variable-length real jumping genes genetic algorithms (VRJGGA) [14], MOGA [15], MOGA (medoid) [16], multiobjective evolutionary strategy [MOES (hybrid)] [17], multiobjective GA with support vector machine (MOGA-SVM) [18], [19], evolutionary multiobjective clustering for overlapping clusters detection (EMCOC) [20], MOGA (mode) [21], dynamic MOGA (DYN-MOGA) [22], multiobjective variable-length genetic algorithm (MOVGA) [23], and multiobjective clustering algorithms (MOCA) [24]. In [25] and [26], strength Pareto evolutionary algorithm-2 (SPEA2) [27] has been used as the underlying optimization tool. The Niched Pareto genetic algorithm (NPGA) [28] has been employed in multiobjective k-means genetic algorithm (MOKGA) [29].

B. Chromosome Representation

The choromosome representation approaches can broadly be classified into two major classes, that is, prototype-based approaches and point-based approaches. In the prototype-based approach, cluster representatives or prototypes, such as cluster centroids, medoids, and modes are encoded in the chromosome. On the other hand, in the point-based approach, a complete clustering solution is encoded in the chromosome.

In a prototype (cluster center)-based approach, the chromosomes are made up of real numbers, which represent the coordinates of the cluster centers. If a chromosome encodes the centers of K clusters in d-dimensional space, then its length l will be $d \times K$. In the case of multiobjective clustering, this encoding scheme was first utilized in [30], and the authors have used this encoding policy in a series of multiobjective clustering algorithms such as MOGA [15],

significant multiclass membership (two-stage) (SiMM-TS) [31], MOGA-SVM [18], [19], and MOVGA [23]. Besides Mukhopadhyay *et al.*, several other researchers have adopted this encoding policy in different multiobjective clustering algorithms such as VRJGGA [14], MOES (Hybrid) [17], and MOCA [24]. In some algorithms, instead of using cluster centers as cluster prototypes, cluster medoids have been encoded in the chromosome. A cluster medoid is the point of the cluster from which the sum of the distances to the other points of the cluster is the minimum. There are some approaches that encode the cluster medoids, or the indices of the points representing the cluster medoids in the chromosomes. Examples of such multiobjective evolutionary clustering algorithms include MOGA (medoid) [16] and EMCOC [20]. Another approach is to encode cluster modes in the chromosomes. Cluster modes are suitable for categorical attributes where the mean centroid of the cluster cannot be computed. Given a set of categorical points, their mode is defined as a vector of the attributes where each component value of the vector represents the most frequent value occurring in the corresponding attribute over all the points. MOGA (mode) [21] is a multiobjective clustering algorithm where cluster modes are encoded in the chromosomes. The advantage of prototype-based encoding is that here the length of the chromosomes is small and, therefore, it takes less time to apply the evolutionary operators such as crossover and mutation. Also, this encoding policy is good for capturing overlapping and fuzzy clusters. However, these algorithms have a tendency to capture round-shaped clusters only. Also, if the chromosomes encode different number of clusters, they have variable lengths that are to be handled while applying the evolutionary operators. Moreover, in this type encoding, the chromosomes may be very large if the number of

attributes is large. Therefore, for higher dimensional datasets, this encoding strategy may not work very well.

Another popular encoding approach is point-based encoding, where the complete clustering of the data points are encoded instead of only the representatives/prototypes of the clusters. Under this scheme, there are two main approaches, the cluster label-based approach and locus-based adjacency representation. The cluster label-based approach is the most common form of point-based encoding. Here, the chromosome lengths are equal to the number of points in the input dataset, and each position represents the cluster label of the corresponding points. If position i of the chromosome contains a value k, then the ith data point is assigned to cluster k. Obviously, the chromosomes can contain only integer values drawn from the set $\{1, 2, \ldots, K\}$, where K is the maximum number of clusters. The multiobjective clustering algorithms that use this encoding policy include VIENNA [8], MOKGA [29], and graph-based sequence clustering (GraSC) [25], [32]. In MOCK, Handl and Knowles [9], [10] used a variant of the cluster label-based encoding strategy. Here, each chromosome consists of n genes (n is the number of data points) and each gene can have integer values in $\{1, \ldots, n\}$. If the gene i is assigned a value j, it represents a link between the data points i and j, and, in the resulting clustering solution, these two points will belong to the same cluster. Thus, a graph is formed with the data points as the vertices and the links between two data points as the edges. Therefore, for decoding a chromosome, it is required that we identify all the connected components of the graph. This can be done in linear time [10]. The data points in the same connected component are then assigned to the same cluster. Hence, this representation encodes the clustering as well as the number of clusters (number of connected components). Many algorithms besides MOCK, such as MECEA [11], AI-NSGA-II [33], and DYN-MOGA [22] have adopted this encoding policy. Although point-based encoding techniques are not biased toward convex-shaped clusters, they suffer from the large length of chromosomes when the number of data points n is large. Thus, the algorithms using this encoding approach require more time to converge. However, unlike prototype-based encoding, here the chromosome length is independent of the encoded number of clusters.

C. Objective Functions

For the clustering problem, usually cluster validity indices [34] are used as the objective functions. Most of such multiobjective clustering algorithms have used two validity indices to be simultaneously optimized. In [8], [10], and [35], the MOCK clustering algorithm minimizes two validity indices: overall cluster deviation [$Dev(C)$] and cluster connectedness [$Conn(C)$]. Some other multiobjective clustering works have also used these two objectives [11], [13], [32]. References [15], [18], and [19], used two validity indices, J_m [36] and XB [37], which are minimized simultaneously to obtain compact and well-separated clusters. In [29], [38], and [39], the two validity indices to be minimized are total within-cluster variance ($TWCV$) and the number of clusters K. In [16], a multiobjective categorical data clustering algorithm is used to optimize overall deviation $Dev(C)$ (with respect to medoids instead of

centroids) and silhouette index [40]. In [41] and [20], the intracluster entropy H and cluster separation $Sep(C)$ are used as the two objective functions. The index $\mathcal{I}$ [34] and XB are simultaneously optimized in [42]. In [25], [32], and [33], the objectives adopted are min-max cut and the silhouette index [40]. In [26], the aim is to obtain compact and well-separated clusters and for that sake, the objectives to be minimized are the validity indices overall deviation $Dev(C)$ and the Edge index $Edge(C)$. In [21], [23], and [43], the objective functions are chosen to be the normalized J_m index ($\mathcal{J}$) and the fuzzy cluster separation $\mathcal{S}$, which are simultaneously minimized. It is to be noted that instead of cluster centroids, cluster modes have been used for computing the validity index values in [21] and [43], since these algorithms have been applied on categorical data. In [44], out of several combinations, DB [45] and $Dunn$ [46] indices have also been chosen as the two objectives to be simultaneously optimized. The indices J_m and cluster separation have been used in [47]. There are also a few multiobjective clustering techniques which use more than two objective functions. For example, in [42] and [48], three cluster validity measures, that is, XB index, $\mathcal{I}$ index and J_m index have been simultaneously optimized. In [24], three objective functions have been simultaneously optimized as well: average cluster variance, average between group sum of squares ($ABGSS$) and cluster connectedness. In [49], four objective functions are considered: overall cluster deviation, cluster separation, cluster dominance and the diameter of the biggest cluster. It is known that MOEAs usually do not perform very well when the number of objective functions increases to four or more [50]. However, in [49], Özyer *et al.* did not address this issue. It should be noted that the choice of a suitable set of objective functions is not a trivial problem and the clustering output may heavily depend on this choice [51]. In view of this, recently, an interactive multiobjective clustering algorithm was proposed in [52]. In this approach, the algorithm interacts with a human decision maker to learn the suitable set of objective functions along with evolving the clustering solution. However, a detailed study that compares the effects of different objective functions is still not available.

D. Evolutionary Operators

Evolutionary operators, such as crossover and mutation, depend on the adopted chromosome representation scheme. Many of the algorithms employing prototype-based representation have adopted single-point crossover. Examples of such multiobjective clustering algorithms include MOGA [15], MOGA-SVM [18], [19], and MOVGA [23]. In [13], two-point crossover has been used. Ripon *et al.* [14], [20] have employed jumping gene crossover in their multiobjective clustering algorithms. Won *et al.* [17] have used a centroid-pool based crossover approach where the centroids encoded in the parent chromosomes are first combined to build a centroid-pool. Thereafter, an offspring solution is generated by randomly selecting a number of chromosomes from the centroid pool. The algorithms that employ a point-based encoding policy have used uniform crossover in most cases [8], [10], [11], [22], [25], [33]. Following the crossover operators, a variety of mutation operators are also employed. Mutation refers to small

changes in the chromosomes and is used for maintaining the diversity of the population. In prototype-based encoding, the predominant mutation operator found is centroid perturbation [13]–[15], [17]–[19], [23]. The basic idea of this mutation operator is to shift a randomly selected centroid slightly from its current position. For medoid-based encoding and mode-based encoding, the mutation operators random medoid replacement [16] and mode perturbation [21] have been used, respectively. In [24], a mutation operator is employed in which either random cluster centers of the chromosomes are perturbed or cluster centers are added/deleted to/from the chromosome with equal probability. For the cluster label-based encoding, the common approach for mutation is to replace the class label of the selected point by a random class label. This mutation operator has been adopted in [32] and [53]. To tackle the problem of dealing with a large chromosome length, a special mutation operator, called directed neighborhood-biased mutation, was proposed in [10]. In this mutation, each point i is linked to its L nearest neighbors $\{nn_{i1}, nn_{i2}, \ldots, nn_{iL}\}$, and thus the effective search space is reduced to L^n. Thus, changing the class label of point i induces the change to all its L nearest neighbors. The mutation probability is also decided adaptively. The same mutation operator has been used in many other algorithms [11], [22], [26], [33].

E. Obtaining the Final Solution

MOEAs-based clustering algorithms also differ in the method for obtaining the final solution from the non-dominated set of solutions yielded by the MOEA. These methods can be broadly classified into three categories, that is, the independent objective-based approach, the knee-based approach, and the cluster ensemble-based approach.

In the independent objective-based approach, an independent cluster validity index, other than those optimized during the clustering process, is used to select a single solution from the non-dominated front. Many of the currently available multiobjective clustering techniques have adopted this approach because of its simplicity. In [15] and [30], the authors used the J_m and XB indices as the objective functions, whereas the final solution was selected using index $\mathcal{I}$. In a similar approach [23], fuzzy cluster compactness and separation were adopted as the two objectives whereas the $\mathcal{I}$ index was used as the selection criterion. In [54], the XB and $\mathcal{I}$ indices have been used as the objective functions whereas the silhouette index was used for selecting the final solution. In [38], the two objective functions are $TWCV$ and the number of clusters, whereas the authors used the DB index and the SD index [55], [56] for selecting the final solution from the Pareto front. In [29], the two objective functions used are $TWCV$ and the number of clusters, and various other validity indices, such as the Dunn index, the DB index, and the silhouette index are adopted for selecting the final solution. The authors also presented a comparative study of their results. Demir et al., in their GraSC algorithm [32], optimized the silhouette index and the min-max cut index, and used the DB index for selecting the final solution. In [24], the authors optimized three objective functions, that is, average cluster variance, average between group sum of squares ($ABGSS$) and cluster connectedness,

and they used the Rand index ($\mathcal{R}$) [5] for selecting the final solution from the Pareto front. Note that computation of $\mathcal{R}$ requires knowing about the true clustering of the dataset. Hence, this method is not applicable when the true clustering information is unknown. Although this approach for selecting the final solution is simple to implement and has low time requirement, the final result may be biased depending on the validity index chosen for selecting the final solution. Moreover, one may criticize this approach by questioning why this independent validity measure is not optimized directly, and the question does not have a very suitable answer.

The second approach is the knee-based approach, where the objective is to select the knee solution from the non-dominated front. A knee solution refers to an interesting solution for which the change of one objective value induces the maximum change in the other one. Handl and Knowles have used this knee-based approach in their MOCK algorithm [9], [10], [57]. This approach is motivated by the GAP statistic [58]. This is done by comparing the generated Pareto front with control fronts generated by applying MOCK on random control data. The solution that corresponds to the maximum distance between the generated Pareto front and the control fronts is selected as the final solution. However, there is no well-formed motivation behind choosing a knee solution as the final solution. It is not well explained why the user should be most interested in this solution. Another major problem is that it is a time consuming approach, because the algorithm has to be executed multiple times with random datasets to generate the control front. Therefore, a few variants of this technique have been proposed in [26], [59], and [60], primarily for improving its scalability for larger datasets.

The third approach is the cluster ensemble-based approach where it is assumed that all the non-dominated solutions contain some information about the clustering structure of the dataset. Therefore, the motivation is to combine this information to obtain a single clustering solution. In [48], some well-known cluster ensemble techniques, such as the cluster-based similarity partitioning algorithm (CSPA), the hypergraph partitioning algorithm (HGPA), and the meta-clustering algorithm (MCLA) [61] have been used to combine the non-dominated front solutions to obtain the final clustering and their performance is compared by the authors. In a similar approach [11], MCLA has been used for ensembling purposes. In [18], [19], and [21], Mukhopadhyay *et al.* proposed a novel approach for combining the nondominated solutions. Here, the points that are put in the same class by most of the non-dominated solutions are first identified. These points are considered to be highly confident and then, some classifier such as SVM or k-nn, is trained using these points. Thereafter, the remaining points are classified by the trained classifier. In this way, the class labels for all the points are generated. It has been shown that ensemble-based techniques work better than the independent objective-based techniques [15] for both satellite image segmentation [18] and microarray data clustering [19]. Although these methods are promising and motivating, the ensemble method takes reasonable time and the final solution depends on the choice of the ensemble technique. Also, sometimes it is necessary to map one non-

TABLE I

COMPARISON OF DIFFERENT MOEAS FOR CLUSTERING

Algorithm	Underlying MOO tool	Data Type	Encoding	Objective functions	Evolutionary operators	Final solution from non-dominated front
Handl and Knowles [7], 2004 (VIENNA)	PESA-II	Continuous	Integer (Label-based)	$Dev(C), Conn(C)$	No crossover, neighborhood-biased mutation	Independent objective-based (F-measure)
Liu et. al. [8], 2005 (MOKGA)	NPGA	Continuous	Integer (Label-based)	$TWCV$, number of clusters K	One-point crossover, probability-based replacement mutation	Independent objective-based ($Dunn$, DB, Silhouette, C, SD, S_Dbw indices)
Chen and Wang [9], 2005 (MOEA(Dynamic))	NSGA-II	Continuous	Real-valued (Centroid-based)	$Dev(C), Conn(C)$	Two-point crossover, centroid perturbation mutation (Gaussian mutation)	Independent objective-based (F-measure)
Handl and Knowles [10], 2007 (MOCK)	PESA-II	Continuous	Integer (Adjacency graph-based)	$Dev(C), Conn(C)$	Uniform crossover, neighborhood-biased mutation	Knee-based (with null model)
Ripon et. al. [11], 2006 (VRJGGA)	NSGA-II	Continuous	Real-valued (Centroid-based)	Entropy H, separation $Sep(C)$	Jumping gene crossover, centroid perturbation mutation (polynomial mutation)	Independent objective-based (Deviation and $Dunn$ index)
Bandyopadhyay et. al. [12], 2007 (MOGA)	NSGA-II	Continuous	Real-valued (Centroid-based)	J_m, XB	One-point crossover, centroid perturbation mutation (uniform distribution)	Independent objective-based ($\mathcal{I}$ index)
Qian et. al. [13], 2008 (MECEA)	PESA-II	Continuous	Integer (Adjacency graph-based)	$Dev(C), Conn(C)$	Uniform crossover, neighborhood-biased mutation	Ensemble-based (Graph-based - MCLA)
Won et. al. [14], 2008 (MOES(Hybrid))	NSGA-II	Continuous	Real-valued (Centroid-based) (variable-length)	$TWCV$, number of clusters K	Centroid pool crossover, centroid perturbation mutation (log normal distribution)	None
Mukhopadhyay et. al. [15], [16], 2009 (MOGA-SVM)	NSGA-II	Continuous	Real-valued (Centroid-based)	J_m, XB	One-point crossover, centroid perturbation mutation (uniform distribution)	Ensemble-based (Majority vote and SVM classifier)
Shirakawa and Nagao [17] 2009 (MOCK variant)	SPEA2	Continuous	Integer (Adjacency graph-based)	$Dev(C), Edge(C)$	Uniform crossover, neighborhood-biased mutation	Knee-based (without null model)
Ripon and Siddique [18], 2009 (EMCOC)	NSGA-II	Continuous	Binary (Medoid-based)	Entropy H, separation $Sep(C)$	Jumping gene crossover, no mutation	Independent objective-based (Entropy and Sepratation)
Mukhopadhyay and Maulik [19], 2011 (MOVGA)	NSGA-II	Continuous	Real-valued (Centroid-based) (variable-length)	Normalized J_m fuzzy separation $\mathcal{S}$	One-point crossover centroid perturbation mutation (uniform distribution)	Independent objective-based ($\mathcal{I}$ index)
Kirkland et. al. [20], 2011 (MOCA)	NSGA-II	Continuous	Real-valued (Centroid-based) (variable-length)	Average deviation, $ABGSS, Conn(C)$	Exchange corresponding prototypes crossover, centroid pool mutation (add/delete/modify centroid)	Independent objective-based (Rand index)
Handl and Knowles [21], 2005 (MOCK-am)	PESA-II	Categorical/ distance matrix	Integer (Adjacency graph-based)	$Dev(C), Conn(C)$	Uniform crossover, neighborhood-biased mutation	Knee-based (with null model)
Mukhopadhyay and Maulik [22], 2007, MOGA(medoid)	NSGA-II	Categorical	Integer (Medoid-based)	$Dev(C)$, silhouette	One-point crossover, medoid replacement (point index)	Independent objective-based (Minkowski score)
Demir et. al. [23], 2007 (GraSC)	SPEA2	Categorical/ distance matrix	Integer (Label-based)	Min-Max cut, silhouette	Modified uniform crossover, random replacement mutation	Non-domination status
Mukhopadhyay et. al. [24], 2009 (MOGA(mode))	NSGA-II	Categorical	Categorical (Mode-based)	Normalized J_m fuzzy separation $\mathcal{S}$	One-point crossover, mode replacement mutation (categorical value replacement)	Ensemble-based (Majority vote and k-nn classifier)
Kim et. al. [25], 2010 (AI-NSGA-II)	NSGA-II	Graph	Integer (Adjacency graph-based)	Entropy H, separation $Sep(C)$	Uniform crossover, neighborhood-biased mutation	Non-domination status
Folino and Pizzuti [26], 2010 (DYN-MOGA)	NSGA-II	Graph	Integer (Adjacency graph-based)	$CS(C), NMI$	Uniform crossover, neighborhood-biased mutation	Independent objective-based (Modularity)

dominated solution to another [21] to ensure that cluster label i means the same cluster in all the solutions. Therefore, the final solution also depends on the mapping technique utilized.

F. Relative Comparison and Applications

We have summarized the approaches of several well-known MOEA-based clustering algorithms in Table I. A total of nineteen different algorithms are considered here. The algorithms are categorized based on the data types considered, that is, continuous data, categorical data and graph data. In each category, we have reported the underlying MOEAs, the encoding strategies, the objective functions, the evolutionary operators, and the final solution selection methods used by the different clustering methods. The algorithms have been arranged in ascending order of their time of publication to illustrate how they have evolved over time. Out of the 19 algorithms, ten used different versions of prototype-based encoding, and the rest used point-based encoding strategies. NSGA-II has been found again to be the most commonly used

approach. However, other MOEAs have also been adopted, including PESA-II, NPGA, and SPEA2.

MOEA-based clustering algorithms have found several applications in real-life domains such as image segmentation, bioinformatics, web mining, and social networks. Usually, the problem of image segmentation can be posed as the problem of clustering the pixels of the images in the intensity space. If the image has multiple bands, then they serve as the different attributes of the dataset. In [26], a few benchmark color images have been segmented. Maulik *et al.* [15], [18], [30] have applied multiobjective fuzzy clustering for segmentation of remote sensing imagery of multispectral satellite images. Besides this, the application of multiobjective evolutionary clustering can also be found in the segmentation of MRI medical imagery [23], [48]. Multiobjective clustering has also been applied in texture image segmentation [11]. Another important application area of multiobjective evolutionary clustering algorithms is bioinformatics, where microarray gene expression data sets are clustered to identify co-expressed

genes. There have been various studies in this area [19], [31], [54], [62], [63]. Multiobjective clustering has also found application in finding gene markers [64], [65] from expression data. Recently, multiobjective clustering has been used in clustering protein-protein interaction networks [66]. Multiobjective clustering algorithms have also been applied in web data mining. For example, in [25], a web-recommender system has been built using multiobjective clustering by extracting web usage patterns. An extension of that is presented in [32], where different multiobjective clustering approaches have been compared for determining a suitable approach for clustering web user sessions, which consist of sequences of web pages visited by the users. In recent times, clustering social networks have gained in popularity and a number of recent studies have applied multiobjective clustering techniques to detect strong communities within social networks [22], [33].

III. MOEAs for Association Rule Mining

An association rule can be considered a general case of classification rule. The consequent of a classification rule consists of the class attribute only, whereas, in association rules, the consequent may consist of a set attributes. Therefore, the number of association rules for a given dataset is much greater than that of classification rules. Most of the classical association rule mining (ARM) algorithms, such as the *a priori* algorithm [4], first generate all frequent itemsets (i.e., itemsets having a support greater than the minimum support threshold), and thereafter, from the frequent itemsets, the association rules that surpass the minimum confidence threshold. Generating all the frequent itemsets is in itself a time consuming task when the number of items is large, because it needs at least a number k of scans of the dataset for k items. Therefore, it would be beneficial if one could generate the association rules in a direct way, skipping the frequent itemset generation step. For this purpose, evolutionary algorithms have been used widely for generating association rules by maximizing the support/confidence of the rules [67]. However, the goodness of an association rule cannot only be represented by its support or confidence. There are many other metrics available to measure the goodness of an association rule [68]. Therefore, the problem of ARM can be posed as a multiobjective optimization problem where the goal is to find association rules while optimizing several such goodness criteria simultaneously. In the past decade, several MOEAs have been proposed for ARM. These techniques can broadly be classified into three categories, namely categorical association rules, numeric association rules, and fuzzy association rules. Here, we discuss several multiobjective evolutionary ARM algorithms from these three categories.

A. Categorical Association Rules

Categorical association rules are generated from a binary or categorical dataset. In a binary dataset, a rule like $ABC \Rightarrow DE$ can be interpreted as follows: if items A, B, and C are purchased, then items D and E are also purchased. Thus, these rules do not say anything about the number of items that are to be purchased; they simply imply the presence or absence of items. For categorical data, if some item has multiple categorical values, then each attribute-value pair is treated as a separate item. In this way the dataset is converted into a binary dataset.

1) Underlying MOEAs: Different standard and non-standard MOEAs have been used in various works on categorical ARM. We call a MOEA non-standard if it does not follow any of the standard MOEA approaches directly, but uses instead some combination of operators. In [69], a multiobjective GA (MOGA) is used. In [70], the authors used a multiobjective co-evolutionary algorithm for this purpose. In [71] and [72], some non-standard MOEAs are used for the ARM problem. NSGA-II has been used in [73] for ARM.

2) Chromosome Representation: There are mainly two chromosome representation techniques for categorical ARM, similar to the ones available for classification rule mining [1]. In the first approach (Pittsburgh approach), a set of possible association rules are encoded in each chromosome. This approach is more suitable for classification rule mining, where the objective is to identify a good set of rules. However, in ARM, the objective is to find a set of rules each of which is good. Therefore, for this case, the Michigan approach, in which each chromosome represents exactly one rule, is more suitable [69]. Most of the MOEA-based categorical ARM techniques use this chromosome representation. In an early work [69], the authors adopted the Michigan approach as follows: each chromosome has length $2k$, where k is the number of items. The chromosomes are binary strings where each attribute is given two bits. If these two bits are 00 or 11, then the attribute appears in the antecedent or consequent parts of the rule, respectively; otherwise, the attribute is absent from the rule. In a similar approach [70], the presence of an attribute in the antecedent and consequent part are represented by bits 10 and 01, whereas other bit combinations represent the absence of the attribute from the rule.

The above encoding schemes [69], [70] can only be adopted for binary datasets, that is, when an item is either present or absent in a transaction. If someone wants to use this encoding for more general categorical data, where an item may be present in a transaction with certain value (a categorical state), the dataset will first need to be transformed into a binary one by considering each attribute-value pair as an item. In view of this, an alternative encoding strategy is presented in [73], which can be used for a categorical dataset directly. Here, each attribute has two parts. The first part represents the position of the attribute in the rule and the second part represents the categorical value it takes. The first part contains two bits and the attribute appears in the antecedent and the consequent of the rule if the bits are 10 and 11, respectively; otherwise, it is absent from the rule. The second part represents categorical values taken by attributes in binary form. However, the authors did not explain how a binary value in the second part represents a categorical state if the number of states for an attribute is not an exact power of two.

The main disadvantage of using a binary encoding scheme is that it gives rise to a large chromosome length when the number of attributes is large, since at least two bits are

needed for each attribute. An integer encoding may come handy in this respect. Such an integer encoding scheme has been proposed in association rule mining using multiobjective genetic algorithm (ARMMGA) [72], where the chromosomes encode the index of the attributes. A chromosome encoding a k-rule, k being the total number of items in the antecedent and the consequent, has $k + 1$ genes. The first gene position indicates the separating position of the chromosome where the antecedent and the consequent attributes are separated. For example, if A_i represents the ith item, then the chromosome {3 | 2 5 4 1 3} represents the rule $A_2A_5A_4 \Rightarrow A_1A_3$. This representation significantly reduces the length of the chromosome, but not effectively the search space, because now for each position, a large number of alternative indices are to be searched. Moreover, this representation scheme gives rise to a variable chromosome length, thus requiring a specialized crossover operator. Also, there remains a possibility of finding duplicate indices in a chromosome after crossover/mutation, which must be taken care of during the evolutionary process.

3) *Objective Functions:* Although support and confidence are two popular objectives that are to be maximized, there are several other metrics to measure the interestingness of association rules. These metrics, which have been used by different algorithms for optimization in a multiobjective framework, include coverage, lift, comprehensibility, cosine, prevalence, recall, Laplace, conviction, surprise, Jaccard, J-measure, and so on [68]. In [69], the rule mining problem has been modeled as a three-objective optimization problem where confidence, comprehensibility, and interestingness have been optimized simultaneously. They defined the comprehensibility of a rule as $log(1 + |C|)/log(1 + |A \cup C|)$, where $|C|$ and $|A \cup C|$ denote the number of attributes in the consequent part and total rule, respectively. They considered that the lower value of comprehensibility, that is, less number of attributes in the consequent of the rule, leads to better understandability of the rule. The interestingness measure, on the other hand, is defined as a product of three probabilities, namely, the probability of generating the rule given the antecedent (ratio of the support of the rule to the support of the antecedent), the probability of generating the rule given the consequent (ratio of the support of the rule to the support of the consequent), and the probability of generating the rule given both antecedent and consequent (ratio of the support of the rule to the total number of transactions). A rule becomes more interesting if it has a high interestingness value. In [70], two objective functions, statistical correlation and comprehensibility, have been simultaneously optimized in a co-evolutionary framework. The statistical correlation measure indicates a better association of the rule. In [71], five objective functions, that is, support, confidence, J-measure, interest, and surprise [68] have been simultaneously optimized. They found five different groups of correlated measures. To make the objective functions contradictory and uncorrelated, they selected these five measures from five different groups. In [73], six different measures (support, confidence, interest, comprehensibility, cosine and attribute frequency) have been considered. Three of these measures have been taken at a time and optimized simultaneously. Measures such as support, confidence, interest

and comprehensibility tend to be better if the rule-length is smaller. To counter this bias, they also maximized attribute frequency, which is the ratio of the rule-length to the total number of items. The reason behind taking three objective functions at a time is that NSGA-II, the underlying MOEA, is known to perform well when the number of objective functions is at most three. Second, due to correlation of the measures, it is unnecessary to use correlated measures for optimization. In [72], the classical measures (support and confidence of the rules) are simultaneously optimized. Thus, it is apparent from the above discussion that different sets of rule-interestingness measures have been chosen by various authors as their objective functions. However, a systematic comparison among the chosen objective functions is still missing in the literature.

4) *Evolutionary Operators:* When binary encoding has been adopted, standard crossover and mutation operators have been used. For example, in [69], multipoint crossover and bit-flip mutation have been used. In [73] bit-flip mutation has been adopted, however, the authors did not specifically mention which crossover operator is used. In [70], the authors proposed Pareto neighborhood crossover, a combination operator and an annexing operator. However, the way in which these operators work is not explained. There is no mention about the motivation for defining these operators, as well as no experimental results have been provided showing their improved effectiveness with respect to the standard operators.

In the encoding strategies, where along with the attributes, their values are also encoded, other types of evolutionary operators are needed. In [71], although the authors did not explain the encoding strategy explicitly, from the description of the evolutionary operators, it appears that they used an approach in which the categorical values of the attributes participating in the rule are encoded. Here, the authors used value exchange and insertion crossover operators. If two parents have some common attributes in the antecedent part, then a value exchange crossover is performed by exchanging the categorical values of one of the common attributes. When the parents do not have any common attribute, then one random attribute selected from one parent is inserted into the other with a probability that is inversely proportional to the length of the latter chromosome. Four mutation operators are applied with equal probabilities. A value mutation randomly replaces a chosen categorical value with another random value from the same domain. An attribute mutation randomly replaces an attribute with another one. An insertion mutation inserts a new attribute-value pair, and a deletion mutation deletes a randomly chosen attribute-value pair. In [72], where integer encoding of the attributes is used, an order-1 crossover strategy is adopted. In this strategy, first a segment is chosen from two parent chromosomes and these are copied to the two offspring. Next, starting from the right side of the segment, the values of the genes that do not exist in the selected segment of the first parent, are copied to the first offspring. The same procedure is repeated for the second offspring as well. The mutation operator replaces a chosen item from the chromosome with a random item not present in the chromosome.

5) *Obtaining the Final Solution:* All the works for categorical rule mining using MOEAs that have been discussed

in this paper use a Michigan type of encoding, where each chromosome encodes one association rule. Hence, the final generation produces a set of non-dominated solutions each of which are given to the user as the association rules generated from the input dataset. Thus, in this case, there is no specific need of selecting a single solution from the non-dominated front.

B. Numeric Association Rules

For datasets having continuous attribute domains, the ARM algorithms designed for categorical attributes do not work well. This is because such algorithms need categorization of the continuous attributes. Hence, the results of the ARM algorithms depend a lot on the categorization technique adopted. To overcome this limitation, many numeric/quantitative ARM algorithms have been proposed and some of them adopted a multiobjective optimization approach.

A quantitative association rule is represented as [74], [75]

$$(l_1 \leq A_1 \leq h_1) \ \wedge \ (l_2 \leq A_2 \leq h_2) \Rightarrow (l_3 \leq A_3 \leq h_3).$$

Here A_i represents the ith attribute. l_i and h_i represent the lower and upper bound of the attribute values, respectively. Thus, $[l_i, h_i]$ defines an interval of values for the attribute A_i. Here, we discuss two different works on quantitative ARM.

1) *Underlying MOEAs:* In this section, we review two multiobjective numerical/quantitative rule mining algorithms. The first is a multiobjective differential evolution based numeric association rule mining algorithm (MODENAR) [74]. In this case, a multiobjective differential evolution (MODE) algorithm is used as the underlying optimization framework. In another work, an NSGA-II-based quantitative association rule mining algorithm (NSGA-II-QAR) is proposed [75].

2) *Chromosome Representation:* The chromosomes representing numeric or quantitative association rules need to encode the lower and upper bounds of the intervals of the attributes participating in a rule. In [74], where the MODENAR algorithm has been proposed, the following encoding technique has been adopted for the chromosomes. They used chromosomes where each attribute has three components. The first component indicates whether the attribute is present or absent in the rule, and if present, in which part (antecedent or consequent) in the rule it is. The second and third components indicate the lower and upper bounds of the ranges of the attribute. The first component can have integer values 0, 1, or 2, which indicate the presence of the attribute in the antecedent of the rule, the presence of the attribute in the consequent of the rule, and the absence of the attribute from the rule, respectively. The second and third components can take real values from the corresponding attribute ranges. It is to be noted that as MODENAR uses differential evolution as an optimizer and works on real-valued chromosomes, the authors used a round-off operator to handle the integer part of the chromosome. A similar encoding scheme is adopted in NSGA-II-QAR. The only difference is that in this case, the first part of the chromosome, instead of using the values 0, 1, 2, adopts the values 0, 1, and -1, respectively, to denote the same meaning. In both cases, the algorithms used a Michigan encoding strategy, that is, each chromosome encodes one rule.

3) *Objective Functions:* MODENAR optimizes four criteria of the rules [74]: support, confidence, comprehensibility, and amplitude of the intervals that make up the itemset and the rule. Comprehensibility is used to bias the search process toward shorter rules, under the assumption that shorter rules provide more non-redundant information. They also proposed that the amplitude of the intervals must be smaller for interesting rules, but the rationale for this is not explained. In NSGA-II-QAR [75], three objective functions are simultaneously optimized: lift, comprehensibility, and performance. Performance is defined by the product of confidence and support. Lift is defined as the ratio of support of the rule to the product of the supports of the antecedent and the consequent of the rule [76]. A high value for the lift measure indicates that the rule is interesting, since its support is high with respect to the supports of its antecedent and its confidence. The comprehensibility is defined simply as the reciprocal of the number of attributes in the rule. In [75], an experimental comparison between NSGA-II-QAR and MODENAR is provided.

4) *Evolutionary Operators:* MODENAR [74] used the standard version of the crossover and mutation operators adopted by the version of differential evolution called DE/rand/1. Additionally, a rounding operator is used to round-off the first part of the attribute that requires an integer (0, 1, 2) for computing the objective function values. In NSGA-II-QAR [75], a multipoint crossover is utilized. The two parts of the chromosome undergo two different mutations. In the first part, where the chromosome can have a value of -1, 0, or 1, a random value is selected from the set {-1, 0, 1} and it replaces the existing value. The other part of the chromosome encodes the lower and upper bounds of the chromosome. A mutation is applied to this part by increasing or decreasing these values randomly. In both [74] and [75], during mutation/crossover, it may happen that the lower bound becomes larger than the upper bound, or they go outside the bounds. For this, some repairing operators are also adopted to make the chromosome a valid one.

5) *Obtaining Final Solution:* Both MODENAR and NSGA-II-QAR use a Michigan approach of rule mining by encoding one rule in one chromosome. Thus, the final non-dominated set gives a set of numeric rules. Thus, there is no need to select any particular solution from the final non-dominated set. All the solutions will serve as the final selected rule set.

C. Fuzzy Association Rules

One of the major problems of mining numeric association rules is that these algorithms deal with sharp boundaries between consecutive intervals. Thus, they cannot represent smooth changes from one interval to another, which can be easily handled by fuzzy association rules. A number of MOEA-based fuzzy ARM techniques have been developed in the past decade. Here, we describe several of these algorithms and discuss different approaches that incorporate them.

The general form of a fuzzy association rule is as [77]

$$\text{If } X = \{x_1, x_2, \ldots, x_p\} \text{ is } A = \{f_1, f_2, \ldots, f_p\}$$

$$\text{Then } Y = \{y_1, y_2, \ldots, y_q\} \text{ is } B = \{g_1, g_2, \ldots, g_q\}.$$

Here X and Y represent two sets of attributes, and $X \cap Y = \phi$. A and B represent the fuzzy sets (linguistic values) of the corresponding attributes in X and Y, respectively. Therefore, if a rule is encoded in a chromosome, both the attributes and their linguistic values should be encoded in it. A number of studies have been done on the application of MOEAs for fuzzy association rule mining. Here we review some of them.

1) *Underlying MOEAs:* Different MOEAs have been employed in various works on fuzzy ARM. Kaya *et al.* [77]–[79] used a variant of SPEA for fuzzy rule mining. In [80], a multiobjective GA (MOGA) is used for this purpose. In another work on fuzzy association rule mining, NSGA-II has been employed [81]. However, in none of these studies, relative comparison among different MOEAs for fuzzy rule mining has been addressed.

2) *Chromosome Representation:* There are two categories of chromosome representations for fuzzy ARM. In the first approach, a chromosome represents a set of fuzzy clusters corresponding to each attribute. The objective is to find a suitable set of fuzzy clusters that partition the range of values in each attribute domain. This approach is adopted in a series of works done by Kaya *et al.* in [77]–[79]. In these works, each chromosome represents the base values of a variable number of membership functions representing the fuzzy sets for each quantitative attribute. Standard triangular membership functions are used to represent the fuzzy sets. Real-valued representation of the chromosomes is used for this purpose. Here, a chromosome does not represent association rules. It represents a suitable fuzzy clustering of the attribute domains. The evolved fuzzy membership functions are then used as the linguistic values of the corresponding attributes. Fuzzy association rules are mined using standard algorithms based on minimum support and minimum confidence criteria. A similar encoding approach is adopted in [80].

The second approach directly encodes fuzzy association rules in the chromosomes. This is a kind of Michigan approach where each chromosome encodes a possible rule. In [81], such an encoding is adopted to mine temporal fuzzy association rules. Here, the authors used a mixed representation of chromosomes combining integer and real values. The chromosome encodes the lower and upper bounds of the temporal interval in the rules as integers. The indices of the items participating in the rule are also encoded as integers. Finally, the real-valued parameters of the triangular membership functions corresponding to each item are encoded in the chromosome. Thus, this representation induces variable-length chromosomes needing special evolutionary operators.

3) *Objective Functions:* In the works of Kaya *et al.* [77]–[79], the authors optimize two criteria, that is, number of large itemsets and time spent to obtain the large itemsets. Thus, here the objective is to evolve a possible fuzzy clustering of the numeric attributes that maximizes the number of large itemsets while minimizing the time required to obtain all large itemsets given the clustering. After optimizing the clustering, the authors then use the membership functions as the linguistic values for the fuzzy association rules extracted based on minimum support and minimum confidence criteria.

In [80], where a similar encoding strategy is adopted as in [77], two objective functions are optimized simultaneously. The first objective function is stability of the encoded membership functions, which has two components, that is, overlap factor and coverage factor. The stability is optimized to avoid generation of too redundant and too separated fuzzy sets for an item. The second objective is to maximize the total number of large 1-itemsets for given minimum support values. Although this paper is a consequence of the works of Kaya *et al.* with modifications in the objective functions and evolutionary operators (described later), the authors did not compare their results with those of Kaya *et al.* So, it is difficult to judge any improvement of the performance over the previous approaches.

In [81], the authors used a direct approach to temporal fuzzy association rule mining by adopting the Michigan form of chromosomes. Thus, here the objective functions are related to the optimization of the encoded rules. In this paper, four objective functions, namely temporal support, temporal confidence, fuzzy support, and membership function widths, are optimized. Whereas the first three objective functions are obvious, the last objective function is used to prevent a membership function from covering the whole range of attribute values. Without this objective function, the solutions could evolve to cover the complete range of attribute values, since this gives higher support values as it includes more number of items.

4) *Evolutionary Operators:* References [77], [78], have used standard multipoint crossover operations. In [79], the authors used arithmetic crossover. Also, they employed standard real-value mutation. In [80], the authors used max-min arithmetical crossover and one-point mutation. This crossover operator generates four offspring at a time out of which the two best offspring are chosen. However, the authors did not describe the crossover process in detail, and did not discuss its advantage over a standard crossover operator. The mutation operator is used to slightly change the center of the fuzzy set being mutated. It is to be noted that when mutation takes place at the center of a fuzzy membership function, it may disrupt the order of the resulting fuzzy membership functions. Hence, these fuzzy membership functions need rearrangement according to their center values after the mutation. In [81], for a Michigan type of encoding, a modified uniform crossover operator is adopted. For mutating the genes representing the lower and upper bounds of the time interval, the values are generated within the endpoint range (epr) where the midpoint is the value of the current gene (g), such that the mutated value is a member of the set $\{-epr/2, \ldots, g, \ldots, epr/2\}$. This is done to reduce the effect of random sampling of the dataset.

5) *Obtaining the Final Solution:* As in [77]–[80], a chromosome encodes a possible fuzzy clustering of the attribute values. It is necessary to select a suitable solution from the final non-dominated set, based on which of the final association rules are extracted. However, in [77], [78], and [80], this issue has been overlooked. In [79], the authors presented an approach based on the lower bound of the objective function values to identify interesting solutions. The authors first determined a lower bound for an objective such that the values under the located lower bound are infeasible

Algorithm	Underlying MOO tool	Type	Encoding	Objective functions	Evolutionary operators	Final solution from non-dominated front
Ghosh and Nath [27], 2004	MOGA	Categorical	Binary (Michigan)	Confidence, comprehensibility, interestingness	Multi-point crossover, bit-flip mutation	None
Hu and Yang-LI [28], 2007	Pareto-based coevolutionary	Categorical	Binary (Michigan)	Statistical correlation, comprehensibility	Pareto neighborhood crossover, combination, annexing	None
Khabzaoui et. al. [29], 2008	Non-standard	Categorical	Not mentioned	Support, confidence, J-measure, interest, surprise	Value exchange crossover, insertion crossover, value/attribute mutation, insertion/deletion mutation	None
Anand et. al. [30], 2009	NSGA-II	Categorical	Binary (Michigan)	Combination (3 at a time) of support, confidence, interest, comprehensibility, cosine, attribute frequency	Crossover not mentioned, bit-flip mutation	None
Qodmanan et. al. [31], 2011 (ARMMGA)	Non-standard	Categorical	Integer (Michigan)	Support, confidence	Order-1 crossover, random replacement mutation	None
Alatas et. al. [32], 2008 (MODENAR)	MODE	Numeric	Mixed (Integer + real) (Michigan)	Support, confidence, comprehensibility amplitude of interval	DE/Rand/1	None
Martin et. al. [33], 2011 (NSGA-II-QAR)	NSGA-II	Numeric	Real-valued (Michigan)	Lift, comprehensibility, performance (support × confidence)	Multi-point crossover, random increase/decrease mutation, random replacement mutation	None
Kaya and Alhajj [34], 2003 Kaya and Alhajj [35], 2004	SPEA variant	Fuzzy	Real-valued (membership functions)	Number of large itemsets, time taken to find all large itemsets	Multi-point crossover, standard real-value mutation	Not mentioned
Alhajj and Kaya [36], 2008	SPEA variant	Fuzzy	Real-valued (membership functions)	Number of large itemsets, time taken to find all large itemsets	Multi-point crossover, standard real-value mutation	Lower-bound based
Chen et. al. [37], 2008	MOGA	Fuzzy	Real-valued (membership functions)	Number of large 1-itemsets, suitability of membership functions	Max-min arithmetic crossover, one-point mutation	None
Matthews et. al. [38], 2011	NSGA-II	Fuzzy (temporal)	Mixed (integer + real) (Michigan)	Temporal support, temporal confidence, fuzzy support, membership function width	Modified uniform crossover, random change mutation	None

solutions for us. The lower bounds are the parameters that are varied by the optimizer to obtain multiple non-dominated sets of solutions. Subsequently, the solution, which maximizes the other objective in feasible space, is chosen. However, as the author mentioned, the lower bound must be chosen carefully and it is not a trivial task. In [81], the authors used a Michigan type of encoding of temporal fuzzy association rules. Therefore, all the rules encoded in the final non-dominated set are considered as extracted rules. There is no specific need of choosing any particular solution from the non-dominated set.

D. Relative Comparison and Applications

In Table II, we provide a comparative overview of different approaches for MOEA-based association rule mining. The approaches are categorized in three types as discussed, that is, categorical rule mining, numeric rule mining and fuzzy rule mining. Different methods are compared with respect to the underlying MOO tool, encoding strategy, objective functions, evolutionary operators, and method for obtaining the final solution from the non-dominated set. It is evident from the table that most of the methods have used a Michigan encoding and thus all the non-dominated solutions are treated as final solutions without needing a particular solution from the set. Although a number of different methods have been discussed here, very few comparative studies of these methods are available in the literature. Only in [75], two numeric rule mining approaches using an MOEA, namely MODENAR and NSGA-II-QAR, have been compared in terms of different rule-interestingness metrics. However, in all the other works, the authors have concentrated on comparing the performance of their approaches with respect to existing single-objective evolutionary and other non-evolutionary methods.

Although MOEA-based ARM algorithms have gained in popularity in recent years, their use in real-life applications is still fairly limited. The authors have mainly preferred to demonstrate their methods on some UCI repository datasets. It would be interesting, however, to see applications of these techniques in domains such as mining gene expression and other biological data, financial databases, and text mining.

IV. MOEAs FOR OTHER DATA MINING TASKS

Most MOEA-based data mining techniques have considered the four areas (feature selection, classification, clustering and association rule mining) as discussed in [1] and this paper. However, besides these, MOEAs have also been applied to many other data mining tasks. These tasks include ensemble learning, biclustering/co-clustering, and so on. In this section, we discuss some of the MOEA-based approaches that have been applied in these areas.

A. MOEAs for Ensemble Learning

Ensemble learning refers to the task of combining the predictions of individual classifiers in some way to obtain more robust predictions. The inherent strength of MOEAs to produce a set of trade-off classifiers in the form of a non-dominated set has made them popular in designing ensembles of classifiers. The general idea is to use MOEAs to yield a set of diverse classifiers encoded in the chromosomes of the final non-dominated front, and then make the final prediction by combining the predictions of these individual classifiers through a majority vote. Integration of diverse classifiers through ensemble learning may prevent overfitting and may provide better classification accuracy and improved robustness compared to the predictions based on a single classifier [82].

The general framework for ensemble classification design is to produce a diverse set of classifiers by optimizing certain

contradictory criteria. A popular approach in this regard is to optimize an artificial neural network-based classifier or MLP with respect to the complexity of the classifier and its predictive accuracy. The complexity of an MLP refers to the number of hidden layer units and weights of the connections. This approach has been adopted in [83]–[87]. In [83], a Pareto-frontier differential evolution (PDE) algorithm [88] is used to develop the memetic Pareto artificial neural network (MPANN) method. In MPANN, the authors performed a comparison between two multiobjective formulations to the formation of neuro-ensembles. In the first formulation, the training set is split into two non-overlapping stratified subsets. The objectives are to minimize the training error on each subset. In the second formulation, they add random noise to the training set to form a second objective. They also compared there algorithm with a negative correlation learning (NCL) algorithm for training an ensemble of ANNs using backpropagation [89]. In [84], the problem of regularization of neural network classifiers is addressed and as a bi-product, a neural network ensemble is generated. They compare the use of NSGA-II and a dynamic weighted aggregation method in generating the ensemble by optimizing two objectives, that is, training mean squared error and number of network connections. A similar approach for the generation of an ensemble of MLPs is found in [85] with different objective functions to be optimized. Here, the authors minimized Type-I and Type-II errors simultaneously, which refer to the number of false positives and number of false negatives, respectively. The algorithm, called MG-Prop, is designed based on the single front genetic algorithm (SFGA) proposed in [90]. The authors showed that this ensemble works well for class-imbalanced data. In [86], an algorithm called diverse and accurate ensemble learning algorithm (DIVACE) is proposed. DIVACE uses ideas from NCL [89] and MPANN [83], and formulates the ensemble learning problem as a multiobjective problem explicitly within an evolutionary setup. The aim of the algorithm is to find good a trade-off between diversity and accuracy to produce an ensemble of neural network classifiers. The diversity is modeled as a correlation penalty [89]. The authors showed that DIVACE performs better than the MPANN algorithm. In a recent work, a multiobjective genetic algorithm based artificial neural network ensemble (MANNE) method is proposed in [87] for intrusion detection. The authors optimized neural network classifiers using NSGA-II with two objective functions, namely detection rate and false positive rate to generate the ensemble. The method was compared with a decision tree and its ensembles using bagging and boosting methods.

Another popular approach for building MOEAs-based classifier ensembles is to encode a feature subset and other parameters in a chromosome and use some classifier as a wrapper to compute the objective functions (usually classification accuracy and feature subset size). The idea is to evolve a set of non-dominated classifiers with respect to the trade-off between accuracy and feature subset size. Each of them works on a specific subspace of the dataset and can be used to form an ensemble of classifiers [91]–[93]. In [91], the authors used MLP as the wrapper and the classification accuracy and feature

subset size as the two objective functions to be optimized. In [92], the authors considered both the supervised and the unsupervised cases. For the supervised case, they have used MLP as the wrapper and as objective functions the same defined in [91]. In the unsupervised case, they have used the K-means clustering algorithm and used DB index and number of features as the objective functions. Experimental studies established performance improvement compared to classical bagging and boosting techniques. In [93], on the other hand, three classifiers have been used as wrappers, namely decision tree, SVM, and MLP. Two objective functions used are average accuracy of these three classifiers and their consensus accuracy. The authors demonstrated that the proposed method outperforms single objective GA-based methods designed with one of these classifiers as wrapper.

B. MOEAs for Biclustering

A variant of clustering, called biclustering or co-clustering [94], aims to capture local structures within a dataset. A clustering algorithm groups similar objects where the similarity is computed based on all attributes. On the contrary, the goal of a biclustering algorithm is to find a group of objects that are not necessarily similar over all the attributes, but are similar based on a subset of attributes. Hence, biclustering can be thought of as the simultaneous clustering of objects and attributes. Biclustering algorithms have several applications in different real-life domains such as text mining [95], recommender systems [96] and collaborative filtering [97]. However, almost all the MOEAs for biclustering are applied for mining biclusters from microarray gene expression data [94]. Here, we review some of these algorithms.

As the biclustering problem requires several objectives to be optimized such as mean squared residue (MSR) (a coherence measure) [98], volume, row variance, and so on, this problem can be posed as a multiobjective optimization problem in a straightforward manner. In recent years, a number of studies have been done in solving biclustering problems using MOEAs. In [99], a multiobjective GA-based biclustering technique is proposed. The authors use a binary string of length $\mathcal{G} + \mathcal{C}$, where $\mathcal{G}$ and $\mathcal{C}$ denote the number of genes and number of conditions/samples/time points, respectively. If a bit position is 1, then the corresponding gene or condition is selected in the bicluster and if a bit position is 0, the corresponding gene or condition is not selected in the bicluster. The algorithm optimizes the MSR and volume of the biclusters simultaneously, in order to obtain coherent and large biclusters. The algorithm uses NSGA-II as the underlying multiobjective optimization tool. Cheng and Church's biclustering algorithm [98] has been used as a local search strategy.

In [100], a different encoding policy is adopted. The algorithm is termed multiobjective GA-based biclustering (MO-GAB). Here, each string has two parts; one for clustering the genes, and another for clustering the conditions. If M and N denote the maximum number of gene clusters and the maximum number of condition clusters, respectively, then the length of each string is $M + N$. The first M positions represent the M cluster centers for the genes, and the remaining N positions represent the N cluster centers for the

conditions. Thus, a string, which looks like the following, $\{gc_1 \ gc_2 \ \dots \ gc_M \ cc_1 \ cc_2 \ \dots \ cc_N\}$, where each gc_i, $i = 1 \dots M$ represents the index of a gene that acts as a cluster center of a set of genes, and each cc_j, $j = 1 \dots N$ represents the index of a condition that acts as a cluster center of a set of conditions. A string that encodes M gene clusters and N condition clusters, represents a set of $M \times N$ biclusters, taking each pair of gene and condition clusters. Each pair $< gc_i, cc_j >, i = 1 \dots M, \ j = 1 \dots N$, represents a bicluster that consists of all genes of the gene cluster centered at gene gc_i, and all conditions of the condition cluster centered at condition cc_j. During the fitness computation, the gene and condition clusters encoded in the chromosome are updated through K-means at each iteration. Two objectives, that is, $\frac{MSR(I,J)}{\delta}$ and $\frac{1}{1+VAR(I,J)}$ are optimized simultaneously. This approach also adopts NSGA-II for optimization. Single-point crossover and random replacement mutation have been used as the evolutionary operators. MOGAB also uses NSGA-II as its underlying optimization tool. In [101], a fuzzy version of MOGAB is proposed. Fuzzy versions of *MSR* and row variance have been simultaneously optimized.

Reference [102] proposed the sequential multiobjective biclustering (SMOB) algorithm. The authors adopted binary encoding in this case. Three objective functions, that is, mean squared residue, volume, and row variance were optimized. In [103], a hybrid multiobjective biclustering algorithm that combines NSGA-II and a estimation of distribution algorithm (EDA) [104] for searching biclusters was proposed. The volume and *MSR* of the biclusters are simultaneously optimized. In [105], an NSGA-II based multiobjective biclustering algorithm was proposed. This approach uses integer encoding. Here, the integers represent the indices of the rows and the columns of the dataset. The objectives optimized are the similarity within the biclusters and the volume of the biclusters.

Although different biclustering approaches are proposed using MOEAs, there has been no effort to compare them systematically. MOEA-based biclustering algorithms have been compared with respect to standard single-objective evolutionary biclustering approaches as well as with respect to other non-evolutionary algorithms based on several criteria. However, comparative studies among different MOEA-based approaches are practically non-existent. These algorithms differ in their encoding strategies, objective functions, evolutionary operators and underlying MOEAs. Therefore, some studies to compare their performance would be beneficial for the users to select the most suitable method for their applications.

C. Other MOEAs-Based Data Mining Approaches

There are a few additional areas of data mining where MOEAs have been applied, but they are not well-studied still now. One such area is feature extraction or construction. Feature extraction or construction refers to the task of creation of new features from functions of the original features. Feature selection can be considered a special case of feature extraction. In [106], the problem of feature extraction for recognizing isolated handwritten symbols is posed as a multiobjective optimization problem, and a multiobjective genetic algorithm is proposed to solve the problem. The proposed algorithm has been shown to outperform human experts. However, not much progress has been noticed in this area, using MOEAs.

Subgroup discovery is another data mining problem where the aim is to mine fuzzy rules for subgroup discovery. These fuzzy rules help to represent the knowledge about patterns of interest which is explanatory and understandable to the expert. A few MOEA-based approaches have been proposed for this purpose over the last few years [107]–[109]. The objective is to optimize different rule-interestingness criteria as in ARM.

MOEAs have also been used for regression. In [110], an MOEA-based approach for obtaining linguistic fuzzy rule-based regression models from imprecise data is proposed. Here, each chromosome encodes one rule (Michigan approach), which competes with others in terms of maximum coverage and fitting. The knowledge base is formed through cooperation of individuals in the population. In a similar work [111], the authors proposed a multiobjective genetic fuzzy system (GFS) to learn the granularities of fuzzy partitions, for tuning the membership functions (MFs), and for learning the fuzzy rules for a regression problem. The proposed method uses dynamic constraints. This enables three-parameter membership function tuning for improved accuracy and guarantees the transparency of fuzzy partitions at the same time.

Another application of MOEAs has been found in outlier detection. In [112], a multiobjective GA is proposed for outlier detection. The MOEA in this case is mainly employed as an effective search method in unsupervised learning for finding outlying subspaces from training data. Besides this, MOEAs have also been used in soft subspace clustering [113], [114]. However, MOEAs have been applied in these areas only very recently and much more work is still needed.

V. FUTURE DIRECTIONS

Although MOEAs are being applied in data mining tasks over the past decade and the literature is already quite rich, still some important future research issues remain open. Here, we discuss some relevant and important research topics to be addressed in the future. First of all, most of the studies have focused on comparing the proposed MOEA-based data mining techniques with existing non-evolutionary or traditional single-objective evolutionary techniques. However, as discussed before, practically none of the studies have compared the performance of different MOEA-based algorithms for different data mining tasks in a systematic way. Thus, for a novice user, it is difficult to judge which algorithm he/she should use for a particular task in hand. Possible reasons for unavailability of these studies may be the lack of publicly available softwares/codes, difficulty in reproducing the results, use of a variety of encoding strategies, objective functions, evolutionary operators, and final solution selection. Thus, a systematic comparison to guide new users in choosing a suitable method for his/her application would be very valuable as it is still missing in the specialized literature.

In the majority of the studies on MOEA-based data mining, the performance of the algorithms has been reported based on

the quality of the obtained result in terms of some metrics. However, to address large scale data mining problems using MOEAs, such as clustering large images or selecting genes from gene expression data containing several thousands of genes, along with the quality measure, the efficiency of the algorithm is also an important concern. Evolutionary algorithms have long been criticized for consuming large amounts of computational time as compared to other heuristics. Moreover, MOEAs typically require more computational time than single-objective evolutionary algorithms. Almost none of the MOEA-based data mining studies reviewed here has considered providing a systematic time complexity analysis. Therefore, it is difficult to compare different MOEAs in terms of time usage. Computational efficiency of MOEAs used in data mining is indeed another promising research area. For example, one could incorporate local search strategies in MOEAs to improve the convergence rate. Many of the MOEA-based data mining techniques currently available have already adopted this strategy, especially in clustering [15] and biclustering [99]. Another possibility is the efficient parallelization of MOEAs using multiple processors. A few studies in this regard have been done for ARM [115] and clustering [116], but more studies are needed to explore other application areas. Another way to reduce the search time for the MOEAs used in data mining is to use some appropriate stop criterion for them, instead of a fixed number of generations (as traditionally done). Some approaches are currently available for defining stop criteria for MOEAs (see, for example, [117]), but none of them have been adopted in data mining yet.

Most of the data mining problems have many objectives to be optimized. For example, a rule mining problem has objectives such as support, confidence, rule length, comprehensibility, interestingness, lift, etc., whereas a clustering algorithm may optimize a number of cluster validity measures simultaneously. However, few MOEA-based data mining problems have been posed with more than three objective functions [49]. Traditional MOEAs such as NSGA-II, SPEA2 and PAES are known to have difficulties solving problems with four or more objectives, and other approaches are required to deal with them (see [50]). The use of such approaches in data mining is, however, still unavailable in the specialized literature.

Another research direction that deserves attention is interactive data mining using MOEAs. In interactive data mining, during the execution of a data mining algorithm, it interacts with a human decision maker to learn in a gradual way. It might be very useful to incorporate such interactions in MOEA-based data mining algorithms when some expert user is available for the problem at hand. Such an approach has been proposed in [52], where the authors have developed an interactive MOEA-based clustering approach called interactive multiobjective clustering (IMOC). In IMOC, the algorithm interacts with a human decision maker during its execution in order to learn the suitable set of cluster validity indices for the input dataset. Thus, different sets of validity measures may be chosen for different datasets. The method has been shown to perform well in clustering of gene expression data. Similar interactive MOEAs may be developed for other data mining tasks such as feature selection, classification and rule mining.

VI. Conclusion

In this two-part paper, we surveyed several MOEAs used for four primary data mining tasks namely feature selection and classification (discussed in Part I [1]), and clustering and association rule mining (discussed in Part II). The main focus has been on the chromosome representation, objective functions, evolutionary operators, and final solution selection from the non-dominated front. Moreover, a comparative overview among different methods in each category along with some real-life applications are provided. Additionally, in this part, several other MOEA-based data mining tasks, such as ensemble learning, biclustering, feature extraction, sub-group discovery etc. have been reviewed. Finally, we have discussed a number of future research areas that deserve attention from the researchers working on the development of MOEAs-based data mining algorithms.

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