New Developments in Fuzzy Sets, Intuitionistic Fuzzy Sets, Generalized Nets and Related Topics
Volume II: Applications

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Differential evolution in clustering with constraints

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Abstract

Computer aided data mining, and in particular methods of clustering, its widely used technique, develop very rapidly nowadays. Basically, clustering is an unsupervised learning technique. However, there is a growing interest in considering the case where there is a partial knowledge on the actual grouping of the objects available. This knowledge may take form of the hints on the co-occurrence of object in the same clusters. In this paper we propose to solve this problem of constrained clustering using the technique of differential evolution (DE). We show the efficiency and usefulness of differential evolution in hard- and soft-constrained clustering tasks. Some practical examples of the clustering problems are examined and results obtained are compared to two variants of a classic clustering technique, the k-means algorithm.

Keywords: differential evolution, metaheuristics, constrained clustering, k-means.

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1 Introduction

In recent years data mining is a very rapidly developing field of modern computer science, mainly due to the rapid growth of computational capabilities of modern computers and growing size and number of data collections available. Data mining's most important goal is to find regularities and patterns of all kinds, which are invisible to humans, mainly due to their limited computing capabilities and the volume and multidimensionality of considered datasets. One of the most widely used techniques of data mining is clustering.

Clustering procedure is basically used for preliminary data processing and unsupervised classification. The task of a clustering algorithm is to divide a set of objects into a number of clusters with the assumption that a single cluster contains objects as similar as possible to each other (*maximising* the similarities) while the objects assigned to different clusters differ significantly (*maximising* the dissimilarities). Thus, clustering problem can be stated as an *optimization task*.

Although clustering is generally considered as unsupervised technique, in many applications there is some background knowledge which should be utilised. Inclusion of that a priori knowledge in the process of clustering allows for significant improvement in quality of solutions and its adaptation to the conditions of the problem. However, it increases the difficulty of the problem, inter alia through forcing many local minima. As a result a new data mining task, a clustering with constraints, is formulated.

The huge size of the solution space and significant computational complexity, along with the size and multidimensionality of the datasets mentioned earlier, results in growing interest in the implementation of metaheuristic optimization methods in clustering problem (see e.g. [2, 3]).

In this paper we present the efficiency and stability of a modern metaheuristic, differential evolution [11], in constrained clustering task. Obtained results are discussed, especially in terms of constraints influence on the clustering accuracy and its robustness, and compared to the results of modifications of classic k-means algorithm - the COP k-means [13] for hard-constrained task, and the KSC [15] for soft approach.

2 Clustering with constraints

The considered data mining task, the clustering with constraints, is a special case of clustering problem [7, 5], which is defined as follow:

Definition 1 ***(Clustering problem)***

Let $\mathbf{O} = \{o_1, o_2, \ldots, o_n\}$ *be a set of* n *p-dimensional data instances and let* $\mathbf{X}_{n\times p}$ *be the matrix describing those data. Each* i*th object is characterised by a* p*-dimensional attributes vector* $\mathbf{x}_i$ $(i = 1, 2, \ldots, n)$*, where each element* x_{ij} *in* $\mathbf{x}_i$ *corresponds to the value of* j*th attribute of the* i*th instance.*

Given $\mathbf{X}_{n\times p}$*, the feasible solution is a partition* $G = \{C_1, C_2, \ldots, C_k\}$ *(i.e.:* $C_i \neq \emptyset$*,* $\forall i$*;* $C_i \cap C_j = \emptyset$*,* $\forall i \neq j$*;* $\bigcup_{i=1}^{k} C_i = \mathbf{O}$*) assigning each instance* o_i $(i = 1, 2, \ldots, n)$ *to a certain cluster* C_j $(j = 1, 2, \ldots, k)$*. The set of all feasible solutions is denoted as* $\mathbf{G} = \{G^1, G^2, \ldots, G^s\}$*.*

As clustering can be stated as an optimisation problem, let $f(G)$ *be the quality function (also called fitness function) of a partition* G*, which basically measures how well similar objects are placed in the same clusters and, at the same time, dissimilar objects are placed in separate clusters.*

Given $\mathbf{G}$ *and* $f(G)$*, the goal of a clustering algorithm is to find a partition* G^* *that* minimises *the function* $f(G)$*:*

$$G^* = \arg\min_{G\in\mathbf{G}} f(G) \tag{1}$$

2.1 Hard and soft pairwise constraints

In clustering with constraints it is assumed that there is a background knowledge available which imposes, or only suggests, some constraints on possible grouping of the objects. These constraints may be expressed in various ways. Now we will discuss one of their general form which will be adopted in this paper.

We consider pairwise constraints, which seems to be a most general representation. Numerous types of relations encountered in the clustering problem can be represented as a set of pairwise constraints [14, 1]. They are commonly implemented as two kinds: *must-link* (denoted *ML* later) and *cannot-link* (*CL*).

ML constraint indicates that the two data instances involved *must /should* be placed in the same cluster, whereas CL indicates two instances which *cannot/should not* belong to the same cluster.

The constraints specified can be stated as *hard* or *soft* constraints, indicating whether it is required or only advisable to preserve them.

Hard constraints are conditions that *must* be satisfied by the feasible solutions (see Def. 1), to be obtained using the clustering algorithm. A ML constraint over a pair of data instances indicates, that the output partition *must* assign those instances to the same cluster. A CL constraint indicates, that involved data instances *cannot* be assigned to the same cluster.

Soft constraints, often referred to as *preferences*, are statements that may or may not be satisfied by the feasible solution. The strength of the soft constraint is modelled by assigning a value $s \in [0, 1]$ ($s \in [-1, 1]$ if we model both ML and CL constraints simultaneously), where 1 indicates hard constraint (that must be satisfied) and 0 means "no constraint". A solution should satisfy as much of the soft constraints as possible.

Definition 2 ***(Must-link and cannot-link constraints)***

Let $\mathbf{Con}_{ML} = \{Con_{ML_1}, Con_{ML_2}, \ldots, Con_{ML_{nML}}\} \subseteq \mathbf{O} \times \mathbf{O}$ *be the* ML constraints set *and* $\mathbf{Con}_{CL} = \{Con_{CL_1}, Con_{CL_2}, \ldots, Con_{CL_{nCL}}\} \subseteq \mathbf{O} \times \mathbf{O}$ *be the* CL constraints set, *where* Con_{*_i} *denotes a triple* $\langle o_k, o_l, s\rangle$, $k \neq l$, *where* s *is the constraint strength (*$s = 1$ *in hard-constrained approach and* $s \in (0, 1]$ *in soft approach) and* o_k *and* o_l *are instances affected by the constraint.*

For each Con_{ML_i}, *if one data instance of the involved pair is assigned to the cluster* C_j *then the second one must/should also belong to it:*

$$\langle o_k, o_l, s\rangle \in \mathbf{Con}_{ML} \wedge o_k \in C_j \Rightarrow o_l \in C_j, \tag{2}$$

and if it is not the case then there is a penalty s.

For each Con_{CL_i}, *if one data instance of the involved pair is assigned to the cluster* C_j *then the second one cannot/should not belong to it:*

$$\langle o_k, o_l, s\rangle \in \mathbf{Con}_{CL} \wedge o_k \in C_j \Rightarrow o_l \notin C_j, \tag{3}$$

and if it is not the case then there is a penalty s.

Equivalently, $\mathbf{Con}_{ML}$ and $\mathbf{Con}_{CL}$ may be treated as fuzzy sets of pairs (o_k, o_l) such that $\mu(o_k, o_l) = s$.

The task of clustering with constraints may be defined as in Def. 1 but assuming that the function $f(G)$ now takes into account a penalty for violating imposed constraints.

3 Differential Evolution and reference methods

3.1 Differential Evolution

Differential Evolution [11] (denoted *DE* later) is a metaheuristic method, which has proved effective in multidimensional, real-valued optimization problems [12]. It is an iterative optimization method based on evolutionary mechanisms. The most important feature of DE, giving an advantage over conventional optimization algorithms (e.g. gradient methods), is the lack of requirements for the existence of a gradient or a continuity of optimised functions, which is essential for clustering task.

DE is a population based technique where a population of possible solutions is represented by real-coded chromosomes. In its basic version, in each iteration, for each individual $\mathbf{x}_i$ three other individuals $\mathbf{x}_{r1}, \mathbf{x}_{r2}, \mathbf{x}_{r3}$ are randomly selected and a new solution candidate $\mathbf{c}_i$ is created by mutating one of them with the difference (also *differential vector*) of the remaining two:

$$\mathbf{c}_i = \mathbf{x}_{r1} + F(\mathbf{x}_{r2} - \mathbf{x}_{r3}). \tag{4}$$

The candidate is then crossed-over with $\mathbf{x}_i$ and individual with higher quality value is selected to next generation.

Algorithm 1 presents the DE procedure.

Algorithm 1: Differential Evolution

Procedure COP-DE

Set $t \leftarrow 0$;
Initialise pop_0 with Np random individuals $\mathbf{x}_1, \ldots, \mathbf{x}_{Np}$;
while *Termination condition* **do**
  foreach $\mathbf{x}_i \in pop_t$ **do**
    Mutation: create candidate $\mathbf{c}_i$;
    Crossover: cross-over candidate $\mathbf{c}_i$ with $\mathbf{x}_i$;
    Selection
      Evaluate $f(\mathbf{x}_i)$;
      Evaluate $f(\mathbf{c}_i)$;
      if $f(\mathbf{c}_i) > f(\mathbf{x}_i)$ **then** Select $\mathbf{c}_i$;
      else Select $\mathbf{x}_i$;
  $t++$;
Return best individual $\mathbf{x}_{best}$;

DE is straightforward to implement, mainly due to the small number of parameters. Apart from the standard ones of this class of algorithms – population size Np and maximum number of generations t_{max} – DE requires two parameters (coefficients): scaling factor $F \in \mathbb{R}$, characterizing the influence of *differential vector* on the mutated individual when generating candidate $\mathbf{c}_i$, and the crossover coefficient $Cr \in \mathbb{R}$, which determines the probability of crossover for each attribute/dimension (for details see [11, 8]).

A number of variants of DE which differ in mutation and crossover operators has been proposed [8]. This work employs the results of our previous studies, indicating that the choice of the variant had a marginal impact on the quality of the results [4]. They confirmed the results obtained by other authors (e.g. [7]). Therefore, in this paper we use the simplest to implement variant: DE/rand/1 with exponential crossover [8].

Selection of DE parameters was also based on our previous studies [4], where we show that precise tuning of them has marginal significance, because results differ only by about 2.5% (for $F \in [0,1]$ and $Cr \in [0,1]$). In all cases the coefficients were set as follow: $F = 0.3$, $Cr = 0.8$.

3.2 Differential Evolution in clustering – chromosome representation

In the present work, we assume that the proper number of clusters k is known. This allows for strict comparison between results obtained by DE and k-means in scope of classification correctness.

To take full advantage of the real-valued character of differential evolution the solution is encoded in the chromosome as a vector of coordinates of the centroids of clusters:

$$\mathbf{x}_i = (\mu_1, \mu_2, \ldots \mu_k)\,, \tag{5}$$

where $\mu_i = \left(\mu_{i1}, \mu_{i2}, \ldots \mu_{ip}\right)$ denotes a vector of coordinates of an ith cluster centroid.

This allows for a direct mutation and crossover of the individuals in line with the assumptions of DE technique.

3.3 Constraint inclusion - fitness function

For all optimisation metaheuristics definition of the fitness function is crucial. Function $f(G)$ (the quality function, see Def. 1) must take into account the conditions of similarity and dissimilarity of data instances belonging to the same/different clusters and the number (or strength in soft approach) of constraints violated.

We use $f(G)$ minimising the combination of classic total variance V of the partition and the penalty for constraints violation, CV, as proposed in [15] for the KSC algorithm:

$$f(G) = (1-w)\frac{V(G)}{V_{max}} + w\frac{CV(G)}{CV_{max}}, \tag{6}$$

where variance $V(G) = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} \mathrm{dist}(\mathbf{x}, \mu_{\mathbf{i}})$, and $CV(G)$ is the number of violated constraints (in hard approach) or the sum of violated constraints strengths (soft) and CV_{max} is its maximum value. The quantities V and CV are then normalised by their maximum values (the V_{max} is calculated for the case of assigning all instances into one cluster). The w parameter, specifying the importance of variance minimisation versus constraint preservation, was set to 0.5 in all cases.

3.4 Reference methods - COP k-means and KSC

As reference methods for constrained clustering task we choose a modifications of classic k-means algorithm. For the hard-constrained approach results are compared with the COP k-means [13], and for soft constraints the KSC [15] was used for comparison. Both methods differ form the classic k-means in the assigning instances to clusters step. The COP k-means assigns each instance to the closest cluster such that no constraints are violated (if no such cluster exists method returns failure), and the KSC chooses the cluster that optimises the function $f(G)$ (6) introduced earlier.

4 Experiments setup

For comparison of the methods the same resources were provided for both the DE and COP k-means/KSC. As the so-called bottleneck of the algorithms' performance in most studies (e.g. [7]) is considered the evaluation of the quality of an individual.

According to this observation and preliminary tests, as a termination condition of DE the maximum number of iterations $t_{max} = 300$ is used, which together with the population size $Np = 50$ requires the 15,000 quality evaluations.

For the COP k-means/KSC methods the number of iterations corresponding to the same number of quality function evaluations were set.

In order to minimise the impact of the stochastic nature of the methods used on the results the tests were run 20 times for each dataset.

4.1 Considered datasets and constraints generation

The effectiveness of the considered methods is studied over the 5 real-world clustering problems. The datasets are obtained from UCI Machine Learning Repository [6]. Prior to clustering, data sets have been pre-processed: non-numeric attributes were mapped by "1-out-of-n" method [9] and the values of attributes were normalised to the interval $[0, 1]$.

Table 1: Description and characteristics of the datasets

No.	k	p	n	Name and URL
1	3	4	150	Iris Data Set `http://archive.ics.uci.edu/ml/datasets/Iris`
2	2	9	683	Breast Cancer Wisconsin (Diagnostic) DS `http://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)`
3	2	9	958	Tic-Tac-Toe Endgame Data Set `http://archive.ics.uci.edu/ml/datasets/Tic-Tac-Toe+Endgame`
4	6	4	4435	Statlog (Landsat Satellite) Data Set `http://archive.ics.uci.edu/ml/datasets/Statlog+(Landsat+Satellite)`
5	6	30	600	Synthetic Control Chart Time Series `http://archive.ics.uci.edu/ml/datasets/Synthetic+Control+Chart+Time+Series`

The description and characteristics of the datasets are presented in Table 1, where n, k and p denote the number of data instances, number of clusters and dimension of data space, respectively.

To prevent the influence of random constraint generation on the results of clustering for each dataset the constraints were randomly chosen for each algorithm's run. Two instances were drawn and constraint was generated according to their labels (the same labels - ML constraint, different - CL constraint).

For the soft-constrained case the strengths of the constraints, s, were randomly chosen depending on the distance between instances involved:

$$s_{ML}(\mathbf{x}_i, \mathbf{x}_j) = 1 - \frac{\mathrm{dist}(\mathbf{x}_i, \mathbf{x}_j)}{2 \cdot \mathrm{dist}(\mathbf{x}_i, \mathbf{x}_j) + \delta}, \tag{7}$$

$$s_{CL}(\mathbf{x}_i, \mathbf{x}_j) = 0.5 + \frac{\mathrm{dist}(\mathbf{x}_i, \mathbf{x}_j)}{2 \cdot \mathrm{dist}(\mathbf{x}_i, \mathbf{x}_j) + \delta}, \tag{8}$$

where $\delta \in [0.5, 1]$ is a random value.

4.2 Clustering evaluation - Rand index

The post-processing step is carried out in order to reliably evaluate results received through the Differential Evolution and k-means algorithm in scope of clustering and classification. To calculate agreement between the results of clustering received and the labels of each data instance the Rand index is used (Rand [10]).

Given a set of n elements $\mathbf{O} = \{o_1, o_2, \ldots, o_n\}$ and two partitions of $\mathbf{O}$, G^i and G^j, each partition is viewed as a $n * (n-1)/2$ pairwise decisions whether o_i and o_j are assigned to the same or to different clusters.

Let a be the number of the pairs of instances with the same label are assigned to the same cluster, and let b be the number of instances with different labels are assigned to different clusters.

The Rand index of partitions G^i and G^j is calculated as follow:

$$R(G^i, G^j) = \frac{a+b}{n * (n-1)/2}, \tag{9}$$

which reaches values in range $[0, 1]$. It represents percentage of correctly grouped instances - $R = 0$ means no agreement with the labels (0%), whereas $R = 1$ represents full agreement (100%).

5 Experimental results

Figures 1-2 present the results averaged for all datasets. The dark curves are the mean values of Rand index obtained for different numbers of constraints imposed (expressed as the percentage of all constraints considered), while the shaded areas show their standard deviation. Darker shading corresponds to the DE results.

Presented results clearly show the advantage of DE over the COP k-means and KSC algorithms, particularly in hard-constrained problem, which is more complex due to introduction of a considerable amount of local minima created by included constraints and instances previously assigned to clusters. The inclusion of constraints provides better results for both hard- and soft-constrained problem when using the DE.

The COP k-means in hard-constrained case provides results worse than DE by about 30-60% (and their 25% higher standard deviation). Its results improve in relation to the unconstrained case only after including $\tilde{1}3\%$ of the constraints, yet still remaining worse than DE's. The main reason for this poor performance of COP k-means method is that it often falls into local minima mentioned earlier. This artificial local minima are avoided by DE, which, by its evolutionary nature, utilises them in the process of evaluating a solution quality.

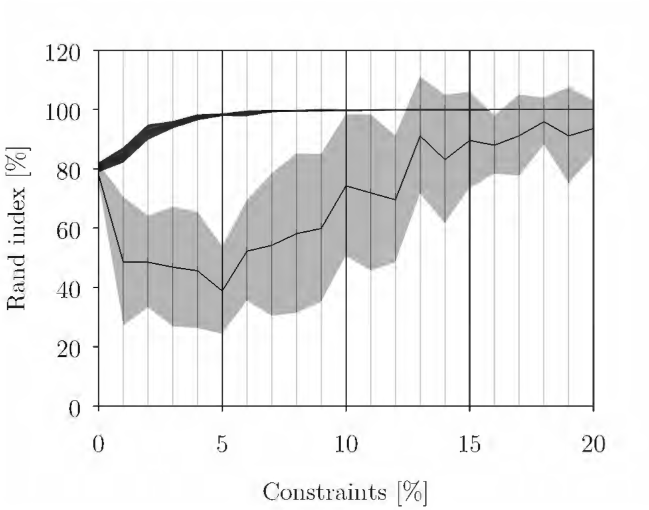

Figure 1: Results for hard-constrained problem. The DE is compared here with the COP k-means algorithm.

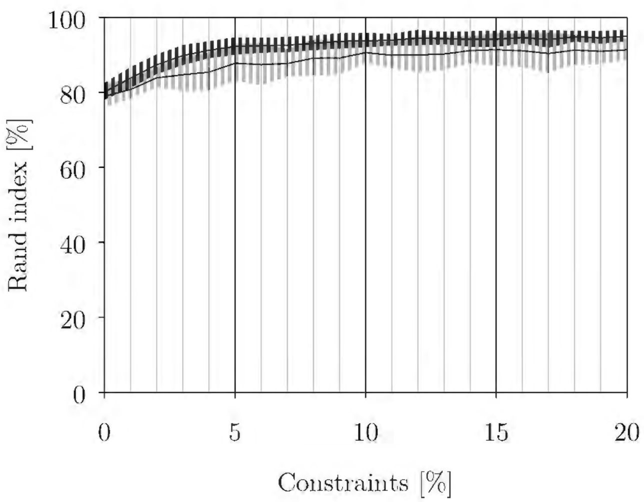

Figure 2: Results for soft-constrained problem. The DE is compared with the KSC algorithm.

In the soft-constrained approach both the DE and KSC benefit from constraints inclusion. But still DE provides results better by about 5% and 2–3% smaller standard deviation. Although this improvement is laden with a substantial increase of resources needed, it is still worth paying attention to DE because of it's great potential of development, which will allow for reduction of the resources needed (parallelisation, self-adjusting of population size, etc.).

6 Conclusions

In this paper the concept of the application of Differential Evolution to pairwise constrained (both hard and soft) clustering is presented. DE is compared to the modifications of the k-means algorithm, the COP k-means and KSC, in terms of results' agreement with original data labels and robustness of results. The real clustering and classification problems based on datasets from the UCI Machine Learning Repository are considered.

Results obtained allow us to consider the usage of novel metaheuristics, such as DE, in considered task as legitimate. DE provides more accurate and robust partitions of datasets both in hard- and soft-constrained approaches. Although this improvement is laden with a substantial increase of resources required, it is advisable in most data mining applications.

Moreover, DE (and other metaheuristics) offer great potential of development in scope of reduction of the resources needed - parallelisation, self-adjusting of population size, etc. Also simplifying DE variants is worth consideration. The results obtained in our earlier studies suggest that this should not significantly affect the quality of the results of clustering.

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The papers presented in this Volume 2 constitute a collection of contributions, both of a foundational and applied type, by both well-known experts and young researchers in various fields of broadly perceived intelligent systems.
It may be viewed as a result of fruitful discussions held during the Tenth International Workshop on Intuitionistic Fuzzy Sets and Generalized Nets (IWIFSGN-2011) organized in Warsaw on September 30, 2011 by the Systems Research Institute, Polish Academy of Sciences, in Warsaw, Poland, Institute of Biophysics and Biomedical Engineering, Bulgarian Academy of Sciences in Sofia, Bulgaria, and WIT - Warsaw School of Information Technology in Warsaw, Poland, and co-organized by: the Matej Bel University, Banska Bystrica, Slovakia, Universidad Publica de Navarra, Pamplona, Spain, Universidade de Tras-Os-Montes e Alto Douro, Vila Real, Portugal, and the University of Westminster, Harrow, UK:

Http://www.ibspan.waw.pl/ifs2011

The consecutive International Workshops on Intuitionistic Fuzzy Sets and Generalized Nets (IWIFSGNs) have been meant to provide a forum for the presentation of new results and for scientific discussion on new developments in foundations and applications of intuitionistic fuzzy sets and generalized nets pioneered by Professor Krassimir T. Atanassov. Other topics related to broadly perceived representation and processing of uncertain and imprecise information and intelligent systems have also been included. The Tenth International Workshop on Intuitionistic Fuzzy Sets and Generalized Nets (IWIFSGN-2011) is a continuation of this undertaking, and provides many new ideas and results in the areas concerned.

We hope that a collection of main contributions presented at the Workshop, completed with many papers by leading experts who have not been able to participate, will provide a source of much needed information on recent trends in the topics considered.

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