Heterogeneous Transfer Learning in Ensemble Clustering

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Abstract. This work proposes an ensemble clustering method using transfer learning approach. We consider a clustering problem, in which in addition to data under consideration, "similar" labeled data are available. The datasets can be described with different features. The method is based on constructing meta-features which describe structural characteristics of data, and their transfer from source to target domain. An experimental study of the method using Monte Carlo modeling has confirmed its efficiency. In comparison with other similar methods, the proposed one is able to work under arbitrary feature descriptions of source and target domains; it has smaller complexity.

Keywords: clustering; transfer learning; ensemble of algorithms; co-association matrix

1 Introduction

In machine learning, there is a fairly large number of models, methods and algorithms based on different approaches. Topical areas of research are transfer learning aimed at improving the quality of decisions by the usage of additional information from similar field of study, and ensemble clustering aspiring to increase the quality and stability of clustering results.

In transfer learning (closely related to domain adaptation and knowledge transfer), the basic idea is to use additional data (called source data) which is similar, in a certain sense, to the data of interest (target data). For example, one may use digital images of the same landscape but at other moments of time, or utilize data and results of text documents classification in a certain language, to documents written in another language.

Within this direction, there are various ways of setting the problem, for example, when one has (or has not) information about class labels in target and source domains; for the same features (homogeneous domain adaptation) or different feature descriptions (heterogeneous domain adaptation). As a rule, it
is assumed that the probability distributions on target and source domains do not coincide. Transfer learning methods are elaborated for pattern recognition problems, regression and cluster analysis [1]. Different approaches to knowledge transfer have been developed, for example, based on the usage of source examples with some adjustable weights for constructing decision functions when predicting the target sample; searching for common feature descriptions; making use of the assumptions about the coincidence of the distribution of some hyperparameters.

Ensemble clustering aims at finding consensus decision from multiple partition variants [2,3,4,5]. As a rule, this methodology gives robust and effective solutions, especially in the case of uncertainty in the data structure. Properly organized ensemble (even composed of "weak" algorithms) significantly improves the overall clustering quality.

We consider a clustering problem, in which, in addition to the target dataset, one may use already classified dataset described by other features and belonging to another statistical population. A practical example is the segmentation of color image using a similar already segmented gray-scale image.

The problem of transfer learning with use of cluster ensembles was considered in [6]. In this work, the authors assume that source and target domains share common feature space and class labels. The authors of [7] suggest a general framework with arbitrary feature descriptions. However, the proposed algorithm has a cubic time complexity with respect to the maximum sample size of source and target domains.

In this paper, we propose an ensemble clustering method using transfer learning approach. The idea of the method is as follows. On the first stage of analysis, both target and source data are examined independently using a cluster ensemble, in order to identify stable structural patterns. This results in obtaining meta-features describing structural data characteristics. On the second stage, the relationships between the elements of coincide matrix of source data and their meta-features are revealed with use of supervised classification. On the next step, a transfer of the found dependencies from source to target domain is performed and the prediction of the coincidence matrix for target data is made. Finally, on the basis of the obtained predictions, the final clustering partition of target data is obtained.

In comparison with other similar methods, the proposed one is able to work under arbitrary feature descriptions of source and target domains; it has smaller complexity.

In the rest of the paper, we give a detailed description of the proposed method and describe the results of its experimental investigation.

2 Cluster analysis and knowledge transfer

2.1 Basic notation and problem statement

Consider a set \( T = \{a_1, \ldots, a_{N_T}\} \) of objects from some statistical population. Each object is described by a set of real-valued features \( X_1, \ldots, X_{d_T} \). Through
$x = x(a) = (x_1, \ldots, x_{d_T})$ we denote a feature vector for an object $a$, where $x_j = X_j(a)$, $j = 1, \ldots, d_T$, and through $X_T$ we denote data matrix $X_T = (x_{i,j})$, $j = 1, \ldots, d_T$, $i = 1, \ldots, N_T$. It is required to obtain a partition $P = \{C_1, \ldots, C_{K_T}\}$ of $X_T$ on some number of $K_T$ groups (clusters) in accordance to a given quality criterion. The number of clusters can be preset in advance or not; in this paper we assume the required number is a fixed parameter.

Suppose there is an additional dataset $S = \{b_1, \ldots, b_{N_S}\}$ where each object $b$ is described by real-valued features $X'_1, \ldots, X'_{d_S}$, and data matrix $X_S$ is given. A categorical attribute $Y$ is specified, denoting a class to which an object $b \in S$ belongs: $Y(b) \in \{1, \ldots, K_S\}$, where $K_S$ is total number of classes. By classification vector we understand a vector $Y = \{y_1, \ldots, y_{N_S}\}$, where $y_i = Y(b_i)$, $i = 1, \ldots, N_S$.

The set $T$ is called target data, and the set $S$ source data. It is assumed that $X_T$ and $X_S$ share some common regularities in their structure, which can be detected by cluster analysis and used as additional information when setting up the desired partition of $X_T$.

### 2.2 Cluster ensemble

Suppose we are able to create variants of the partitioning of $X_T$ into clusters using some clustering algorithm $\mu$. The algorithm works under different parameter settings, or, more generally, "learning conditions" such as initial centroids locations, subsets of selected features, number of clusters or random subsamples. On the $l$th run it gives a partition of $X_T$ on $K_l$ clusters, $l = 1, \ldots, L$, where $L$ is total number of runs.

For each pair of points $a_i, a_j \in X_T$ we define the value $h_T^l(i, j) = \mathbb{I}[\mu_l(x_i) = \mu_l(x_j)]$, where $\mathbb{I}[\cdot]$ is an indicator function: $\mathbb{I}[true] = 1$; $\mathbb{I}[false] = 0$, $\mu_l(x)$ is an index of the cluster assigned to a point $x \in X_T$ by the algorithm $\mu$ on $l$-th run. Let us calculate the averaged co-association matrix $H^T = (\bar{h}_T(i, j))$ with elements $\bar{h}_T(i, j) = \frac{1}{L} \sum_{l=1}^{L} h_T^l(i, j)$, $i, j = 1, \ldots, N_T$.

The next stage is aimed at constructing the final partition of $X_T$. Elements of the matrix $H^T$ are considered as measures of similarity between pairs of objects. To form the partition, any algorithm which uses these measures as input information can be used. In this paper, we apply ensemble spectral clustering algorithm \cite{8} based on a low-rank decomposition of the averaged co-association matrix which has near-linear time and storage complexity.

The basic steps of the used ensemble clustering algorithm EC are described below.

**Algorithm EC:**

**Input:**
- $X_T$: target data;
- $L$: the number of runs of the ensemble clustering algorithm;
- $\Omega$: the set of algorithm’s parameters;
- $K_T$: The required number of clusters in the partition of $X_T$.
Output: \( P = \{C_1, \ldots, C_{K_T}\} \): partition of \( X_T \).

Steps
1. Get \( L \) variants of clustering partition for objects from \( X_T \) by randomly choosing the algorithm’s parameters from \( \Omega \);
2. Calculate the averaged co-association matrix \( H^T \) in low-rank representation;
2. Using spectral clustering with low-rank represented matrix \( H^T \) as input, find a final partitioning \( P = \{C_1, \ldots, K_T\} \).

end.

2.3 Probabilistic properties of cluster ensemble

Suppose we have iid sample \( X = \{x_1, \ldots, x_N\} \) generated from a mixture of \( K \) distributions (classes). Suppose there also exists a ground truth (latent, directly unobserved) variable \( Y \) that determines to which class an element \( x_i \) belongs: \( Y_i \in \{1, \ldots, K\} \). Let \( Z(i, j) = I[Y_i \neq Y_j] \), where \( i, j = 1, \ldots, N \). Let algorithm \( \mu \) be randomized, i.e. it depends on a random set of parameters \( \Omega \in \Omega \), and the sample partitions are formed using independently selected statistical copies of \( \Omega \).

Each ensemble algorithm contributes to the overall collective decision. Denote by \( v_1(i, j) \) the number of votes for the union of \( x_i, x_j \) into same cluster; and by \( v_0(i, j) \) the number of votes for their separation. The value \( c(i, j) = I[v_1(i, j) > v_0(i, j)] \) shall be called the ensemble solution for \( x_i \) and \( x_j \) obtained in accordance with the voting procedure. Conditional probability of classification error for each pair is defined as \( P_{\text{err}}(i, j) = P[c(i, j) \neq Z(i, j)|X] \). The following property was proved in [9].

**Theorem.** Let us suppose that for any \( i, j \) \( (i \neq j) \) the symmetry condition is satisfied: \( P[h(i, j) = 1|Z(i, j) = 1] = P[h(i, j) = 0|Z(i, j) = 0] = q(i, j) \) where \( q(i, j) \) is the conditional probability of correct decision. If the condition of weak learnability \( 0.5 < q(i, j) \leq 1 \) holds, \( P_{\text{err}}(i, j) \rightarrow 0 \) as \( L \) approaches infinity.

Therefore, under certain regularity conditions, the quality of ensemble decisions improves with an increase in ensemble size. However, in case of the violation of the assumptions, as well as with a small number of ensemble elements, the quality of the decisions can turn into a degenerate. To improve the ensemble quality, it is possible to use information contained in the additional (source) data.

2.4 Usage of source data

For source data \( X_S \), classification vector \( Y \) is known. Therefore it is possible to calculate the coincidence matrix \( Z^S = (z^S(i, j)) \), where \( z^S(i, j) = I[y_i = y_j] \), \( i, j = 1, \ldots, N_S \). Despite the fact \( X_T \) and \( X_S \) belong to different statistical populations, we may assume that some general structural regularities characterizing both populations exist. The regularities can be found using cluster analysis. To get more robust results, we apply cluster ensemble algorithm independently for
source and target data (for simplicity, we assume equal number \( L \) of runs in the ensemble for each dataset). As the analysis proceeds, the averaged co-association matrix \( H^S \) is determined for \( X_S \).

For specifying the types of regularities under interest, one may use different approaches. In this paper, we consider characteristics of mutual positions of data points with respect to the found clusters and use them as meta-features describing common properties of source and target domains.

As the first type of meta-feature, we use frequencies of the assignment of object pairs to the same clusters (elements of matrix \( H^S \)). These values belong to interval \([0, 1]\) and do not explicitly depend on initial feature dimensions.

Another meta-feature suggested in this work is based on Silhouette index which is defined for each data point and reflects its similarity to other points in the same cluster and dissimilarity to points from different clusters. Let \( \text{Sil}(x_i) \), \( \text{Sil}(x_j) \) denote Silhouette indices, averaged over ensemble partitions, respectively for points \( x_i, x_j \in X_S \). Denote \( P^S(i, j) = \frac{1}{2}(\text{Sil}(x_i) + \text{Sil}(x_j)) \); matrix \( P^S \) is determined for all pairs of points of source data. Similarly, matrix \( P^T \) is defined for target data.

Consider a problem of finding a decision function

\[
f: (P^S(i, j), H^S(i, j)) \mapsto Z^S(i, j)
\]

for predicting elements of \( Z^S \) viewed as new class labels (0 or 1). A classifier can be found by usage of existing machine learning algorithms such as logistic regression or support vector machine. Then the found classifier can be transferred to target domain for predicting \( \hat{Z}^T = f(P^T, H^T) \).

The resulting coincidence matrix \( \hat{Z}^T \) cannot be directly used for clustering (for example, by finding connected components), since it can lead to metric properties violation in feature space. For example, if for some \( i, j, k \), it holds \( \hat{Z}^T(i, j) = 1 \) and \( \hat{Z}^T(i, k) = 1 \), there is no guarantee that \( \hat{Z}^T(j, k) \neq 0 \). For this reason, we propose to search for a partition by solving the following optimization problem:

\[
\text{find } \hat{Z}^* \in \Psi_{K_T}: \hat{Z}^* = \arg \min (\hat{Z}^* - \hat{Z}^T)_2
\]

where \( \Psi_{K_T} \) is a set of Boolean coincidence matrices corresponding to all possible partitions of \( X_T \) into \( K_T \) clusters, \((\cdot)_2\) is the Frobenius norm of a matrix.

For an approximate solution, one may apply a procedure which starts from some initial partition of \( X_T \) (in our implementation, found with \text{EC} algorithm), and sequentially corrects it by finding such points, which give the best improvement of functional in \([2]\) when migrating to another cluster. The iterations continue until the optimized functional becomes less than a given parameter \( Q_{\min} \), or the number of iterations (migrated points) exceeds the preset value \( I_{\max} \).

The main steps of the proposed algorithm \text{TrEC} (Transfer Ensemble Clustering) are described below.

**Algorithm \text{TrEC}:**

**Input:**

- \( X_T \): target data;
$X_S$: source data;  
$Y$: class labels for source data;  
$L$: number of runs for clustering algorithm $\mu$;  
$\Omega_S, \Omega_T$: parameters of algorithm $\mu$ working on $X_S$ and $X_T$, respectively;  
$K_T$: required number of clusters in $X_T$. 

**Output:**  
$P = \{C_1, \ldots, C_{K_T}\}$: clustering partition of $X_T$.  

**Steps:**  
1. Generate $L$ variants of clustering for $X_S$ and $L$ variants of clustering for $X_T$ by random choice of parameters from $\Omega_S, \Omega_T$, respectively;  
2. Calculate co-association matrices $H^T, H^S$ and matrices $P^T, P^S, Z^S$;  
3. Find a decision function $f(P^S, H^S)$ for predicting elements of $Z^S$;  
4. Calculate matrix $\hat{Z}^T = f(P^T, H^T)$;  
5. Find matrix $\hat{Z}^*$ and corresponding partition $P$, using the above-mentioned approximate procedure of solving (2);  

end.

In the implementation of TrEC, we use k-means to design the cluster ensemble. To find a solution to the problem $\mathbb{I}$, we apply Support Vector Machine (SVM). The overall complexity of the algorithm with respect to sample size is $O(\max(N_T, N_S)^2)$.

### 3 Numerical experiment

To verify the applicability of the suggested approach, we have designed Monte Carlo experiments with artificial datasets. To generate target data, we use the following distribution model. In 24-dimensional feature space, the two of modeled classes have spherical form, and another two have strip-like form. First and second classes are of Gauss distributions with unit covariance matrix $\mathcal{N}(\nu_1, I)$, where $\nu_1 = (0, \ldots, 0)^T, \nu_2 = (8, \ldots, 8)^T$. The coordinates of objects from other two classes are determined recursively: $x_{k+1} = x_k + \gamma_1 \cdot 1 + \varepsilon$, where $1 = (1, \ldots, 1)^T, \gamma_1 = 0.2, \varepsilon$ is a Gauss random vector $\mathcal{N}(0, \gamma_2 \cdot I), \gamma_2 = 0.25, k = 3, 4$. For class 3, $x_3 = (-6, 6, \ldots, -6, 6)^T + \varepsilon$; for class 4, $x_4 = (6, -6, \ldots, 6, -6)^T + \varepsilon$.

The number of objects for each class equals 20.

Source data set has a similar structure, with the following differences: feature space dimensionality equals 16; the first and second classes follow Gauss distribution $\mathcal{N}(\lambda_i, I), i = 1, 2$, where $\lambda_1 = (0, \ldots, 0)^T, \lambda_2 = (6, \ldots, 6)^T$; the third and fourth classes are determined as follows: $x_{k+1} = x_k + \gamma_1 \cdot 1 + \varepsilon$; where $\gamma_1 = 0.2, \varepsilon$ is normally distributed vector $\mathcal{N}(0, \gamma_2 \cdot I), \gamma_2 = 0.2, k = 3, 4$. For the third class $x_3 = (-5, 5, \ldots, -5, 5)^T + \varepsilon$; for the fourth class $x_4 = (5, -5, \ldots, 5, -5)^T + \varepsilon$.

The sample size for each class equals 25.

Examples of generated data are shown in figure 1.

To design the ensemble, we use random subspace method: each clustering variant is built on three randomly selected features. The number of elements in the ensemble equals 10; the number of clusters $K_T = 4$.  


For training on \((P^S, H^S)\), \(\hat{Z}^S\) and predicting elements of \(\hat{Z}^T\) using \((P^T, H^T)\), we apply SVM with the following parameters: RBF kernel \((\sigma = 4)\), penalty parameter \(C = 10\). Parameter \(Q_{\text{min}} = 5\), \(H_{\text{max}} = 40\).

In the process of Monte Carlo modeling, artificial datasets are repeatedly generated according to the specified distribution model.

Figure 2 shows an example of SVM decision on the coordinate plane with axes determined by values of \(P^S, P^T\) (horizontal axis) and \(H^S, H^T\) (vertical axis).
To evaluate the quality of clustering, we use Adjusted Rand index $ARI$ \cite{10}. The index varies from values around zero to 1; $ARI$ close to 1 means a high degree of matching between the found partition and the true one; $ARI$ close to zero indicates nearly random correspondence. To increase the reliability of the results, the accuracy estimates are averaged over 40 experiments. Two data processing strategies are compared: a) with use of the suggested TrEC algorithm, and b) using EC algorithm, in which no transfer learning is utilized. The statistical analysis of the significance of the differences between the estimates is carried out using a paired Student’s t-test.

As a result of the experiment, the following averaged quality estimates are obtained: for TrEC: $ARI = 0.73$, and for EC: $ARI = 0.56$. The paired Student’s t-test shows significant differences between the two estimates (p-value 0.0003). Thus, despite the fact that the data distribution is quite difficult for k-means (which is oriented on spherical-shaped clusters), the suggested method shows a statistically significant increase in decision quality.

We also estimate a significance of meta-features with respect to clustering quality. To this end, we try to exclude one of the features from the analysis and repeat the experiment. When co-association matrix-based meta-feature is used alone in TrEC, the averaged $ARI$ equals 0.68. If only Silhouette-based meta-feature is employed, the averaged $ARI$ degrades to 0.31. One can conclude from the experiment that the former meta-feature is more important than the latter, however, both of them are useful in combination.

4 Concluding Remarks

This work has introduced an ensemble clustering method using transfer learning methodology. The method is based on finding meta-features describing structural data characteristics and their transfer from source to target domain. The proposed method allows one to consider different feature sets describing source and target domains, as well as a different number of classes for both of them. The complexity of the method is of quadratic order, and is smaller than the complexity of analogous algorithm.

An experimental study of the method using Monte Carlo modeling has confirmed its efficiency.

In the future, we plan to continue studying the theoretical properties of the proposed method and its further development aimed at faster processing speed. Determining of useful types of meta-features, in addition to such as those proposed in the present work, is another important problem. A detailed comparison with existing combined ensemble clustering and transfer learning methods is our next objective. Application of the method in various fields is also planned.

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