CLASSIFICATION AT INCOMPLETE TRAINING INFORMATION: USAGE OF GROUP CLUSTERING TO IMPROVE PERFORMANCE

[1,2]VLADIMIR BERIKOV, [3]YEDILKHAN AMIRGALIYEV , [4]LYAILYA CHERIKBAYEVA, [5]DIDAR YEDILKHAN, [6]BAKYT TULEGENOVA

[1] Sobolev Institute of Mathematics, Novosibirsk, Russia

[2]Novosibirsk State University, Novosibirsk, Russia

[3]Suleyman Demirel University, Kazakhstan

[4]Institute of Information and Computational Technologies CS MES RK, Kazakhstan

[5]Al-Farabi Kazakh National University, Kazakhstan

[6]Kazakh National Research Technical University after K. Satpayev, Kazakhstan

E-mail: [1]berikov@math.nsc.ru, [2]amir_ed@mail.ru, ainur79@mail.ru, [3]lailash01@gmail.com
[4]yedilkhan@gmail., [5]tulegenova_bakhit@mail.ru

ABSTRACT

In this paper, we propose a method for semi-supervised classification based on a group solution to cluster analysis in combination with Laplacian regularization of similarity graph. The averaged co-association matrix obtained with the cluster ensemble is considered as a similarity matrix in the regularization context. We use a low-rank representation of the matrix that allows us to speed-up computations and save memory in the solution of the derived system of linear equations. Both theoretical studies and numerical experiments on artificial data and hyperspectral imagery confirm the efficiency of the method.

Keywords: *Co-Association Matrix, Cluster Ensemble, Low-Rank Representation, Semi-Supervised Learning.*

1. INTRODUCTION

In pattern recognition problems, an ultimate goal is to perform a classification of sample objects described with a given feature set. With that, it is necessary to obtain an optimal value of a certain quality criterion (for example, to minimize the estimated error probability). A classifier is found using a training sample consisting of precedents – the objects with known classes they belong to. In the basic variant of the problem, class labels are known for all sample objects (*fully supervised classification*).

In the given work we consider another variant – the task of *semi-supervised classification*. In this problem, class labels are known only for a part of the given sample; it is necessary to classify either available unlabeled objects or formulate a decision rule for new objects attributing to classes. This task is urgent due to the following reasons: as a rule, unlabeled data “are cheap” (in the case when the identification of classes is an expensive procedure); usage of unlabeled data jointly with labeled samples often allows one to involve additional information and provide significant improvement of the classification quality.

Problems of such type arise in many applied areas, for example, in the analysis of tomographic images, when a specialist indicates the belonging of some image area to one or another class (tumor, degenerative changes, etc.). Manual segmentation of the images is rather time-consuming; often only a small part of available images, therefore, can be annotated.

In the field of Earth remote sensing [1] and the problems of allocation in recovery well logging [2] the tools and technologies for hyperspectral imaging are actively used in the visible and near-infrared ranges of the spectrum. The hyperspectral image features are a large number of spectral channels (up to several hundred) under a small spectral width of each channel (of the order of several nanometers). Hyperspectral images are three-dimensional data arrays, in which two dimensions correspond to spatial coordinates, and the third one corresponds to a spectral coordinate; therefore a hyperspectral image is called a spatial-spectral cube [3]. In many cases, the attributing of pixels to classes (vegetation or urban area types, etc.) requires field research and labeling for that reason is incomplete.

There exist a large enough number of approaches and algorithms for semi-supervised classification [4]. Currently, there are widely used self-training heuristic algorithms, probabilistic methods, transduction support vector machine (TSVM), as well as the theoretic-graph approach (Graph Laplacian Regularization) [5-8]. This approach (known also as manifold regularization) assumes that if two data points belong to the same manifold, then with a large probability they share their class labels. Laplacian graph is used for measuring the smoothness degree in the manifold including both labeled and unlabeled data. To get an efficient solution, a combination of supervised and *unsupervised classification* (clustering) is acknowledged in the literature [9].

In cluster analysis, a group (ensemble) approach is actively developing [10-11]. The application of this approach allows one to reduce the dependence of grouping results on the choice of algorithm parameters and to obtain more stable solutions in the conditions of noisy data. The idea of constructing group solutions based on the composition of simple algorithms is actively used in modern theory and practice of machine learning and data mining. A collective decision function combines the advantages of each of the methods used in constructing a classifier. Besides that, the area of its best “competence” can be determined for each of the basic decision functions.

Conceptually, the optimization model of applying the group solutions (cluster ensemble) is proposed in the following scheme below. The basis of the model has been offered in [12].

In Figure 1 the points $M_1,M_2,...,M_\alpha$ denote input data, which can be represented both as numeric values and images. A={A_1, A_2,…, A_m} is a set of classification algorithms, operating on different principles. $z_c^1, z_c^2,\ldots, z_c^t$ are algorithms of group solutions (cluster ensemble). Every $z^i \in z_c$, i=1,2,...,t makes a decision based on outcomes of the set of algorithms *A*. Further, through F={F_1, F_2,…,F_n} we denote the quality criteria (validity) of algorithms both of the first level from A, and the second level from z_c. The offered model allows scaling the multitudes A and z_c dimensionality. The arrows directions in the model show the data stream subject to processing. As it is shown in Figure 1, the optimization model is presented as the networking model. One might exit from the network upon obtaining an appropriate result in terms of performance functionals.

A practical application of cluster analysis has been contemplated in the work [13]. The authors have applied a tree-like Bayesian network and *k*-means for computing the conventional linear Gaussians for classification of positions in motion in a dance. The basic task for using cluster analysis is recognizing a dancer’s head motions, which in turn, play a considerable role in recognizing the whole body’s gestures.

The works [14-15] offer an approach to neural network construction, which is not supported with a traditional one, based on the functional minimization. Rather, that approach is based on the operator’s theory, developed by Yu.I. Zhuravlyev [16] for solving the tasks of identification and classification.

The above-mentioned network’s distinctive feature is the usage of diagonal functions activation in the inner layers, which considerably facilitates intermediate calculations in outer and inner cycles. Similar researches on applying the neural networks CNN for image identification have been described in the work [17]. The work studies a complete withdrawal of an intermediate layer and creation of an image descriptor with a lower dimensionality, excluding the activation of filters, corresponding to the media changes. Thus, there is attained the objects’ visual recognition reliability. Interesting cluster analysis and ensemble algorithms for practical applications are described in [18-19]. The works solve the tasks of data interpretation, stratigraphy borders classification and lithology based on of the data of geophysical logging for uranium deposits. In [18] the problem is solved using several computer-aided learning algorithms: random forest, logistic regression, gradient rise of k nearest neighbor and XGBoost. The work [19] applies such algorithms as the artificial neural network (ANN), linear discriminant analysis classifier (LDAC), support vector machine (SVM) and k-Nearest-Neighbor (kNN).

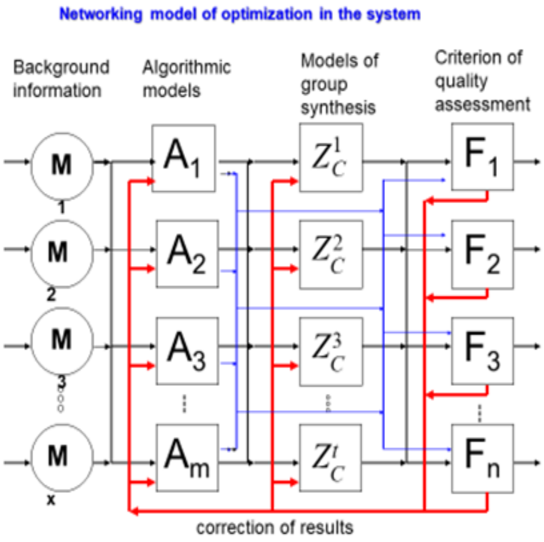


Figure 1. Concept scheme (networking model) of cluster ensemble optimization results

The main limitations of the existing methods for semi-supervised classification are in the following:

- large computational complexity and memory demands;
- poor resistance to noise.

One of the serious problems in constructing an ensemble solution is the considerable complexity of the used search procedures. Existing algorithms are unable to analyze large-volume data.

In this paper, a computationally efficient ensemble algorithm is proposed that is able to work with a large amount of data being analyzed. This article develops a collective approach in the context of its application to the analysis of hyperspectral images. We suggest a new method of semi-supervised classification using a combination of theoretical-graph approach, regularization technique and cluster ensemble. The idea of the method is in the usage of the averaged co-association matrix as a similarity matrix in the regularization context, as well as in a low-rank presentation of the matrix to decrease the demanded memory and computation cost. The usage of group clustering aims at increasing the quality and stability of results.

In [20-21], a novel approach combining ensemble clustering and kernel-based learning was suggested for classification and regression analysis. The main idea is to consider the averaged co-association matrix calculated on the outputs of the ensemble as a similarity (kernel) matrix. Such a replacement has several grounds. Firstly, it might be assumed that objects from the same dense region (cluster) in the feature space have common class attributes, even if the given region has a complex form. From that point of view, such points are more similar to each other, than other points which are remote from each other on the same distance but belonging to different clusters. Secondly, it is known that the averaged co-association matrix defines a semi-metric on observation space [22]; it means that the frequencies of assigning object pairs to common clusters can be considered as similarity measures for corresponding data points. The obtained matrix depends on the outputs of clustering algorithms and often is less dependent on outliers than a conventional similarity matrix.

Theoretical analysis using different kinds of ensemble models [24-25] shows that the usage of group approach allows one to raise the stability of clustering results in case of uncertainty in data structure which occurs, for instance, when the true number of clusters is unknown; or when unnecessary, noisy features are used; if data have unknown complex structures (e.g., spiral-like, spherical clusters).

The work [26] suggests an algorithm of semi-supervised classification using a low-rank representation of the co-association matrix and linear algebraic transformations. However, in many applied tasks, these transformations are intractable due to large complexity of the problem and consequently a large size of the ensemble. In this work, we suggest the usage of efficient iterative algorithms of solving a system of linear equations instead of troublesome matrix inversion procedures.

The main contribution of this paper, in comparison with other works in the field, is in the involving efficient gradient descent iterative algorithms for an approximate solution of systems of linear equations to find the predicted class labels. We also consider a new application of the developed algorithm in the problem of hyperspectral imagery semi-supervised classification.

The paper aims at validating the proposed methodology and summarizing our previous work. Further, in the article we give a mathematical problem statement, made a short overview of existing methods for semi-supervised classification. We describe the suggested method, discuss its properties and carry out an experimental evaluation. Finally, we give some concluding remarks.

2. MATHEMATICAL PROBLEM STATEMENT FOR SEMI-SUPERVISED

CLASSIFICATION AND RELATED WORK

Let there be an entire population Γ of recognizing objects and finite set of class labels $C=\{c_{1},...,c_{k},...,c_{K}\}$. Each object $a\epsilon\Gamma$ is described with attributes (feature set) $X=(X_1,..., X_d)$. Let us denote through $X_j(a)$ the X_j attribute value for the object a. Depending on the values and admissible operations with them, the attributes are of the following types:

- binary feature: $X_j(a) \in \{0,1\}$;
- quantitative feature: $X_j(a) \in R$;
- categorical feature: $X_j(a) \in G_j$: a finite set of unordered values;
- ordered feature: $X_j(a) \in D_j$: a finite ordered set.

In this work, we will consider only quantitative attributes. Under the prescribed attributes, the set $x(a) = (X_1(a), \dots, X_d(a))$ is called a feature description (observation) of the object $a \in \Gamma$. Let there be a data sample $\boldsymbol{X} = \{ x_1, \dots, x_n \}$ of observations for objects $a_1, \dots, a_n$, where $x_i=x(a_i)$. In the problem of semi-supervised classification there are two types of samples:

– $\boldsymbol{X_1} = \{x_1, \dots, x_{n_1}\}$: describes objects $a_1, \dots, a_{n_1}$ with known class labels $\boldsymbol{Y_1} = \{y_1, \dots, y_{n_1}\}$, where $y_i \in C$ is the label of the class to which the object a_i, $i=1,...,n_1$ belongs;

– $\boldsymbol{X_0} = \{x_{n_1+1}, \dots, x_n\}$ is a description of unlabeled objects (without loss of generality, we assume, that the first n_1 sample objects are labeled, and the next in ones are unlabeled).

There exist two main versions of the problem statement. In the first version it is demanded to conduct inductive teaching, i.e., to construct a classifier $f: X \to Y$ which attributes class labels to objects from **X₀** and arbitrary new observations. In the second variant of the problem statement it is necessary to carry out transduction learning, that is to define the class labels $\boldsymbol{Y_0} = \{y_{n_1+1}, \dots, y_n\}$ only for the objects from $\boldsymbol{X}_0$. Both in the first and second cases there is used some quality functional of classification. The given work considers the second version of the problem statement.

Let us consider some most frequently used approaches to supervised learning.

2.1. Self-training

In this approach, there is used some basis fully supervised classification algorithm. At the first step, the algorithm is trained at the labeled sample and further classifies the unlabeled part. For each classified object there is computed a recognition quality estimate (for instance, the distance to the separating hyperplane). At the next step, those observations for which the quality estimate is higher than the prescribed threshold, are excluded from **X₀** and added to **X₁**, and their labels replenish the set **Y₁**. Subsequently, the basic algorithm is applied again to training on the integrated sample and classification of the remained unlabeled part. The procedure is repeated until no unlabeled objects remain.

The methods based on this heuristic procedure, as a rule, are enough effective, however theoretical analysis of their properties is a troublesome problem.

2.2. Probabilistic approach

For the given approach, it is assumed that for each class c_k there exists a conditional distribution $p_j(x|\theta_k)$ in feature space, where θ_k is a set of distribution parameters, $k=1,...,K$. It is supposed the distribution type is known (for instance, normal), and its parameters should be evaluated by sample. Let us denote $\theta = (\theta_1, \dots, \theta_K)$, and let $q = q_1, \dots, q_K$ be a set of classes prior probabilities. Then for the labeled point $x_i \epsilon \boldsymbol{X_1}$, for which $y_i=c_k$, according to the chain rule, we obtain:

$$p(x_i,y_i\,|\theta) = q_k p_k(x_i \mid \theta_k)$$

According to total probability formula, for unlabeled point $x_i \in \boldsymbol{X}_0$

$$p(x_i\,|\theta) = \textstyle\sum_{k=1}^{K} q_k p_k(x_i \mid \theta_k).$$

It is possible to consider the problem of likelihood maximization:

$$(q^*,\theta^*)=arg\max_{q,\theta}\{\textstyle\sum_{x_i\epsilon X_1}\log p(x_i,y_i|\theta) + \\ +\textstyle\sum_{x_i\epsilon X_0}\log p(x_i|\theta)\}$$

s.t.: $\sum q_i = 1, \forall i, q_i \geq 0.$

The solution can be found by iterative algorithms, for example, EM algorithm for distribution mixtures [27]. After specifying the optimal $q^* = (q_1^*, \dots, q_K^*)$, $\theta^* = (\theta_1^*, \dots, \theta_K^*)$, the classification of the unlabeled objects is performed according to

Bayes formula:

$$f(x_i) = c_{k^*},$$

where

$$k^* = arg\,\max_k\{\,q_k^*\,p_k(x_i|\theta_k^*)\},\ i=n_1+1,\dots,n$$

A disadvantage of the approach is in the fact that upon the significant violation of the assumptions on the probabilistic model, the found decisions have poor accuracy.

2.3. Transduction support vector machine

The basis of the given method is Support Vector Machine (SVM) methodology for binary classification (which can be extended to a multiclass problem). In the basic statement, it is needed to find the hyperplane for which the separating margin width is maximal. The input is a training sample $\boldsymbol{X}$ with class labels $\boldsymbol{Y}=\{y_1,\dots,y_l\}$, $y_i \in \{-1,+1\}$, $i=1,\dots,n$. In the case of linear separability, there exists an infinite number of separating hyperplanes. It is reasonable to select the hyperplane, the distance from which to both classes is maximal. The points lying at the margin border are called support vectors.

Let us present the hyperplane equation in the form $\langle w, x\rangle + b = 0$, where $\langle\cdot,\cdot\rangle$ is a scalar product, w is a vector perpendicular to the separating hyperplane and b is a parameter. SVM constructs a decision function in the following form

$$f(x)=sign(\textstyle\sum_{i=1}^{n}\alpha_i y_i\,\langle x_i, x\rangle + b$$

where $\alpha_1,\dots,\alpha_n \geq 0$ are some parameters; at that, the normalization condition $\langle w, x_i\rangle + b = \pm 1$ for support vectors should be fulfilled. It is important to note that the summation is carried out only for those support vectors for which $\alpha_i \neq 0$.

For the transductive SVM, the hyperplane shall be drawn in the way it separates with a maximum margin width not only labeled points $\boldsymbol{X}_1$, but also unlabeled points $\boldsymbol{X}_0$. Consequently, the hyperplane should pass through the area with the lowest density. The optimization task can be formulated as follows:

find

$$\boldsymbol{Y}_0,\ w,\ b,\ \xi :\ \frac{1}{2}\|w\|^2 + C\sum_i \xi_i \to \min_{Y_0,w,b,\xi}\ ,$$

s.t.:

$$y_i(\langle w, x_i\rangle + b) \geq 1 - \xi_i, i = 1, \dots, n,$$

$$\xi_i \geq 0,\ i=1,\dots,n$$

where $\xi_1,\dots,\ \xi_n$ are variables which have the meaning of the penalty value for the margin border violation, $C \geq 0$ is a prescribed parameter. Consequently, there is maximized the margin width (one may show that the condition herein is equivalent to minimization of $\|w\|^2$), and the total penalty for the margin borders violation is minimized.

There exist algorithms for the given task approximate solution [28]; for this purpose, there is solved a corresponding dual problem for parameters $\alpha_1,\dots,\alpha_n$.

Upon a linear inseparability of classes, the transformation φ: $X \to X'$ of the initial space X into a new space X' of higher dimensionality can be performed. In the new space, the objects can already be linearly separable. A decision function $f(x)$ depends on the vector scalar product, not on the objects immediately. Therefore the scalar product $\langle x, z\rangle$ can be replaced with the products of the type $\langle\varphi(x), \varphi(z)\rangle$ in the rectifying space X'. In this case, the decision function has the form:

$$f(x)=sign(\textstyle\sum_{i=1}^{n}\alpha_i y_i\langle\varphi(x_i), \varphi(x)\rangle + b$$

Function $K(x,z)=\langle\varphi(x), \varphi(z)\rangle$ is called a kernel. The transition from a scalar product to a kernel is a "kernel trick".

The selection of a kernel defines an implicit transformation to rectifying space and allows applying linear algorithms (in particular, SVM) to linearly inseparable sample. For kernel-based methods, the Mercer's theorem [29] is widely known. It establishes necessary and sufficient conditions for a function to be a kernel. According to the theorem, continuous (or defined on a finite set) function $K(x,z)$ is a kernel then and only then, when it is symmetric: $K(x,z)=K(z,x)$ and positive semi-definite: for any finite sample ($x_1,\dots x_p$), given matrix $K=(K(x_i,x_j))$ and any $z \in \mathrm{R}_\mathrm{p}$, it holds true: $z^T Kz \geq 0$.

It is known that the optimization problem for transductive SVM is nonconvex, and known algorithms of its approximate solution are of polynomial cost. Therefore the approach can be applied to samples of comparatively small size (about a thousand observations).

2.4. Graph Laplacian regularization

Let us consider a weighted non-directed complete graph *G=(V,E)*, in which the set of vertices *V* corresponds to observations from **X**, and the set of edges *E* corresponds to pairs (x_i,x_j), $i, j=1,\dots,n,\ i\neq j$. Each edge (x_i,x_j) is associated with a nonnegative number (weight) W_{ij}, having the meaning of the given pair degree of similarity. For example, the weight can be defined using RBF function:

$$W_{ij}=exp\left(-\frac{\|x_i-x_j\|}{2\sigma^2}\right)$$

where σ is a prescribed parameter.

Let $Y_i = (Y_{i1},\dots,Y_{iK})$ denote a Boolean vector of the observed associations with classes: $Y_{ik} = \boldsymbol{I}[y_i=c_k]$, where $\mathbf{I}[\cdot]$ is a predicate function: $\mathbf{I}[true]$=1, $\mathbf{I}[false]$=0, $i=1,\dots,n_1$, $k=1,\dots,K$. Let us denote through $F_i=(F_{i1},\dots,F_{iK})$ a classification vector, in which the element $F_i \geq 0$ has a sense of the degree of belonging of point x_i to class c_j, and let the classification matrix of dimensionality $n \times K$ be specified as $\mathrm{F} = (F_1,\dots,F_n)^T$.

Let us consider the following optimization task: find

$$F^* = \arg\min_{F\in R^{n\times K}} Q(F) = \frac{1}{2}\left(\sum_{x_i\in X_1}\|F_i - -Y_i\|^2 + \beta\sum_{x_ix_j\in \boldsymbol{X}} W_{ij}\left\|\frac{F_i}{\sqrt{D_{ii}}} - \frac{F_j}{\sqrt{D_{jj}}}\right\|^2\right), \qquad (1)$$

providing $F \geq 0$, where $\beta > 0$ is a regularization parameter. The first sum in the right part of (1) is aimed at minimizing the labeled data fitting error; the second component plays the role of a smoothing function: its minimization means that if two points x_i, x_j (labeled or unlabeled) are similar, then their classification vectors shall not differ much. It is known that the function being optimized is convex.

Let us introduce a diagonal matrix *D* with components $D_{ii} = \sum_j W_{ij}$. The matrix

$$L = I - D^{-1/2}WD^{-1/2}$$

is called the normalized Laplacian, *I* is an identity matrix. The matrix has dimensionality $n \times n$; its element L_{ij} equals $L_{ij} = \delta_{ij} - \frac{W_{ij}}{\sqrt{D_{ii}}\sqrt{D_{jj}}}$, where $\delta_{ij=}\boldsymbol{I}[i=j]$ is the Kronecker symbol. Note that there are other variants of graph Laplacian definition [3].

To find the optimal solution, we differentiate (1), and after simple transformations obtain:

$$\frac{\partial Q}{\partial F_{ik}}|_{F_{ik}=F^*_{ik}} = F^*_{ik} - Y_{ik}+\beta F^*_{ik} - L_{i,\cdot}F^*_{\cdot,k} = 0 \qquad (2)$$

$$i = 1,\dots,n_1,$$

$$\frac{\partial Q}{\partial F_{ik}}|_{F_{ik}=F^*_{ik}} = \beta F^*_{ik} - \beta L_{i,\cdot}F^*_{\cdot,k} = 0, \qquad (3)$$

$$i = n_1+1,\dots,n$$

where $L_{i,\cdot}, F^*_{\cdot,k}$ is the *i*th row of matrix *L* and *k*th column of matrix F^* accordingly, $i=1,\dots,n_1$, $k=1,\dots,K$. Let us denote through $Y_{1,0}$ the matrix

$$Y_{1,0} = (Y_1,\dots,Y_{n_1},\underbrace{0,\dots,0}_{n-n_1})^T$$

of dimensionality $n\times K$, and through $I_{1,0}$ the diagonal $n\times n$ matrix:

$$I_{1,0} = diag(I_{11}\dots,I_{nn}), I_{ii} = \begin{cases} 1, i = 1,\dots,n_1 \\ 0, i = n_1+1,\dots,n. \end{cases} \qquad (4)$$

Then (2) and (3) can be rewritten in matrix form:

$$(I_{1,0} + \beta L)F^* = Y_{1,0}, \qquad (5)$$

from which

$$F^* = (I_{1,0} + \beta L)^{-1}Y_{1,0}, \qquad (6)$$

if the inverse matrix exists (note that the regularization parameter β can be chosen in the way to ensure well conditioning of the obtained task).

To find the solution, one may use iterative methods. For example, the work [6] describes Label Spreading iterative algorithm used for solving the task analogous to (6). Apart from that, we may apply existing methods for solving linear equations systems, where each system is considered concerning corresponding columns $F^*, Y_{1,0}$ in (5). After computing $F = F^*$, the final classification is defined according to the formula:

$$y_i = c_{k^*}$$

where

$$k^* = arg \max_{k=1,\dots,K} F_{ik}, i = n_1 + 1, \dots, n. \quad (7)$$

A limitation of the given approach is that it operates with non-sparse graph Laplacian matrix of dimensionality $n \times n$ which results in a large cost of matrix operations and memory demand.

3. SUGGESTED METHOD

The method is based on a combination of collective cluster analysis and theoretical graph approach. The main idea is in the usage of the averaged co-association matrix of cluster ensemble as a similarity matrix in (1).

3.1. Cluster ensemble and averaged co-association matrix

According to group approach in clustering, we consider several different clustering partitions of the same data and integrate them to find the overall consensus partition.

As a rule, each partition variant is formed according to the parameters of the clustering algorithm selected at random from an admissible set of parameters. One can also vary the algorithm's settings (such as distance type, initialization, feature subspace) to get different variants of partitioning.

In our task, we do not need to partition data: our primary goal is to perform a classification of the unlabeled sample. The used information obtained by multiple clustering can be presented in the form of the averaged co-association matrix.

Let us consider r partition variants $\{P_l\}_{l=1}^{r}$, where $P_l = \{C_{l,1}, \dots, C_{l,K_l}\}$, $C_{l,K_l} \subset \boldsymbol{X}$, $C_{l,K_l} \cap C_{l,k'} = \emptyset$, K_l is the number of clusters in the partition variant. For each P_l we define matrix H_l=$(H_l(i,j))_{i,j=1}^{n}$, the elements of which indicate wether a pair x_i, x_j belongs to the same cluster in the l-variant or not:

$$H_l(i,j) = \boldsymbol{I}[\mathrm{c}_l(x_i) = \mathrm{c}_l(x_j)],$$

where $c_l(x)$ denotes the cluster label assigned to point x. Weighted averaged coassociation matrix is defined as follows:

$$H = \left(H(i,j)\right)_{i,j=1}^{n}, H(i,j) = \sum_{l=1}^{r} w_l H_l(i,j)$$

where $w_1,\dots,w_r$ are weights, $w_l \geq 0$, $\sum w_l = 1$. The weights can be identical or can be selected proportionally to some quality index of each clustering variant.

It was shown in [11] that matrix H is symmetric and positive semi-definite. Thus, according to Mercer's condition, it is possible to use it as a kernel matrix in kernel-based classification methods such as SVM or kNN. Below we describe basic steps of algorithms CASVM and CANN which implement the combination scheme.

Algorithm CASVM

Input: data set $\boldsymbol{X_1}$ with known class labels $\boldsymbol{Y_1}$; unlabeled data $\boldsymbol{X_0}$; number of clustering variants *r*;
Output: predicted class labels $\boldsymbol{Y_0}$.
Steps:

```
1. Generate $r$ variants of the partition of $\boldsymbol{X} = \boldsymbol{X_1} \cup \boldsymbol{X_0}$ using a given clustering algorithm with randomly chosen parameters; calculate quality indices and weights $w_1,\dots,w_r$;
2. Calculate the averaged co-association matrix $H$.
3. Train $SVM$ at labeled data $\boldsymbol{X_1}$ using matrix $H$ as a kernel matrix.
4. Predict $\boldsymbol{Y_0}$ using the trained $SVM$.
end
```

Algorithm CANN:

Input: data set $\boldsymbol{X_1}$ with known class labels $\boldsymbol{Y_1}$; unlabeled data $\boldsymbol{X_0}$; number of clustering variants *r*;
Output: predicted class labels $\boldsymbol{Y_0}$.
Steps:

```
1. Generate $r$ variants of the partition of $\boldsymbol{X} = \boldsymbol{X_1} \cup \boldsymbol{X_0}$ using a given clustering algorithm with randomly chosen parameters; calculate quality indices and weights $w_1,\dots,w_r$;
2. Calculate the averaged co-association matrix $H$.
3. Apply nearest neighbor method: for each unlabelled object $x \in \boldsymbol{X_0}$ find a class label of the most similar (according to $H$) labeled object $x' \in \boldsymbol{X_1}$:
       $x' = arg \max_{i=1,\dots,n_1} H(x_i, x).$
end
```

As a basic clustering algorithm, we use *k*-means that has a linear cost. Note that elements of matrix *H* can be computed dynamically which allows one to save memory in case of large sample size *n* (however, the calculation time grows consequently).

It was proved in [25] that under some natural assumptions on the probabilistic properties of the ensemble, the probability error in classifying an arbitrary pair of points to clusters approaches zero at increasing the ensemble size.

3.2. Low-rank representation of averaged co-association matrix

By the definition, the averaged co-association matrix requires quadratic memory with respect to sample size. Nevertheless, this requirement can be relaxed using the matrix low-rank representation.

The next property allows one to sufficiently decrease the computation cost.

Proposition. Weighted averaged co-association matrix admits low-rank representation in the form:

$$H = BB^T,\ B = [B_1 B_2 \dots B_1] \tag{8}$$

where B is a block matrix, $\mathrm{B}_l = \sqrt{\mathrm{w}_l \mathrm{A}_l}$; A_l is an association matrix for *l*th clustering partition which has a dimensionality $n \times K_l$: $\mathrm{A}_l(i,k) = \mathbf{I}[\mathrm{c}(\mathrm{x}_i) = k]$, *i*=1,…,*n*, *k* =1,…,$K_l$.

As a rule, $m = \sum_l K_l \ll n$; thus (8) gives us a possibility to save memory by storing sparse matrix *B* of dimensionality $n \times m$ instead of full matrix *H*. The cost of matrix multiplication $H \cdot x$ is reduced from $O(n^2)$ to $O(nm)$.

3.3. Cluster ensemble and graph Laplacian regularization

We consider matrix *H* as a similarity matrix *W* in (1) and define the normalized Laplacian of the corresponding graph in the form: $\tilde{L} = I - \widetilde{D}^{-1/2} H \widetilde{D}^{-1/2}$, where $\widetilde{D} = diag(\widetilde{D}'_{11}, \dots, \widetilde{D}_{nn})$, $\widetilde{D}'_{ii} = \sum_j H(i,j)$. We obtain:

$$\widetilde{D}_{ii} = \sum_{j=1}^{n} \sum_{l=1}^{r} w_l \sum_{k=1}^{K_l} A_l(i,k) A_l(j,k) = \sum_{l=1}^{r} w_l \sum_{k=1}^{K_l} A_l(j,k) = \sum_{l=1}^{r} w_l\, n_l(i) \tag{9}$$

where $n_l(i)$ is the size of the cluster which includes the point x_i in *l*-variant of partitioning. Substituting $\tilde{L}$ in (5), we obtain a linear equations system:

$$\left(I_{1,0} + \beta L\right) F^{**} = Y_{1,0}. \tag{10}$$

Using (8), the system can be transformed into a form that uses more effective operations with low-rank matrices. For that purpose, let us denote $U = \widetilde{D}^{-1/2} B$, then $\tilde{L} = I - UU^T$. From (6) and (8) we obtain the system:

$$\left(I_{1,0} + \beta I - UU^T\right) F^{**} = Y_{1,0}. \tag{11}$$

For the numerical solution, one can use any of the existing iterative algorithms. In the given work we use algorithm GDSolve [30] based on gradient descent. The GDSolve algorithm convergence for symmetrical positive definite system matrix was proved in [30]. Let us describe the main steps of the given GDSolveLR algorithm modification, which uses low-rank graph Laplacian representation.

GDSolveLR algorithm:

Input:
U, $I_{1,0}$: sparse matrices in the left part of (11);
$Y_{1,0}$: matrix in the right part of (11);
$\delta > 0$: required accuracy parameter.
Output:
F^{**}: classification matrix.
Steps:

```
1. t:=0; $F^{**}(0) := 0$;
2. for $k:=1 \rightarrow K$ do
3.    b:= $Y_{1,0 \cdot k}$ (kth column of matrix $Y_{1,0}$);
4.    repeat
5.       compute residual error $r(t) := b - (I_{1,0} \cdot F^{**}_{\cdot,k}(t) + \beta F^{**}_{\cdot,k} - \beta U(U^T \cdot F^{**}_{\cdot,k}(t)))$;
6.       find the optimal step length $\eta(t) := \frac{r(t)^T r(t)}{r(t)^T (I_{1,0} \cdot r(t) + \beta r(t) - \beta U(U^T \cdot r(t)))}$;
7.       $F^{**}_{\cdot,k}(t+1) := F^{**}_{\cdot,k}(t) + \eta(t) \cdot r(t)$;
8.    until r(t)< $\delta$;
9. end for
10. return $F^{**}(t+1)$.
```

Note that at the steps 5,6 the algorithm performs a multiplication by Laplacian matrix represented in a low-rank form; thus it is not required to save in the memory full matrix of $n \times n$ size. Below we describe the main steps of the proposed algorithm SSC-LR-GD for semi-supervised classification based on Laplacian similarity graph, low-rank representation of co-association matrix and gradient method.

Algorithm SSC-LR-GD:

Input:
data set $\boldsymbol{X_1}$ with known class labels $\boldsymbol{Y_1}$; unlabeled

data $\boldsymbol{X_0}$; number of clustering variants *r*;
Output:
predicted class labels $\boldsymbol{Y_0}$.
Steps
1. Generate *r* variants of the partition of $\boldsymbol{X} = \boldsymbol{X_1} \cup \boldsymbol{X_0}$ using a given clustering algorithm with randomly chosen parameters; calculate quality indices and weights $w_1,\ldots,w_r$;
2. Calculate normalized graph Laplacian in a low-rank representation, using matrices B in (6), $\widetilde{D}$ in (9) and $I_{1,0}$ in (4).
3. Find classification matrix F^{**} with GDSolveLR algorithm;
4. Define labels for **Y₀**, using matrix $F = F^{**}$ in (7).
end.

In the computer implementation, we use *k*-means as a base clustering algorithm.

4. EXPERIMENTAL STUDY

The suggested algorithm SSC-LR-GD was evaluated in numerical experiments. The first experiment employs Monte Carlo simulation to estimate the accuracy and time complexity of the algorithm under various sample size and noise levels for a given example of data distribution. The second experiment demonstrates the applicability of the method in the real task of hyperspectral image analysis.

4.1. Mixture of normal distributions

In this example we consider data sets generated from the mixture of five multidimensional normal distributions *N(a*$_i$*,σ*$_X$*I)* at equal weights; $a_i \in \boldsymbol{R}^d$, *i=1,…,5*, *d=8*; value σ_X is a parameter. To study the algorithm robustness under noise conditions, two independent random features are additionally generated according to the uniform distribution $U(0, \sigma_2)$ where noise parameter $\sigma_2 = 5$. Figure 2 illustrates the generated data. In the simulation process, we repeatedly generate samples of size *n* with the given distribution.

10% of points selected at random from each component compose a labeled part of the sample; the remaining points are included in an unlabeled subsample. Cluster ensemble variants are generated using random initialization of centroids in *k*-means (number of clusters equals 10). The number of ensemble elements *r=10*. The weights of ensemble variants are identical: $w_l \equiv 1/r$. Regularization parameter β is evaluated by cross-validation and grid search in the interval [0.001,0.5] with a step 0.005; the best prediction has been obtained for β=0.1. Parameter δ=10^{-5}.

We also apply an algorithm (denoted SSC-RBF) which uses a standard similarity matrix found with RBF kernel (parameter $\sigma = 4$), in which the predictions are calculated according to (6). To raise the reliability of the comparison, quality estimates (frequency of correct predictions on test sample) are averaged over 40 experiments. Analysis of the statistical significance of the differences between the estimates is performed using a paired two-sample Student's *t*-test.

Table 1 presents the results of the experiments. The table shows the averaged accuracy estimates, as well as the averaged operation time (on the dual-core Intel Core i5 processor with a clock frequency 2,8 GHz and 4 Gb RAM). For SSC-LR-GD, we separately indicate ensemble generation time and matrix operation time (in seconds). Accuracy evaluations that are statistically significantly better than those of the compared algorithm (p-value $< 10^{-5}$) are in bold.

Table 1. Results of experiments with distribution mixture for various sample size n and parameter σ_X *values.*

n	σ_X	SSC-LR-GD			SSC-RBF	
		accuracy	t_{ens} (sec)	t_{matr} (sec)	accuracy	time (sec)
1000	1	1.000	0.06	0.10	1.000	0.32
	3	0.985	0.07	0.02	0.982	0.32
	5	**0.874**	0.13	0.11	0.817	0.35
3000	1	1.000	0.10	0.48	1.000	5.42
	3	0.986	0.13	0.10	0.984	5.29
	5	**0.878**	0.23	0.48	0.848	5.48
10^5	1	1.000	2.05	25.69	-	-
10^6	1	1.000	49	443	-	-

The results demonstrate that SSC-LR-GD shows comparable or even higher accuracy than SSC-RBF. For large data size (*n=10*^{5}*, n=10*^{6}), SSC-RBF failed due to unacceptable memory demands (74.5 Gb and 7450.6 Gb correspondingly).

One can see that SSC-LR-GD spend the most time in the stage of iterative computations. The average operation time for SSC-LR-GD is much less than that for SSC-RBF which does not use low-rank operations.

4.2. Analysis of hyperspectral images

For the experimental research of the developed algorithm, we use the Indian Pines hyperspectral image [30]. This scene was gathered by AVIRIS sensor over the Indian Pines test site in North-western Indiana. The image size is 145×145 pixels; each pixel is characterized by the vector of 224 spectral intensities in the 400-2500 nm range. Figure 3(a) shows the RGB-composite, and Figure 3(b) presents the ground truth map with 16 classes (different vegetation types). The image has unlabeled pixels which are not assigned to any of the classes. These pixels are excluded from the analysis.

In the experiment, the labeled part comprises 1% of points selected at random for each component. To reduce the spectral channels correlation effect, we use PCA to decrease the dimensionality up to 10 features.

The transformed data is used as input for SSC-LR-GD. Ensemble size r=10; base ensemble elements are generated with cluster number variation in the interval [1000, 1000+r]. The other parameters coincide with the described ones in the previous experiment.

We also perform a comparison with multiclass SVM which uses standard RBF kernel (with parameters recommended by default).

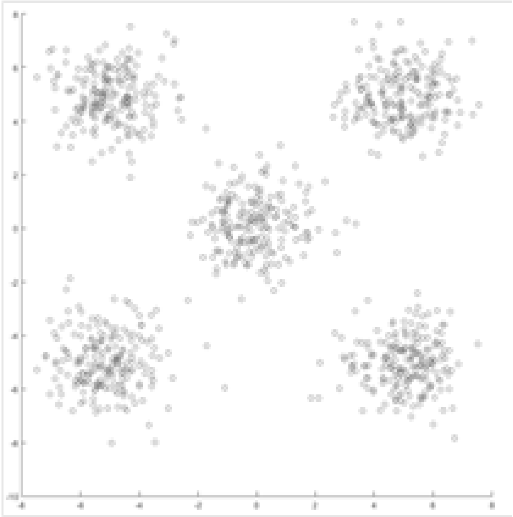


Figure 2. Generated data (projection on axes X_1, X_2): n=1000, $\sigma_x = 1$

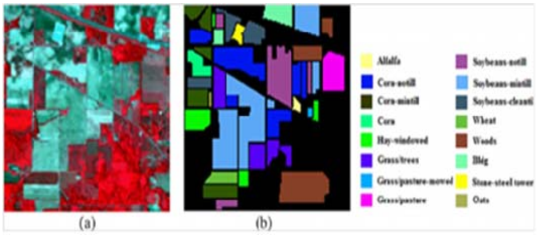
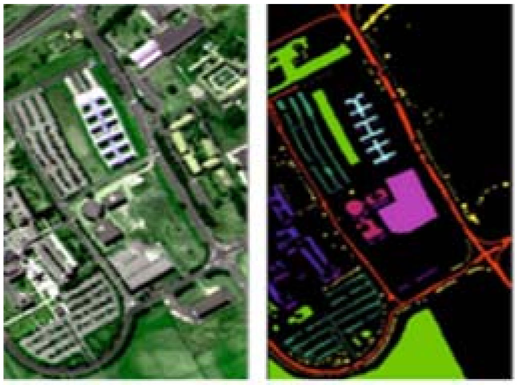


Figure 3. Indian Pines hyperspectral image: (a) composite image of hyperspectral data; (b) ground-truth map

To increase the statistical reliability of the comparison, we average the accuracy estimates over 20 runs for each algorithm with randomly selected labeled subsamples. At each run, we calculate classification accuracy estimate on the unlabeled pixels which are not used at the training stage. For SSC-LR-GD, the average operation time is about 1.5 minutes, and for SVM about 0.3 minutes. As a result, the SSC-LR-GD average accuracy is 0.657, and that of SVM 0.613. A paired Student's t-test has shown a significant improvement in the accuracy of SSC-LR-GD (p-value < 10^{-5}).

We also have examined CASVM performance on another hyperspectral image. We use Pavia University scene [31], which has a size of 610 × 340 pixels, containing 103 spectral channels. The spatial resolution of the scene is 1.3 m. Figure 4a) shows the image's RGB-composite (channels 40, 50 and 70), and Figure 4b) presents the ground truth map.

There are unlabeled pixels in the image which are not assigned to one of the nine classes. The given pixels are excluded from the consideration.



a) b)

Figure 4. Hyperspectral image Pavia University scene (RGB composite)(a) and labeled data (b)

In the experimental study, 1% of the pixels selected at random for each class compose a labeled sample; the remaining ones are included in the unlabeled part. To study the effect of noise on the quality of algorithms, we add normally distributed noise to the spectral brightness values: a corresponding value x is replaced by a quantity $x(1+p\varepsilon)$, where p is a parameter, ε follows standard normal distribution.

An obtained data consisting of the spectral intensity values of the pixels over all channels is an input of CASVM. K-means is chosen as a base algorithm for constructing a cluster ensemble. Different variants of the partitioning are generated by varying the number of clusters in the interval $[30,30+r]$ where r=120. To speed up the operation time of k-means and obtain more diverse results, the number of iterations is limited to 1.

Table 2 shows the accuracy estimates in the classification of unlabeled pixels for some pairs of noise parameters.

Table 2. Accuracy of CASVM and SVM at some values of noise parameters

Noise parameter p	0.05	0.1	0.25	0.5
CASVM	0.78	0.76	0.74	0.68
SVM	0.79	0.72	0.68	0.62

The running time of the algorithm is about 2 minutes. As can be seen from the table, CASVM algorithm is more noise resistant than SVM.

6. CONCLUSION

In this work, we have considered a pattern recognition problem in case of incomplete training information. Using a combination of the methodologies, based on the regularization of Laplacian similarity graph, collective cluster analysis, and a low-rank matrix representation, a method for the solution of the given task was suggested.

The main idea of the method is in the usage of the averaged co-association matrix of cluster ensemble as a similarity matrix in graph Laplacian regularization context. The matrix admits a low-rank representation that has allowed us to speed-up computations and save memory in the solution of the derived system of linear equations (from quadratic to linear concerning sample size).

We have performed an experimental study of the suggested method by the usage of Monte Carlo simulations. In the experiments, the method has shown comparable or even significantly better accuracy estimates than an analogous algorithm, not using group clustering and a low-rank representation of the co-association matrix. In the case of a big volume of data (up to a million points), the standard algorithm failed due to the infeasible memory requirements, and the proposed method gave an accurate solution in a few hundred seconds running on an ordinary computer. Even for a small amount of data, the average working time of the suggested algorithm turned out to be much less than that of the analogous standard one.

In the experimental study on the real hyperspectral image in noise conditions, the suggested methodology has allowed obtaining more accurate solutions than the existing SVM technique.

Further, we plan to continue the theoretical study of the suggested method (to investigate the problem of theoretical convergence to an optimal solution in the probabilistic context, to obtain classification quality estimates). To accelerate the computations, there are good reasons to vectorize the proposed algorithm upon forming a cluster ensemble and use more effective procedures for solving a linear equations system.

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