DEVELOPMENT AND COMPARATIVE ANALYSIS OF SEMI-SUPERVISED LEARNING ALGORITHMS ON A SMALL AMOUNT OF LABELED DATA

The paper is dedicated to the development and comparative experimental analysis of semi-supervised learning approaches based on a mix of unsupervised and supervised approaches for the classification of datasets with a small amount of labeled data, namely, identifying to which of a set of categories a new observation belongs using a training set of data containing observations whose category membership is known. Semi-supervised learning is an approach to machine learning that combines a small amount of labeled data with a large amount of unlabeled data during training. Unlabeled data, when used in combination with a small quantity of labeled data, can produce significant improvement in learning accuracy. The goal is semi-supervised methods development and analysis along with comparing their accuracy and robustness on different synthetics datasets. The proposed approach is based on the unsupervised K-medoids methods, also known as the Partitioning Around Medoid algorithm, however, unlike K-medoids the proposed algorithm first calculates medoids using only labeled data and next process unlabeled classes – assign labels of nearest medoid. Another proposed approach is the mix of the supervised method of K-nearest neighbor and unsupervised K-Means. Thus, the proposed learning algorithm uses information about both the nearest points and classes centers of mass.

The methods have been implemented using Python programming language and experimentally investigated for solving classification problems using datasets with different distribution and spatial characteristics. Datasets were generated using the scikit-learn library. Was compared the developed approaches to find average accuracy on all these datasets. It was shown, that even small amounts of labeled data allow us to use semi-supervised learning, and proposed modifications are expected to improve accuracy and algorithm performance, which was demonstrated during experiments. And with the increase of available label information accuracy of the algorithms grows up. Thus, the developed algorithms are using a distance metric that considers available label information.  

Keywords: Unsupervised learning, supervised learning, semi-supervised learning, clustering, distance, distance function, nearest neighbor, medoid, center of mass.

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Introduction. A large amount of data was produced recently, and nowadays humanity had the opportunity to store and process all this data. In all spheres of life people try to use these data for optimizing business and life-improving using AI and data mining.

There are several approaches to data processing and analysis problem within the framework of machine learning paradigms. One of them is unsupervised learning [1] when we try to detect inner structure or patterns without human supervision. The most efficient approach in machine learning is supervised learning, when we have some data with labels and try to learn a function on data points as label pairs. In many cases, there is no opportunity to label all data from different cases, causes are too complex and expensive experiments, data streaming with large frequency, or just high cost of data labeling. Therefore, in this case a satisfactory compromise is semi-supervised learning when we use datasets with a small amount of labeled that allows learning better inner structure (fig 1).

![Fig. 1. Example of unlabeled data in semi-supervised learning](image)

Semi-supervised learning includes different approaches, and can be used for any popular data analysis problems, such as clustering [3], anomaly detection, latent variables models.

The object of the study is the process of the data points classifications, namely, identifying to which of a set of categories a new observation belongs using a training set of data containing observations whose category membership is known.

The subject of the study is development of semi-supervised methods for data classification.

The purpose of the work is to develop an improved semi-supervised method using already exist supervised and unsupervised approaches and compare their accuracy and robustness.

Problem statement. Given a set of \( l \) labeled examples \( \{< x_1, y_1 >, ..., < x_l, y_l >\} \), where \( x_i \) — feature vector of \( i \)-th example and \( y_i \) — its label (class), and a set of \( u \) unlabeled data \( \{x_{i+1}, ..., x_{i+u}\} \), \( x_1, x_2, ..., x_{i+u} \in X \) and \( y_1, y_2, ..., y_l \in Y \). The goal is to determine some function using given sets, that will correct map points from \( X \) to \( Y \): \( f(x_i) = y_j \) for any point from \( X \).

Related work. The semi-supervised learning described in literature not so widely as unsupervised or supervised, especially algorithms implementation.

In [4] Jesper E. van Engelen and Holger H. Hoose gives an overview of semi-supervised approaches describes assumptions of semi-supervised learning especially: smoothness, low-density and manifold.

Semi-supervised approach demonstrates high efficiency in solving clustering problems, the idea of using of clustering algorithm was described in the review [5]. The majority of these methods are modifications of the popular \( k \)-means clustering method.

One of the simplest unsupervised approach is \( K \)-Medoids also known as Partitioning Around Medoid algorithm was proposed in 1987 by Kaufman and Rousseeuw in [6]. A medoid is a point in the cluster, whose average dissimilarities with all the other points in the cluster is minimum.

\( K \)-medoid is a partitioning technique of clustering, which clusters the data set of \( n \) objects into \( k \) clusters, with the number \( k \) of clusters assumed known a priori.

Both the \( k \)-means and \( k \)-medoids algorithms are partitional, which breaking the dataset up into groups, and both attempt to minimize the distance between points labeled to be in a cluster, and a point designated as the center of that cluster. In contrast to the \( k \)-means algorithm, \( k \)-medoids choose data points as centers and can be used with arbitrary distances, while in \( k \)-means the center of a cluster is the average between the points in the cluster (fig 2). Consequently, \( K \)-medoids is more robust to noise and outliers as compared to \( K \)-means.

![Fig. 2. Mean and medoid difference](image)
One of the popular semi-supervised methods is kernels based methods \cite{8}, especially Transductive support vector machines \cite{9,10}. This method has the same pros and cons as classic Support Vector Machine, but the main cons are that the algorithm works only with binary classification and has exponential computation time while a data set to increase.

**Semi-supervised methods.** As a baseline was chosen clustering algorithms implemented in the scikit-learn library \cite{11,12}. Algorithms use different approaches and library has interfaces for using custom metrics.

The proposed algorithm uses the $K$-medoid approach as a base idea. However, unlike $K$-medoids the proposed algorithm first calculates medoids using only labeled data and next process unlabeled classes – assign labels of nearest medoid.

This algorithm has the following pros:

- reduced processing time, because required only multiple iteration throw points unlike standard $K$-medoid;
- more robustness to wrong assigned labels, because the algorithm gives higher weights to labeled data in the medoids calculation step.

Another proposed approach uses the idea of $K$-nearest neighbors and $K$-Mean algorithm, for because classifying we use both information about the nearest points and classes centers of mass (algorithm 1).

As a distance metric was used Euclidean distance but any metric could be used.

Classes’ centers do not recalculate after each assignment, because experiments show that it does not bring results but takes more computation time. So, the described above method allows:

- consider information about the nearest point, because in most cases point has the same label as its neighbors;
- combine a different kind of information;
- tune weight of different sources using input parameters.

**Experiments.** For experiments purpose was generated multiple datasets using sklearn library. Each dataset contains 250 points in 2D space. Available only 10% of labels as default. In addition, datasets have multiple clusters with different distributions and shapes (fig. 3).

We will compare different approaches to find average accuracy on all these. In Tab. 1 we can see that the best-unsupervised method is $K$-nearest neighbors based algorithm has higher average accuracy. The fig. 4 shown the same result. Especially the $K$-nearest neighbors based approach has better accuracy in case of closely located clusters with the same distribution.

Another required feature of a semi-supervised algorithm is quality versus a number of labels dependency: more labels – higher quality and vice versa. However, fig. 5 shows that the proposed methods perform more accuracy with increasing number of available labels.

| Method name                | Dataset name | Average accuracy |
|----------------------------|--------------|------------------|
| $K$-medoids based          | Moons        | 0.860            |
| $K$-nearest neighbors based| Aniso        | 0.864            |
| $(N = 5, C = 2)$            | Varied       | 0.904            |
|                            |              | 0.904            |
|                            |              | 0.912            |
|                            |              | 0.905            |

**Algorithm 1.** Object classification using K-NN based approach

**Input:**

$X$ – feature matrix $n \times m$, $n$ – number of objects, $m$ – number of features

$y$ – labels vector of length $n$, $y[i] = -1$ if no label data for $i$-th object

$K$ – number of nearest points

$C$ – weight of nearest class center

**Output:**

$y_{predicted}$ – vector of length $n$ with object labels

1. $y_{predicted} \leftarrow \emptyset$
2. $unlabeled\_idxs \leftarrow \{\text{indexes where } y = -1\}$
3. $labeled\_idxs \leftarrow \{\text{indexes where } y > -1\}$
4. $center\_coordinates \leftarrow \{\text{center coordinates for each class, calculated using available labels}\}$
5. random shuffle $unlabeled\_idxs$
6. for $i$ in $unlabeled\_idxs$
7. $distances\_i \leftarrow \{\text{distances from } i$-th object to each object with indexes in $labeled\_idxs\}$
8. $distances\_i \leftarrow \text{argsort} \{\text{distances}_i\}$
9. $nearest\_idxs \leftarrow \{\text{indexes of first } K \text{ elements from } distances\_i\}$
10. $classes\_dist\_i \leftarrow \{\text{distance from } i$-th object to each classes' center\}$
11. $nearest\_class\_idxs \leftarrow \{\text{index of nearest class to } i$-th object\}$
12. $cls\_counts \leftarrow \{\text{where } j$-th element denote numbers of points belong to $j$-th class among $nearest\_idxs\}$
13. $cls\_counts[nearest\_class\_idxs] \leftarrow \text{cls\_counts[nearest\_class\_idxs]} + C$ // add additional value for class with nearest center
14. $label \leftarrow \text{argmax}(cls\_counts)$
15. $y_{predicted}[i] \leftarrow label$
16. end for
17. for $i$ in $labeled\_idxs$
18. $y_{predicted}[i] \leftarrow y[i]$
19. end for
20. return $y_{predicted}$
Fig. 3. Datasets visualization; the legend shows classes’ label; -1 – unlabeled point;

- $a, b$ – moons dataset, 2 classes, with non-convex and separable shapes;
- $c, d$ – aniso dataset, 3 classes, convex shape with same class variation, not separable;
- $e, f$ – varied dataset, 3 classes with a convex shape and different class variation, also not separable
Fig. 4. Predicted labels visualization; a, c, f – unsupervised $K$-Medoids; 
  $b, d, f$ – semi-supervised $K$-nearest neighbors based method.
Conclusions. In this study, we had shown that even small amounts of labeled data allow using of semi-supervised learning and improving accuracy. In addition, semi-supervised learning can improve algorithm performance too. Multiple approaches to semi-supervised learning were proposed, they are using a distance metric that considers available label information.

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