On using Additional Unlabeled Data for Improving Dissimilarity-Based Classifications*

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- Keywords: Dissimilarity-Based Classification (DBC), One-Shot Similarity Metric (OSS), Semi-Supervised Learning (SSL).
- Abstract: This paper reports an experimental result obtained with additionally using unlabeled data together with labeled ones to improve the classification accuracy of dissimilarity-based methods, namely, dissimilarity-based classifications (DBC) (Pękalska, E. and Duin, R. P. W., 2005). In DBC, classifiers among classes are not based on the feature measurements of individual objects, but rather on a suitable dissimilarity measure among the objects. In image classification tasks, on the other hand, one of the intractable problems is the lack of information caused by the insufficient number of data. To address this problem in DBC, in this paper we study a new way of measuring the dissimilarity distance between two object images by using the well-known one-shot similarity metric (OSS) (Wolf, L. et al., 2009). In DBC using OSS, the dissimilarity distance is measured based on unlabeled (background) data that do not belong to the classes being learned, and consequently, do not require labeling. From this point of view, the classification is done in a semi-supervised learning (SSL) framework. Our experimental results, obtained with well-known benchmarks, demonstrate that when the cardinalities of the unlabeled data set and the prototype set have been appropriately chosen using additional unlabeled data for the OSS metric in SSL, DBC can be improved in terms of classification accuracies.

1 INTRODUCTION

In dissimilarity-based classifications (DBC), designing a classifier is not based on the feature measurements of individual objects, but rather on a suitable dissimilarity measure among the individual objects (Pękalska, E. and Duin, R. P. W., 2005). The advantage of this strategy is that it can avoid the problems associated with feature spaces, such as the curse of dimensionality and the issue of estimating a number of parameters on data distributions (Kim, S. -W. and Oommen, B. J., 2007). Another characteristic of the dissimilarity approach is that it offers a different way to include expert knowledge on the objects in classifying them (Duin, R. P. W., 2011). One of the questions we encountered when designing DBC is: How can the (dis)similarities between object examples be efficiently measured? To explore this question, various strategies have been proposed in the literature, including (Bicegoa, M. et al., 2004), (Pękalska, E. and Duin, R. P. W., 2005), (Pękalska, E. and Duin, R. P .W., 2008), (Orozco-Alzate, M. et al., 2009), (Duin, R. P. W., 2011), and (Millán-Giraldo, M. et al., 2012). In these strategies, investigations have focused specifically on generalizing the dissimilarity representation by using various methods, such as feature lines and feature planes (Orozco-Alzate, M. et al., 2009) and hidden Markov models (Bicegoa, M. et al., 2004).

On the other hand, when designing a DBC with a measuring system, we sometimes suffer from the difficulty of collecting sufficient (labeled) training data for each class. Labeled instances, for example, are often difficult, expensive, or time-consuming to obtain, as they require the services of an experienced expert. Meanwhile, unlabeled data, defined as the samples that do not belong to the classes being learned, may be relatively easy to collect, but the use of this type of data is limited. To address this problem, in a learning framework of *semi-supervised learning* (SSL) (Chapelle, O. et al., 2006), a large amount of unlabeled data, together with labeled data, can be utilized to build better classifiers. Because SSL requires less human effort and results in higher accuracy, it is of great interest in practice. However, it is also well known that the utilization of unlabeled data is not al-

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ways helpful for SSL. Specifically, it is not guaranteed that adding unlabeled data to the training data leads to a situation in which we can improve the performance (Ben-David, S. et al., 2008). Several strategies have been investigated to address this, including self-training (McClosky, D. et al., 2008), co-training (Blum, A. and Mitchell, T., 1998), SemiBoost (Mallapragada, P. K. et al., 2009), etc.

Recently, one-shot similarity (OSS) (Wolf, L. et al., 2009) was proposed to exploit both labeled and unlabeled (background) data when learning a classification model. In OSS, when given two vectors, x_i and x_j , and an additionally available (unlabeled) data set, A, a measure of the (dis)similarity between x_i and x_j is computed as follows: First, a discriminative model is learned with x_i as a single positive example and A as a set of negative examples. This model is then used to classify x_j , and to obtain a confidence score. Next, a second such score is obtained by repeating the same process with the roles of x_i and x_j switched. Finally, the (dis)similarity of the two vectors can be obtained by averaging the above two scores.

In DBC, on the other hand, when a limited number of objects are available, it is difficult to achieve the desired classification performance. To overcome this limitation, in this paper we study a way of exploiting additionally available unlabeled data when measuring the dissimilarity distance with the OSS metric. As in SSL, we use the easily collected unlabeled data as the background data set, A, with which we can enrich the representational capability of the dissimilarity measures. The main contribution of this paper is to demonstrate that the classification accuracy of DBC can be improved by employing the OSS metric based on additional unlabeled data. More specifically, experiments on an artificial and real-life data sets have been carried out to demonstrate better performance than selected baseline approaches.

The remainder of the paper is organized as follows: In Section 2, after providing a brief introduction to DBC and OSS, we present an explanation for the use of OSS in DBC and a modified DBC algorithm. In Section 3, we present the experimental setup and the results obtained with the experimental data. Finally, in Section 4, we present our concluding remarks as well as some feature works that deserve further study.

2 RELATED WORK

2.1 Dissimilarity Representation

A dissimilarity representation of a set of objects, $T = \{x_i\}_{i=1}^n \in \mathbb{R}^d$ (*d*-dimensional samples), is based on

pair-wise comparisons, and is expressed, for example, as an $n \times m$ dissimilarity matrix, $D_{T,P}[\cdot, \cdot]$, where $P = \{p_j\}_{j=1}^m \in \mathbb{R}^d$, a prototype set, is extracted from *T*. The subscripts of *D* represent the set of elements, on which the dissimilarities are evaluated. Thus, each entry, $D_{T,P}[i, j]$, corresponds to the dissimilarity between the pairs of objects, $\langle x_i, p_j \rangle$, where $x_i \in T$ and $p_j \in P$. Consequently, when given a distance measure between two objects, $d(\cdot, \cdot)$, an object, $x_i, (1 \le i \le n)$, is represented as a new vector, $\delta(x_i, P)$, as follows:

$$\delta(x_i, P) = [d(x_i, p_1), d(x_i, p_2), \cdots, d(x_i, p_m)].$$
(1)

Here, the generated dissimilarity matrix, $D_{T,P}[\cdot, \cdot]$, defines vectors in a *dissimilarity space*, on which the *d*-dimensional object, *x*, given in the input feature space, is represented as an *m*-dimensional vector, $\delta(x, P)$ or shortly $\delta(x)$. On the basis of what we have just explained briefly, a conventional algorithm for DBC is summarized as follows:

1. Select the prototype subset, P, from the training set, T, by using one of the prototype selection methods described in the related literature.

2. Using Eq. (1), compute the dissimilarity matrix, $D_{T,P}[\cdot, \cdot]$, in which each dissimilarity is computed on the basis of the given distance measure $d(\cdot, \cdot)$.

3. For a testing sample, *z*, compute a dissimilarity feature vector, $\delta(z)$, by using the same prototype subset and the distance measure used in Step 2.

4. Achieve the classification by invoking a classifier built in the dissimilarity space and operating it on the dissimilarity vector $\delta(z)$.

2.2 One-shot Similarity

Assume that we have two vectors, x_i and x_j , and an additionally available (unlabeled) data set, A. To measure OSS, we first generate a hyperplane that separates x_i and A (and also x_j and A). Then, we count the distance from x_j (and also x_i) to the hyperplane decision surface. For a 2-class classification problem, for example, we begin with a simple case of designing a linear classifier described by $g(x) = w^T x + w_0$. To make it clear, we focus again on the binary LDA (Fisher's linear discriminant analysis) (Duda, R. O. et al., 2001). Then, after deriving a projection matrix, w, by maximizing the Rayleigh quotient, we can classify an unknown vector, z, to class-1 (or class-2) if g(z) > 0 (or g(z) < 0).

Using the above LDA-based OSS, the dissimilarity distance between the pairs of x_i and x_j can be computed as follows (Wolf, L. et al., 2011):

1. By assuming that the class-1 contains a single vector x_i and the class-2 corresponds to the set of A,

we compute the absolute distance of x_i to the hyperplane that separates x_j and A, $\frac{|g(x_i)|}{||w||}$, where $|\cdot|$ (and $||\cdot||$) denotes the absolute value of a scaler (and the Euclidean norm of a vector), as follows:

$$\gamma(x_i, x_j, A) = \frac{|(x_j - \mu_A)^T S_W^{-1}(x_i - \frac{x_j + \mu_A}{2})|}{\|S_W^{-1}(x_j - \mu_A)\|}, \quad (2)$$

where μ_A (and S_W^{-1}) denotes the mean of all vectors (and the pseudo-inverse of the within-class covariance matrix) of *A*. Also, the bias term is computed using *w* and the mean of x_j and μ_A , as: $w_0 = -w^T \frac{x_j + \mu_A}{2}$.

2. By repeating the same process with the roles of x_i and x_j switched, we compute the distance of x_j to the hyperplane that separates x_i and A as follows:

$$\gamma(x_j, x_i, A) = \frac{|(x_i - \mu_A)^T S_W^{-1}(x_j - \frac{x_i + \mu_A}{2})|}{\|S_W^{-1}(x_i - \mu_A)\|}.$$
 (3)

3. Finally, by averaging these two distances, we can compute the dissimilarity of Eq. (1) as follows:

$$d_{OSS}(x_i, x_j) = \frac{1}{2} (\gamma(x_i, x_j, A) + \gamma(x_j, x_i, A)), \quad (4)$$

where x_j plays as a p_j , $(1 \le j \le m)$.

2.3 The Use of OSS for DBC

When given an unlabeled data set, $A \in \mathbb{R}^d$, l = |A|(where $|\cdot|$ denotes the cardinality of a set), in addition to the existing prototype set, P, m = |P|, the cardinality of the representation set, $P' (=P \cup A \in \mathbb{R}^d)$, is m+lwhen the entire set of the training data is selected as the prototypes. Thus, each entry of the dissimilarity matrix, $D_{T,P'}[i, j]$, $(1 \le i \le n; 1 \le j \le m+l)$, is represented as an augmented vector, $\delta(x_i, P')$, as follows:

$$\delta(x_i, P') = [d(x_i, p_1), d(x_i, p_2), \cdots, d(x_i, p_{m+l})], \quad (5)$$

where $p_j \in P'$ and m+l = |P'|.

In DBC, another way of utilizing *A* is to measure the dissimilarity in OSS metric by employing *A* as the background data. When measuring the OSS together with *A*, each entry of $D_{T,P}[i, j]$, $(1 \le i \le n; 1 \le j \le m)$, is computed as follows:

$$\delta_{OSS}(x_i, P) = [d_{OSS}(x_i, p_1), \cdots, d_{OSS}(x_i, p_m)], \quad (6)$$

where $p_i \in P$ and m = |P|.

On the basis of what we explained briefly, an algorithm for SSL-type DBC is summarized as follows:

1. Obtain labeled training set *T*, prototype subset *P*, and unlabeled set *A* as input data sets.

2. Using Eq. (5) or (6), rather than Eq. (1), compute $D_{T,P}[\cdot, \cdot]$, in which each dissimilarity is computed on the basis of a distance metric.

3. This step is the same as Step 3 in DBC.

Table 1: Characteristics of the experimental data sets. Here, the dimensionality of the data set marked with a † symbol is reduced into 10% value using a PCA.

Data	Datasets	# of	# of	# of
types	names	features classes		objects
	Auto_mpg	6	2	392
	Dermatology	34	6	366
UCI	Diabetes	8	2	768
	Heart	13	2	297
	Laryngeal1	16	2	213
	Liver	6	2	345
	Nist38	1024	2	1000
	Sonar	60	2	208
	Yeast	8	10	1484
	BCI	117	2	400
SSL	COIL	241	6	1500
	COIL2	241	2	1500
	USPS	241	2	1500
	Text [†]	11960	2	1500

4. This step is the same as Step 4 in DBC.

From a comparison of the algorithms of DBC and SSL-type DBC given in Sections 2.1 and 2.3, it can be seen that the required CPU-time for the latter is more sensitive to the dimensionality and the cardinality of T, P, and A than that for the former.

3 EXPERIMENTAL RESULTS

3.1 Experimental Setup

The proposed method has been tested and compared with the conventional ones. This was done by performing experiments on an artificial data, namely, the Difficult (a normally distributed *d*-dimensional 2-class) data (Duin, R. P .W. et al., 2004)² and other multivariate data sets cited from the UCI machine learning repository (Frank, A. and Asuncion, A., 2010)³ and SSL-type benchmarks (Chapelle, O. et al., 2006)⁴. Characteristics of the UCI and SSL-type data sets are summarized in Table 1.

The experiment focuses on a few simple binary and multi-class classification problems, where all data sets are initially split into three subsets: labeled training data, L, labeled test (evaluation) data, E, and unlabeled data, U. The training and test procedures are then repeated ten times and the results obtained are averaged.

In this experiment, classifications are carried out in four ways, which are named F_{input} , $D_{exclude}$,

²http://prtools.org/

³http://www.ics.uci.edu/~mlearn/MLRepository.html ⁴http://www.kyb.tuebingen.mpg.de/ssl-book/

 $D_{include}$, and D_{OSS} . In F_{input} , classification is carried out in the original input-feature space as the traditional one does. In the other schemes, however, classifications are performed in three dissimilarity representations differently constructed as follows: First, in $D_{exclude}$ approach, the entire L (or its subset) serves as a prototype set P, and the dissimilarity between the pairwise objects, $\delta(\cdot, P)$, is measured with Eq. (1), in which $d(\cdot, \cdot)$ is the Euclidean distance (l_2 metric). Here, U is precluded. Second, in $D_{include}$, the prototype set, P, is randomly selected from $L \cup U$ and the dissimilarity, $\delta(\cdot, P)$, is measured with Eq. (5), in which $d(\cdot, \cdot)$ is also l_2 metric. Finally, in D_{OSS} , L works as the prototype set P, and the dissimilarity, $\delta_{OSS}(\cdot, P)$, is measured with Eq. (6), in which $d_{OSS}(\cdot, \cdot)$ is the averaged OSS confidence, $\bar{\gamma}(\cdot, \cdot, \cdot)$, utilizing U as a A. Here, to select prototypes from Lor $L \cup U$, the *Random* selection is utilized in the experiment. However, other various methods described in the literature (Pękalska, E. and Duin, R. P. W., 2005), (Kim, S. -W. and Oommen, B. J., 2007), such as RandomC, KCentres, ModeSeek, LinProg, FeatSel, KCentres-LP, EdiCon, etc, can also be considered.

Finally, to evaluate the classification accuracies of all the four approaches, a classifier based on the *k*-nearest neighbor rule is employed to classify the evaluation test data, *E* (or the corresponding dissimilarity representations), and will be denoted as *knnc* (where k = 1) in subsequent sections.

3.2 Experiment # 1 (Difficult Data)

First, the experimental results obtained with the three classifiers trained in the four approaches for an artificial data set, the Difficult data set (Duin, R. P. W. et al., 2004), were probed into. We first generated a 5-dimensional 2-class Difficult data set of the positive and negative samples of [300, 300], and divided them into L, E, and U subsets at a ratio of 20% : 10% : 70%. Then, we performed the experiment as mentioned previously.

Fig. 1 (a) shows a comparison of the error rates obtained with *knnc* trained in the four approaches for seven different cardinalities of P of Difficult data, under the condition A = U. Also, Fig. 1 (b) shows a comparison of the error rates obtained with the same classifier, but designed with different cardinalities of A of Difficult, having P = L. Here, the x and y axes represent the seven different cardinalities of P (and A) and the averaged error rates, respectively.

The observations obtained from the two pictures shown in Fig. 1 (a) and (b) are the followings: First, in Fig. 1 (a), it should be pointed out that the estimated error rates obtained with the $D_{exclude}$, $D_{include}$,



Figure 1: Error rates obtained with *knnc* trained in the four approaches for Difficult data: (a) top and (b) bottom; (a) and (b) are obtained with different cardinalities of the prototype set, *P*, and the unlabeled data set, *A*, respectively.

and D_{OSS} approaches, marked with the \triangleright , \Box , and \diamond symbols, decrease *uniformly* as the cardinality of *P* increases, i.e., the three graphs have the same shape in general, maintaining a consistent difference from each other. This comparison demonstrates that the classification accuracy of D_{OSS} , marked with the \diamond symbol, is always the lowest among the four rates when having an appropriate number of prototypes.

Next, in Fig. 1 (b), the two error rates obtained with $D_{exclude}$ and $D_{include}$ are almost the same for different numbers of unlabeled samples, from which we can see that the addition of an available unlabeled data set, U, to the existing prototype set, i.e., $P = L \cup U$ or its randomly selected subsets, did *not* succeed in enhancing the classification performance.

Finally, in Fig. 1 (b), it should be mentioned that, in evaluation of the error rates, the cardinality of the prototype set is more sensitive than that of the unlabeled background set; the curves of the latter are more flat than those of the former.

From these observations, it can be mentioned that

the accuracy of certain kinds of DBC classifiers, such as *knnc*, can be improved by using the available unlabeled data in a SSL fashion through measuring the dissimilarity with a OSS metric. This characteristic can be observed again in subsequent experiments.

3.3 Experiment # 2 (UCI / SSL Data)

Second, to further investigate the characteristics of the proposed method, and, especially, to find out which kinds of significant data sets are more suitable for the scheme, we repeated the experiment with a few of UCI and SSL-type benchmark data sets. After dividing each data set into the L, E, and U subsets at a ratio of 40% : 30% : 30%, we performed the training and evaluation procedures 30 times and computed the error rates by averaging the results obtained.

Table 2 shows a numerical comparison of the mean error rates (\pm standard deviations) obtained with the classifier, knnc, trained in a traditional feature-based and four dissimilarity-based approaches. Here, the results shown in the fifth and the sixth columns, i.e., those of $D_{includeP}$ and $D_{includeW}$, are obtained with two specific cases of $D_{include}$. In the latter case, the prototype set is the whole set of labeled samples and unlabeled ones, i.e., $P = L \cup U$, while, in the former case, it is the (randomly chosen) par*tial* subset of the cardinality of |L|. Besides, in both $D_{exclude}$ and D_{OSS} , the entire set of L is served as a P, while, in D_{OSS} , U is utilized as a A. Also, in order to facilitate the comparison in the tables, the lowest error rate in each data set is bold-faced. Especially, the values highlighted with a * marker are the lowest one among the four error rates of the DBC approaches.

Table 2 presents the error rates obtained with *knnc* designed in the five approaches for the data sets, showing the similar characteristics as the ones we obtained in the figures (see the bold-faced and/or * marked numbers). In the table, we observed that almost all of the lowest error rates (* marked) were achieved with D_{OSS} except for Auto_mpg.

From this consideration, a question arises: *Why* does D_{OSS} not work in certain applications? The theoretical explanation for this remains unchallenged.

In addition, to simplify the classification task for the experiment and because of the limit on the number of pages, only a classifier of the *k*-nearest neighbor rule was experimented and analyzed. However, other classifiers, including the AdaBoost algorithm, support vector machines, and neural networks, can also be considered.

Also, in the above two experiments # 1 and # 2, it was observed that using U can lead to increasing the classification accuracy of DBC. Although the classlabels of the U was not used in the training phase, it had been selected from a given training data set. Thus, the characteristics of U are the same as those of the training data set. From this point of view, the following question is an interesting issue to investigate: Is the classification accuracy of D_{OSS} superior or inferior to that of the conventional scheme when U is collected from a different data set? The experimental results on these issues will be appeared in a subsequent journal paper.

In review, it is not easy to decide which kinds of significant methods are more suitable for DBC to use unlabeled data in a SSL fashion. However, by comparing the numbers of the highlighted values among the DBC approaches, the reader should observe that the classification accuracies of certain kinds of classifiers designed with D_{OSS} , representing the use of OSS for DBC, are marginally better than those of the classifiers designed in $D_{exclude}$, $D_{includeP}$, and $D_{includeW}$. So, the classifier of D_{OSS} , albeit not always, seems to be more helpful for certain kinds of data sets than the Euclidean distance does.

4 CONCLUSIONS

In our efforts to improve the classification performance of DBC in a SSL fashion, we used the wellknown OSS measuring scheme based on the background information of available extra (unlabeled) data. To achieve this improvement, we first computed the confidence levels of the training data with the OSS metric. We then constructed the dissimilarity matrices, where the dissimilarity was measured with the averaged confidence levels. This measuring technique using unlabeled data was employed to solve the problems caused by the insufficient number of labeled data. The proposed method was tested on an artificial data and the UCI / SSL-type data sets, and the results obtained were compared with those of a feature-based classification and three dissimilarity-based ones.

Our experimental results demonstrate that the classification accuracy of DBC, albeit not always, is improved when the cardinalities of the prototype subset P and the unlabeled background set A have been appropriately chosen. Also, the results show that the accuracy is superior to that of the conventional schemes when A is collected from data samples that are different in nature. Although we have shown that DBC can be improved by employing the OSS metric, many tasks remain open. One of them is to further improve the classification efficiency by selecting an optimal, or nearly optimal, cardinality of P (and A) and utilizing various distance learning techniques in

Table 2: A numerical comparison of the mean error (\pm std) rates obtained with <i>knnc</i> implemented in the five approaches
for the UCI and SSL-type data sets. In order to facilitate the comparison, for each row, the lowest error rate is bold-faced.
Especially, the values highlighted with a * marker are the lowest one among the four error rates of the DBC approaches.

Data	Dataset	Input feature-based	Dissimilarity-based classification (DBC)			
types	names	classification (Finput)	Dexclude	$D_{includeP}$	$D_{includeW}$	D _{OSS}
	Auto_mpg	15.00 ± 2.49	15.00 ± 2.71	15.20 ± 2.68	$*14.94 \pm 2.62$	14.97 ± 3.16
	Dermatology	16.35 ± 3.78	32.86 ± 4.37	34.00 ± 3.89	32.79 ± 4.11	* 14.44 ± 3.59
	Diabetes	28.60 ± 2.62	29.80 ± 2.40	29.99 ± 2.41	29.51 ± 2.42	*27.22 ± 1.85
UCI	Heart	36.78 ± 4.59	40.45 ± 4.27	40.42 ± 4.16	40.68 ± 4.27	* 35.11 ± 3.84
	Laryngeal1	25.22 ± 5.38	32.90 ± 5.42	33.49 ± 5.55	32.90 ± 6.12	* 24.62 ± 5.26
	Liver	34.51 ± 5.11	40.03 ± 4.36	40.26 ± 4.16	40.39 ± 4.32	*36.50 ± 5.37
	Nist38	2.90 ± 0.75	2.98 ± 0.90	4.44 ± 1.31	3.06 ± 0.92	* 2.66 ± 1.03
	Sonar	24.44 ± 6.10	28.28 ± 5.76	29.89 ± 4.75	28.94 ± 7.04	$*24.72 \pm 6.74$
	Yeast	43.55 ± 2.23	46.04 ± 2.11	46.03 ± 2.03	46.17 ± 2.38	* 43.45 \pm 2.33
	BCI	46.06 ± 4.97	46.89 ± 4.58	47.00 ± 4.98	47.78 ± 4.18	* 44.72 \pm 4.99
	COIL	5.72 ± 1.35	6.44 ± 1.07	6.58 ± 1.17	6.56 ± 1.11	* 4.93 ± 1.08
SSL	COIL2	0.81 ± 0.51	1.90 ± 0.83	2.01 ± 0.79	1.92 ± 0.79	* 0.60 ± 0.43
	USPS	3.73 ± 0.94	4.81 ± 1.01	4.79 ± 0.95	4.81 ± 0.87	* 3.52 ± 0.81
	Text	23.67 ± 1.86	24.22 ± 1.98	26.44 ± 2.36	24.36 ± 2.10	$\textbf{*22.35} \pm 2.06$

the OSS scheme. Also, it is not yet clear which kinds of significant data sets (and classifiers) are more suitable for the use of OSS for DBC.

Finally, the proposed method lacks of details to support its technical soundness, and the experiments performed are very limited. Therefore, the problem of theoretically investigating the measuring method developed for DBC remains to be challenged.

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