Dissimilarity-Based Ensembles for Multiple Instance Learning

Veronika Cheplygina, David M. J. Tax, and Marco Loog

***Abstract*— In multiple instance learning, objects are sets (bags) of feature vectors (instances) rather than individual feature vectors. In this paper, we address the problem of how these bags can best be represented. Two standard approaches are to use (dis)similarities between bags and prototype bags, or between bags and prototype instances. The first approach results in a relatively low-dimensional representation, determined by the number of training bags, whereas the second approach results in a relatively high-dimensional representation, determined by the total number of instances in the training set. However, an advantage of the latter representation is that the informativeness of the prototype instances can be inferred. In this paper, a third, intermediate approach is proposed, which links the two approaches and combines their strengths. Our classifier is inspired by a random subspace ensemble, and considers subspaces of the dissimilarity space, defined by subsets of instances, as prototypes. We provide insight into the structure of some popular multiple instance problems and show state-of-the-art performances on these data sets.**

***Index Terms*— Combining classifiers, dissimilarity representation, multiple instance learning (MIL), random subspace method (RSM).**

I. Introduction

NOWADAYS, many applications face the problem of using weakly labeled data for training a classifier. For example, in image classification, we may only have an overall label for an image (such as a tiger), not where the tiger is actually located in the image. Such problems are often formulated as multiple instance learning (MIL) [1] problems. MIL is an extension of supervised learning, and occurs in cases when class labels are associated with sets (bags) of feature vectors (instances) rather than with individual feature vectors. The bag labels provide weak information about the instance labels. For example, the label tiger could apply to only some of the image patches, because patches of sand, sky, or other surroundings could be present as well. This is a natural representation for many real-world problems, therefore, MIL has been successfully used to address molecule [1] or drug [2] activity prediction, image classification [3], [4], document categorization [5], computer-aided diagnosis [6], and many other problems.

Manuscript received September 30, 2013; revised December 10, 2014 and March 30, 2015; accepted April 7, 2015. Date of publication May 25, 2015; date of current version May 16, 2016.

The authors are with the Pattern Recognition Laboratory, Delft University of Technology, Mekelweg 4, 2628CD Delft, The Netherlands (e-mail: v.cheplygina@tudelft.nl; d.m.j.tax@tudelft.nl; m.loog@tudelft.nl).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/TNNLS.2015.2424254

We can group methods that learn in this weakly supervised setting in two categories. The first category, which we call instance-based methods, relies on different assumptions [7] about the relationship of the bag labels and the instance labels to build instance classifiers. A bag is classified a bag by first classifying that bag's instances, and then fusing these outputs into a bag label. For example, the standard assumption is that a bag is positive if and only if at least one of its instances is positive or inside a concept [1]. The second category, which we call bag-based methods, often uses the collective assumption. They assume all instances contribute to the bag label, and that bags with the same label are somehow similar to each other. Therefore, the bags can be classified directly using distances [8] or kernels [9], or by converting bags to a single-instance representation and using supervised learners [4], [10], [11]. The bag-based methods have frequently demonstrated the best performances on a wide range of data sets.

One of the ways to represent structured objects, such as bags, in a feature space, is to describe them relative to a set of reference objects or prototypes. This approach is called the dissimilarity representation [12] and is in contrast to traditional pattern recognition, because the dimensions of this space are defined in a relative way. The dissimilarity to the jth prototype can, therefore, be seen as the jth feature in the transformed space. A successful approach we studied uses training bags as prototypes [10], [13], whereas an alternative approach called multiple instance learning via embedded instance selection (MILES) [4] uses all the training instances as prototypes. Both alternatives have demonstrated the best performances on a wide range of MIL problems, and, as we show in this paper, are, in fact, strongly related. However, both approaches are extremes with respect to the dimensionality and the information content of the resulting dissimilarity space. The bag representation reduces the dimensionality from the number of instances to the number of bags, but risks losing information contained in the individual instances. The instance representation preserves more information, but increases the dimensionality dramatically, possibly including many redundant features.

We propose a third alternative, which combines the advantages of using bags and instances as prototypes. We train classifiers on different subspaces of the instance dissimilarity space, where each subspace is formed by the instances of a particular bag, and combining the decisions of these classifiers in the test phase. This way, the information provided by different dissimilarities is preserved, but the dimensionality

of each subspace is lower. Therefore, the ensemble has the potential to be more robust than a single classifier, but still has the ability to provide interpretation for which instances are important in classification. Note that the bag, instance, and subspace representations are analogous to different ways—averaging, concatenating, and ensembles—of combining information from different sources [14]–[16]. The informativeness of these sources is central to this paper, and we focus on investigating which prototypes—bags, instances, or subspaces—are more informative in MIL problems.

We first introduced dissimilarity-based subspace ensembles in [17]. We now present an extended analysis of our approach, as well as significantly improved results on many MIL data sets. With respect to [17], this paper has several differences. In Section II, we explain the preliminary tools used in our method, and relate our method to other dissimilarity-based approaches in MIL. In Section III, we more formally define the proposed approach and explain the parameter choices that need to be made that were treated as defaults in [17]. In Section IV, we provide understanding of the relationship between these parameters and the ensemble performance, which also explains our earlier results. We then demonstrate the effectiveness of the proposed approach with competitive results on several benchmark data sets.[1] In addition to these results, we provide insight into the structure of some popular MIL problems, and why the dissimilarity space is a successful approach for such problems in general.

II. Dissimilarity-Based Multiple Instance Learning

A. Data Representation

In MIL, an object is represented by a bag $B_i = \{\mathbf{x}_{ik} | k = 1, \ldots, n_i\} \subset \mathbb{R}^d$ of n_i feature vectors or instances. The training set $\mathcal{T} = \{(B_i, y_i) | i = 1, \ldots, N\}$ consists of positive ($y_i = +1$) and negative ($y_i = -1$) bags, although multiclass extensions are also possible [18]. The standard assumption for MIL is that there are instance labels y_{ik}, which relate to the bag labels as follows. A bag is positive if and only if it contains at least one positive, or concept instance: $y_i = \max_k y_{ik}$. In this case, it might be worthwhile to search for only these informative instances. Alternative formulations, where a fraction or even all instances are considered informative, have also been proposed [7].

We can represent an object, and therefore also an MIL bag B_i, by its dissimilarities to prototype objects in a representation set $\mathcal{R}$ [12]. Often $\mathcal{R}$ is taken to be a subset of size M of the training set $\mathcal{T}$ of size N ($M \leq N$). If we apply this to MIL, each bag is represented as $\mathbf{d}(B_i, \mathcal{T}) = [d(B_i, B_1), \ldots, d(B_i, B_M)]$: a vector of M dissimilarities. Therefore, each bag is represented by a single feature vector $\mathbf{d}$ and the MIL problem can be viewed as a standard supervised learning problem.

The bag dissimilarity $d(B_i, B_j)$ is defined as a function of the pairwise instance dissimilarities $[d(\mathbf{x}_{ik}, \mathbf{x}_{jl})]_{n_i \times n_j}$. There are many alternative definitions (see [10], [19]), but in this paper, we focus on the average minimum instance distance, which tends to perform well in practice. Suppose that we are only given one prototype B_j. With the proposed bag dissimilarity, the bag representation of B_i using prototype B_j is

$$d^{\text{bag}}(B_i, B_j) = \frac{1}{n_i} \sum_{k=1}^{n_i} \min_l d(\mathbf{x}_{ik}, \mathbf{x}_{jl}). \tag{1}$$

Note that the dissimilarity between bag B_i and B_j is now reduced to a scalar, and $\mathbf{d}(B_i, \mathcal{T})$ becomes an M-dimensional vector.

A related method, MILES [4], considers a different definition of prototype, using the training instances rather than the training bags. The motivation is that, when we assume just a few concept instances per bag, it is better to consider just these informative instances rather than the bag as a whole. MILES is originally a similarity-based approach, where the similarity is defined as $s(B_i, \mathbf{x}) = \max_k \exp(-(d(\mathbf{x}_{ik}, \mathbf{x})/\sigma^2))$ and σ is the parameter of the radial basis function kernel. However, by leaving out kernel and the need to choose σ, we get a dissimilarity-based counterpart. The instance representation of B_i using the instances of B_j is then defined as

$$\mathbf{d}^{\text{inst}}(B_i, B_j) = \Big[\min_l d(\mathbf{x}_{i1}, \mathbf{x}_{jl}), \min_l d(\mathbf{x}_{i2}, \mathbf{x}_{jl}), \ldots, \min_l d(\mathbf{x}_{in_i}, \mathbf{x}_{jl}) \Big]. \tag{2}$$

Now, the dissimilarity between B_i and B_j is summarized in a n_i-dimensional vector, resulting in a representation $\mathbf{d}(B_i, \mathcal{T})$ that has a dimensionality of $\sum_{k=1}^{M} n_k$.

From this point onward, we will discuss the dissimilarity matrices D^{bag} and D^{inst}, which look as follows:

$$D^{\text{bag}} = \left[d^{\text{bag}}(B_*, B_*) \right]_{N \times M} \tag{3}$$

and

$$D^{\text{inst}} = \left[\mathbf{d}^{\text{inst}}(B_*, B_*) \right]_{N \times \sum_{k=1}^{M} n_k}. \tag{4}$$

D^{bag} and D^{inst} are two extremes with respect to the amount of information that is preserved. In cases where only a few instances per bag are informative, D^{bag} could suffer from averaging out these dissimilarities. D^{inst} would preserve these dissimilarities, but it could be difficult for the classifier to select only these relevant dissimilarities due to the high dimensionality of the representation. As an example, consider an image categorization problem, where an image is a bag, and an image region or patch is an instance. If many images in the training set contain regions that include the sky, the dissimilarities to the sky instances in D^{inst} will provide heavily correlated information about the bags. Therefore, D^{inst} could contain many redundant (but not necessarily uninformative) dissimilarities.

On the other hand, when most instances in a bag are informative, we would expect D^{bag} to perform well. D^{inst} would still have access to all the informative dissimilarities, however, selecting a few relevant dissimilarities, as in [11], where a single instance per bag is selected, might not

[1] Data sets available online at http://www.miproblems.org.

be the best strategy if most instances are, in fact, relevant for the classification problem. The problem of being unable to specify how many dissimilarities are informative, still holds in this case.

B. Classifier and Informative Prototypes

In this paper, we consider linear classifiers $(\mathbf{w}, w_0)$ such that $f(\mathbf{d}) = \mathbf{w}^\intercal\mathbf{d} + w_0$ and $\mathbf{w}$ is an M-dimensional vector. The entries of $\mathbf{w}$ correspond to the weights assigned to each of the prototypes, either bags or instances. These weights are found by minimizing an objective function of the form

$$\min_{\mathbf{w}} \mathcal{L}(\mathbf{w}, \mathcal{T}) + \lambda\Omega(\mathbf{w}) \tag{5}$$

where $\mathcal{L}$ is the loss function evaluated on the training set, such as the logistic (for a logistic classifier) or hinge loss [for a support vector classifier or support vector machine (SVM)]. Ω is a regularization function of the weight vector and is often the l_2 norm or the l_1 norm. The l_2 norm typically results in most coefficients of $\mathbf{w}$ being nonzero, whereas the l_1 norm promotes sparsity, i.e., only some of the coefficients have nonzero values. λ is a parameter that trades off the loss with the constraints on the weight vector, and therefore influences the final values in $\mathbf{w}$.

A larger coefficient in $\mathbf{w}$ means the dissimilarity was found to be discriminative by the classifier, we, therefore, can examine the coefficients to discover which prototypes are more informative. However, the low sample size and high dimensionality/redundancy of feature space can make it difficult to find the $\mathbf{w}$ that leads to the best performance on a held-out test set.

There are several alternatives for dealing with the redundancy of the prototypes, which are similar to the filter, wrapper, and embedded methods in feature selection, which we describe in this section.

In the filter approach, (subsets of) prototypes are evaluated prior to training a classifier, therefore reducing the dimensionality of the training set. Such methods include clustering the prototypes and then selecting the cluster centers as prototypes. In [20] and [21], clustering of instances is performed. Erdem and Erdem [20] first rely on the standard assumption to cluster and prune the instances of negative bags, creating negative prototypes. The positive prototypes are created by selecting from each bag the instance that is furthest from the negative prototypes. In [21], the prototypes are initialized as the k-means cluster centers of the instances. The prototypes are then updated by letting the prototypes take any value in the instance space $\mathbb{R}^d$. However, note that in both cases, clustering instances has the risk of excluding informative instances in sparsely populated parts of the feature space, because these would not have any neighbors to form a cluster with. On the other hand, Zhang and Zhou [22] use clustering of bags, by performing k-centers with a bag dissimilarity measure, such as (1), and selecting cluster centers as prototypes. Note that the dissimilarity in (1) is nonmetric in which case clustering may lead to unpredictable results [23]. A more general disadvantage of filter approaches is that the informativeness of the filtered prototypes is not available.

In a wrapper approach, the classifier is used to determine which prototypes are more informative. The less informative prototypes are then removed, and the classifier is trained again on a smaller subset of prototypes. This procedure is repeated several times. This approach is used in multiple instance learning with instance selection [11] and is, in fact, an application of the popular SVM with recursive feature elimination [24] on the D^{inst} representation. Again, a disadvantage is that in the final model, the informativeness of the removed prototypes is not available.

An example of an embedded approach is a sparse classifier that performs feature selection and classification simultaneously, such as the l_1-norm SVM [25] or Liknon classifier [26], used in MILES. This way, each prototype is associated with a weight, representing its informativeness. However, such sparse classifiers require cross validation to set λ, which is ill advised in case the training set is small already. A common consequence of such problems is that a poor set of features might be chosen for the testing phase.

We would like to stress that it is not our purpose to focus on a selection of prototypes, whether instances or bags. Next to the methods described above, there are many works on prototype selection in dissimilarity spaces [27], [28] that could be applied on either D^{bag} or D^{inst} representations. However, from the perspective of MIL, we are instead interested in the more general question of which prototypes—bags, instances, or subspaces—are more informative, and which particular (for example, positive or negative) prototypes this might be.

III. Proposed Approach

A. Random Subspace Ensembles

We can see the bag and instance representations as two alternative ways of combining dissimilarities of different instances: 1) by averaging and 2) by concatenating. If we view these approaches as ways of combining different sources of information, a third alternative, ensembles, springs to mind.

The random subspace method (RSM) [29] is one way to create an ensemble that is particularly geared at small-sample-size, high-dimensional data. Each classifier is built on a lower dimensional subspace of the original, high-dimensional feature space. This strategy addresses both aspects of a successful ensemble: 1) accurate and 2) diverse classifiers [30], [31]. Subsampling the feature space reduces the dimensionality for the individual base classifiers, therefore allowing for more accurate classifiers. Resampling of features introduces diversity [30], i.e., decorrelates the classifier decisions, which improves the performance of the overall ensemble.

More formally, the RSM ensemble consists of the following components.

1) The number of subspaces L to be sampled.
2) The numbers of features $\{s_1 \dots s_L\}$ (or just s if $s_i = s_j \forall i, j$) to be selected for each subspace.
3) Base classifier f, which is applied to each subspace. We denote the trained classifiers by $\{f_1, \dots, f_L\}$.
4) Combining function g, which for a test feature vector $\mathbf{d}$, combines the outputs into a final classifier $F(\mathbf{d}) = g(f_1(\mathbf{d}), \dots f_L(\mathbf{d}))$.

RSM is interesting in high-dimensional problems with high feature redundancy [32]. For example, the expression levels of coregulated (both influenced by another process) genes will provide correlated information about whether a subject has diabetes or not. Other genes may be irrelevant to diabetes, only adding noise. We typically do not have prior knowledge about the number of underlying processes that are responsible for diabetes, i.e., the amount of redundancy is unknown. This increases the number of possible relevant feature sets, and makes selecting only the relevant features more difficult. RSM decreases this risk, simplifying the feature selection problem for each individual classifier, and by still allowing access to all the (possibly relevant) features, thus letting the classifiers correct each other. Other examples where RSM is a successful approach include functional magnetic resonance imaging data [33], microarray data [34], and hyperspectral data [35].

The different prototypes in MIL may also provide redundant information, but we do not know in advance how many such redundant prototypes there might be. Furthermore, many MIL problems are small-sample-size problems in the number of bags, so additional classifier evaluations during training are undesirable. Therefore, we believe that RSM can be an attractive method to address dissimilarity-based MIL, and to combine the strengths of the dissimilarity space with those of ensemble classifiers.

B. Choice of Subspaces

There are two alternatives for how the subspace classifiers can be defined as follows.

1) By choosing each prototype bag as a subspace, i.e., the subspace is formed by the dissimilarities to the instances of a prototype bag. This representation immediately follows from our intuition about bags and instances being analogous to averaging and concatenating different information sources. We denote this representation by D^{BS}, where BS stands for bag subspace. The RSM parameters are straightforward here. $L = M$ and the subspace dimensionalities s_i correspond to the bag sizes n_i.
2) By choosing each subspace randomly. We denote this representation by D^{RS}, where RS stands for random subspace. D^{RS} offers more flexibility with regard to the RSM parameters. In [17], we used default parameters $L = M$ and $s = (1/N)\sum_i n_i$. However, alternative settings are possible as well, and we will demonstrate further on in this paper that other choices (which can be set by rules of thumb rather than cross validation) can, in fact, improve the results significantly.

Equations (6) and (7) show the choices in matrix format

$$D^{\text{BS}} = \left\{ \left[d^{\text{inst}}(B_*, B_1) \right]_{N \times n_1}, \ldots, \left[d^{\text{bag}}(B_*, B_M) \right]_{N \times n_M} \right\} \quad (6)$$

and

$$D^{\text{RS}} = \left\{ \left[d^{\text{inst}}(B_*, R_1) \right]_{N \times s}, \ldots, \left[d^{\text{bag}(B_*, R_M)} \right]_{N \times s} \right\} \quad (7)$$

where R_i are prototype bags, generated randomly from all available instances in the training set.

TABLE I

DIFFERENT WAYS FOR CONSTRUCTING DISSIMILARITY REPRESENTATIONS. D^{bag} CONSISTS OF DISSIMILARITIES TO BAGS IN THE TRAINING SET (ONE FOR EACH BAG), WHEREAS D^{inst} CONSISTS OF DISSIMILARITIES TO INSTANCES IN THE TRAINING SET. IN D^{BS}, A SEPARATE CLASSIFIER IS BUILT ON EACH PROTOTYPE'S INSTANCE DISSIMILARITIES. IN D^{RS}, CLASSIFIERS ARE BUILT ON RANDOM SELECTIONS OF ALL AVAILABLE INSTANCES

Representation	Dimensionality	Classifiers
D^{bag}	M	1
D^{inst}	$\sum_i n_i$	1
D^{BS}	$\{n_1, \ldots n_M\}$	M
D^{RS}	any	any

Note that these alternatives are both slightly different from RSM because the dissimilarity representation depends on the training set. In traditional RSM, all features are available to the classifier at any split of the training and test data, whereas with D^{BS} and D^{RS}, the features are defined through dissimilarities to the training set, which obviously changes with every training-test split. However, we still expect there to be a relationship between how RSM parameters, and the choices in D^{BS} and D^{RS}, affect ensemble performance.

We provide a summary of the ensembles, as well as the single classifier dissimilarity representations in Table I.

C. Illustrative Example

The basic intuition about the benefit of the proposed ensembles is illustrated by the artificial problem in Fig. 1 (top). This is the classical MIL problem from [36]. This data set contains bags with 50 2-D instances. The instances from the bags are uniformly distributed in a square, and the positive bags contain at least one feature vector from a concept region that is located in the middle of the square. Only the dissimilarities of the concept instances are informative. Averaging over the dissimilarities as in D^{bag} dilutes these informative features, and indeed, the learning curves in Fig. 1 (bottom) show that D^{bag} performs poorly here. D^{inst} has trouble selecting only the informative dissimilarities, because many dissimilarities are uninformative, and because dissimilarities of the informative instances are correlated. The ensemble methods are more robust against these problems and achieve the best performances [Fig. 1 (bottom)].

IV. EXPERIMENTS

A. Data and Setup

We provide a list of data sets we used in Table II. The *Musk* problems [1] are traditional benchmark MIL problems about molecule activity, *Mutagenesis* [37] is a drug activity prediction problem. *Fox*, *Tiger*, and *Elephant* [3] are benchmark image data sets. *African* and *Beach* are also image data sets originating from a multiclass scene recognition problem [4], but here formulated as one-against-all problems. The data set *Alt.atheism* originates from the Newsgroups data [5],

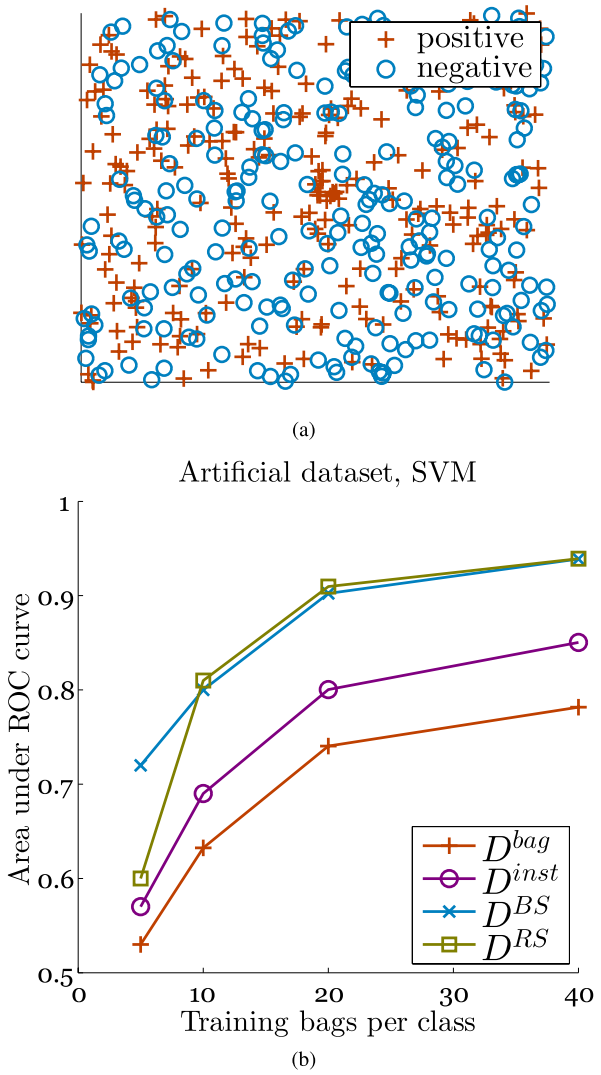


Fig. 1. Top: artificial 2-D MIL problem with informative instances in the center. Bottom: learning curves for dissimilarity-based classifiers on this data set. The amount of uninformative, and redundant instances deteriorates performances of D^{bag} and D^{inst}, but the ensemble methods D^{BS} and D^{RS} are more robust against these problems. (a) Artificial data set, SVM. (b) Training bags per class.

TABLE II
MIL DATA SETS, THE NUMBER OF BAGS, INSTANCES, THE AVERAGE NUMBER OF INSTANCES PER BAG. THE DATA SETS ARE AVAILABLE ONLINE AT http://www.miproblems.org

Dataset	+bags	-bags	total	average
Musk 1	47	45	476	5
Musk 2	39	63	6598	65
Fox	100	100	1302	7
Tiger	100	100	1220	6
Elephant	100	100	1391	7
Mutagenesis 1	125	63	10486	56
African	100	1900	7947	8
Beach	100	1900	7947	8
Alt.atheism	50	50	5443	54
Brown Creeper	197	351	10232	19
Winter Wren	109	439	10232	19

and is concerned with text categorization. *Brown Creeper* and *Winter Wren* are both bird song [38] data sets, where the goal is to classify whether a particular bird species can be heard in an audio recording.

We preprocess the data by scaling each feature to zero mean and unit variance. The scaled data are used to compute the dissimilarity representations. The instance dissimilarity function is defined as the squared Euclidean distance: $d(\mathbf{x}_i, \mathbf{x}_j) = (\mathbf{x}_i - \mathbf{x}_j)^\intercal(\mathbf{x}_i - \mathbf{x}_j)$.

For the base classifier f, we consider linear classifiers, as described in Section II. We used several linear classifiers: 1) logistic; 2) 1-norm SVM; and 3) a linear SVM, where the primal formulation is optimized [39]. The tradeoff parameter λ is set to 1 by default. The common characteristic of these classifiers is that we can inspect the weight vector $\mathbf{w}$ to determine which dissimilarities are deemed to be more important by the classifier. Although the individual performances of the classifiers differ, we observe similar trends (such as relative performances of two different ensembles) for these choices. We, therefore, only show the results for the linear SVM.

For the combining function g, we average the posterior probabilities, which are obtained after normalizing the outputs of each classifier to the [0, 1] range. We also considered majority voting, and using the product and the maximum of the posterior probabilities as combining schemes. With the product and maximum rules, the performances were lower, especially deteriorating toward larger ensemble sizes (thus being more sensitive to outlier, inaccurate base classifiers). With majority voting, the results were slightly lower than with averaging, but the standard deviations across different folds were larger. Therefore, we chose averaging as a more robust combining strategy. Furthermore, averaging posterior probabilities perform well in practice in other problems as well [40], [41]. It could be argued that the fixed g can be replaced by a more flexible function, such as a linear classifier, trained on the outputs of the base classifiers. However, as discussed in [42], this would ideally require splitting the training data into two parts: 1) for training the base classifiers and 2) for training the combiner. This is undesirable because we are already faced with a low object-to-feature (i.e., bag-to-instance) ratio. Indeed, our earlier experiments [17] with the nearest mean classifier as a combiner did not lead to improved results.

The metric used for comparisons is area under the receiver-operating characteristic [area under the receiver operating characteristic curve (AUC)] [43]. This measure has been shown to be more discriminative than accuracy in classifier comparisons [44], and more suitable for MIL problems [45].

B. Subspace Experiments

We start by comparing the two alternatives of creating the subspaces, D^{BS} and D^{RS}. For simplicity, we base the parameters of D^{RS} on those for D^{BS}, as in [17]: M subspaces, each subspace with dimensionality $(1/N)\sum_i n_i$. We use a linear SVM as the classifier (C-parameter is set to 1 by default) and perform tenfold cross validation. Fig. 2 shows the distributions of the individual classifier performances and the ensemble performance for both representations.

The results show that overall by the following.

1) The RSs are more informative than BSs.
2) The RS ensemble is better at improving upon the base classifiers.

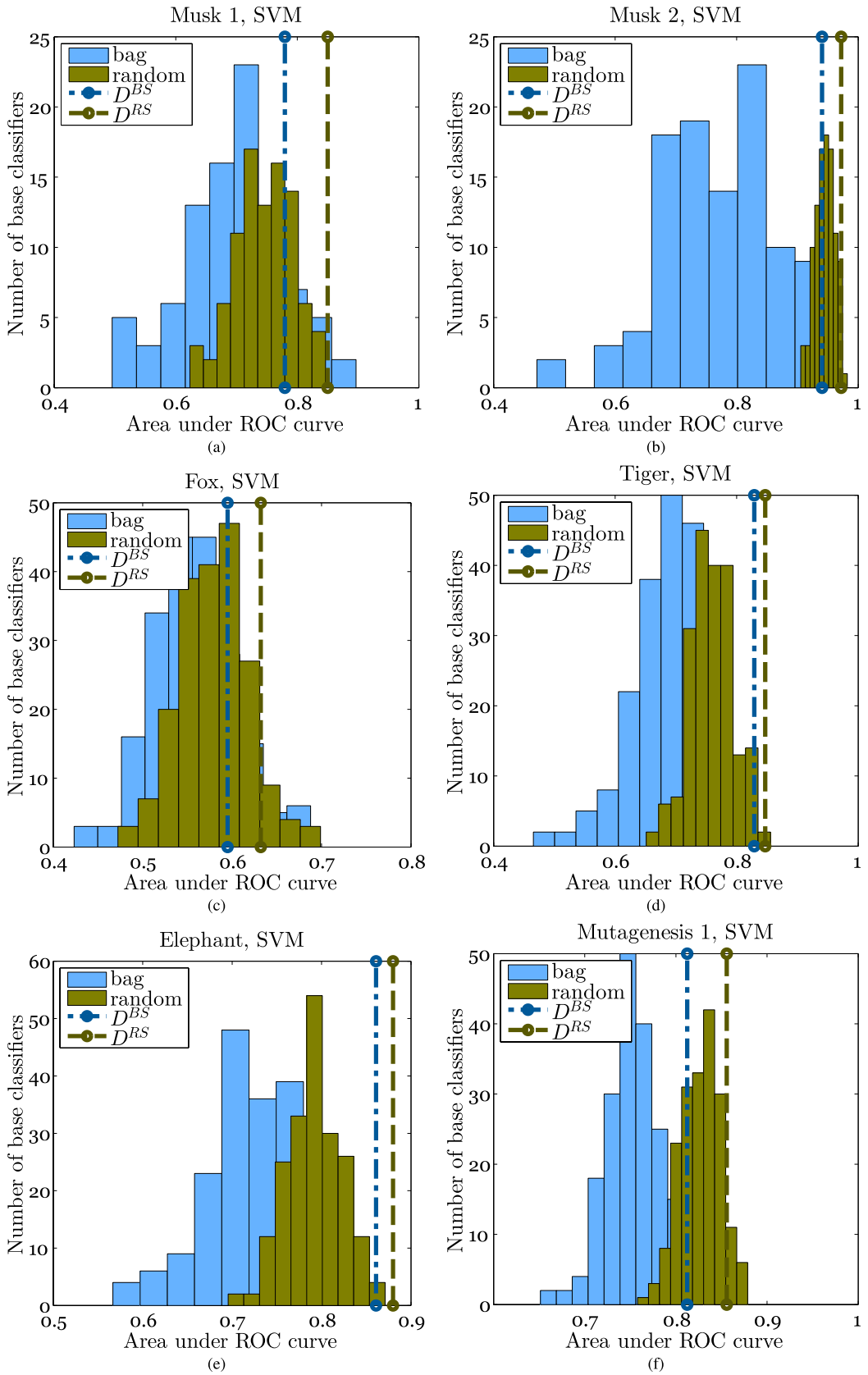


Fig. 2. Distributions of AUC performances of individual BS classifiers. (a) *Musk1*, SVM. (b) *Musk2*, SVM. (c) *Fox*, SVM. (d) *Tiger*, SVM. (e) *Elephant*, SVM. (f) *Mutagenesis1*, SVM.

Why do the RSs perform better than the BSs? One difference might be the subspace size. The BSs have variable dimensionalities, whereas the RSs are equally large. For D^{BS}, we plot the bag size against the performance of that subspace. A few of the results are shown in Fig. 3. In all data sets except *Alt.atheism*, we find medium to high correlations between

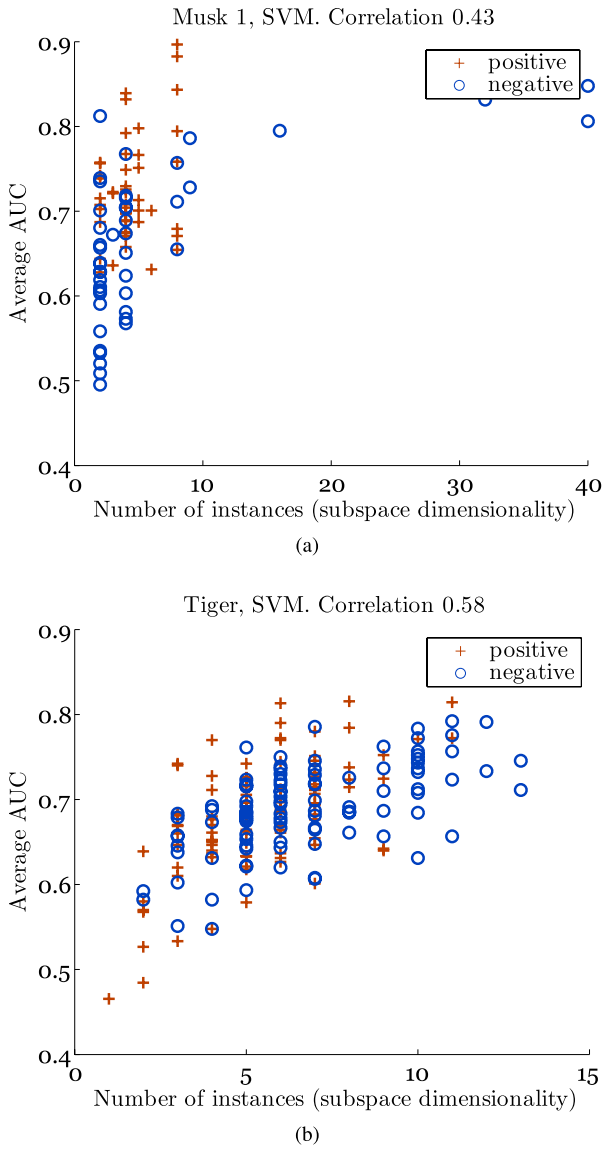


Fig. 3. Relationship of bag size, bag label, and AUC performance of the dissimilarity subspace formed by that bag. (a) *Musk1*, SVM. Correlation 0.43. (b) *Tiger*, SVM. Correlation 0.58.

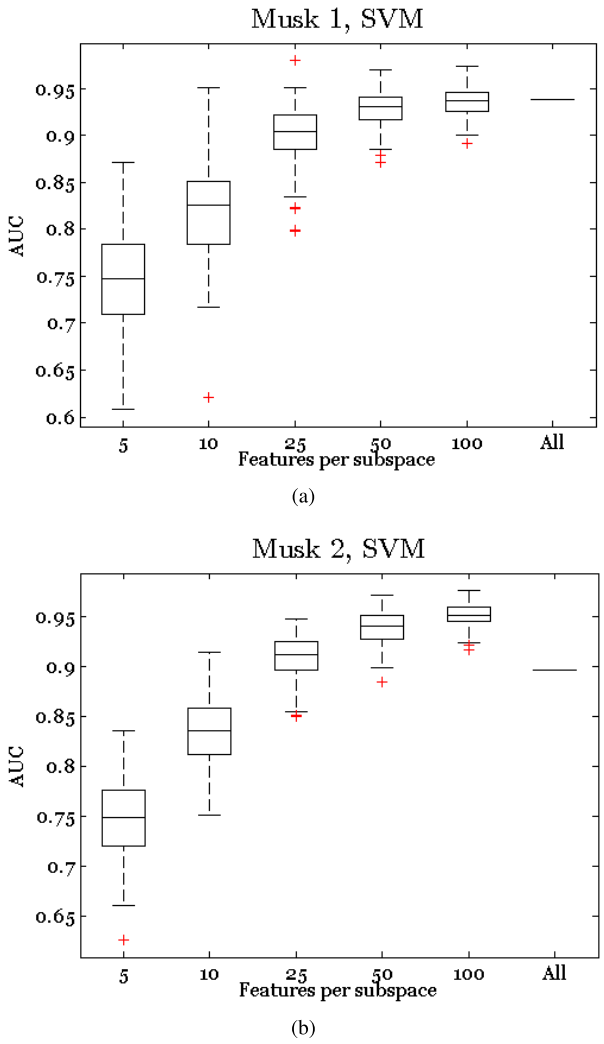


Fig. 4. Distributions of AUC performances of individual subspace classifiers, for different dimensionalities of the subspaces. The degradation of performance using all features is larger in *Musk2*, because instance/bag (and thus feature/object) ratio is larger than in *Musk1*. Similar trends can be observed in other data sets. (a) *Musk1*, SVM. (b) *Musk2*, SVM.

these quantities. Therefore, as prototypes, small bags are not very informative. This might seem counterintuitive in a MIL problem, because small bags are less ambiguous with respect to the instance labels under the standard assumption. The fact that large, ambiguous bags are better at explaining the class differences suggests that most instances are informative as prototypes.

The informativeness of most instances as prototypes is supported by the relationship between the bag label and the subspace performance in the plots. Although for a fixed bag size, positive BSs perform better on average, negative bags can also be very good prototypes. This is also true for random bags, for which we do not have labels, but for which we can examine the percentage of instances, which were sampled from positive bags. We found no correlations between the positiveness of the RSs and their performance. This provides opportunities for using unlabeled data in a semisupervised way. Unlabeled bags can be used to extend the dissimilarity representation to improve performance, similar to the approach in [46].

The results with respect to the bag size suggest that it is advantageous to combine classifiers built on higher dimensional subspaces. We, therefore, investigate the effects of subspace dimensionality in D^{RS}, where this parameter can be varied. We vary the subspace size for each classifier from 5 to 100 features, which for most data sets, would be larger than the default dimensionalities used previously, as shown in Table II. We generate 100 subspaces of each dimensionality, and train a linear SVM on each subspace. The classifiers are then evaluated individually. Some examples of performance distributions at different subspace dimensionalities are shown in Fig. 4. For most data sets (except Newsgroups, as will be explained later), larger subspaces lead to more accurate classifiers. However, increasing the dimensionality too much, eventually using all the features, decreases the performance. This can be more clearly seen in the results of *Musk2*,

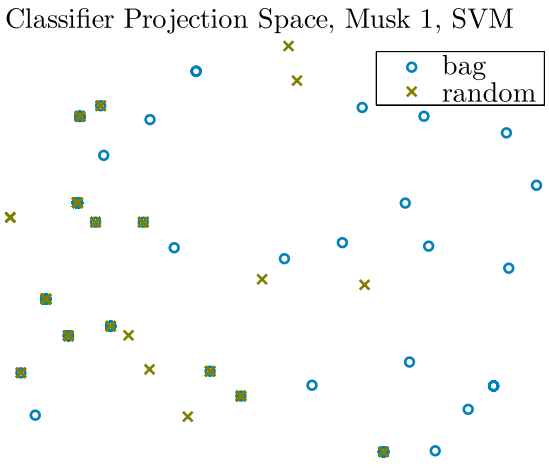


Fig. 5. Classifier projection spaces. Plots: relative disagreement of trained subspace classifiers on a test set. The higher the disagreement of two classifiers on the labels of the test set, the larger their distance in the plot. (a) Classifier projection space, *Musk1*, SVM. (b) Classifier projection space, *Tiger*, SVM.

where the total number of instances (and thus dimensionality) is larger than in *Musk1*. The results of other data sets show similar trends depending on the bag/instance ratio, for example, the results of *Mutagenesis* are quite similar to *Musk2*.

Why is D^{RS} better than D^{BS} at improving upon the individual classifiers? A possible explanation is that the classifiers created by D^{RS} are more diverse than the classifiers of D^{BS}. For each set of classifiers, we examine their $L \times L$ disagreement matrix C, where each entry $C_{i,j}$ corresponds to the number of test bags for which the ith and the jth classifier provide different labels. $C_{i,j}$ can be seen as the distance of the two classifiers. We perform multidimensional scaling with each of these distance matrices and map the classifiers into a 2-D classifier projection space [47].

The classifier projection spaces for two data sets are shown in Fig. 5. These results are surprising, because the classifiers in D^{BS} actually cover a larger part of the space, and are, therefore, more diverse. This diversity alone, however, is not

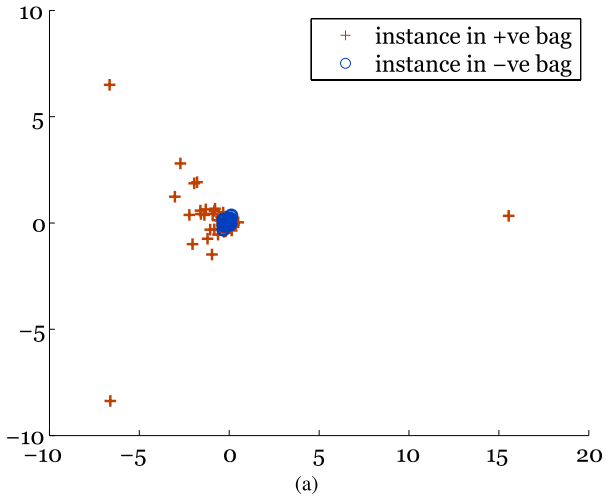


Fig. 6. Multidimensional scaling of the instances in the *Alt.atheism* data set.

able to improve the overall performance of the ensemble. A possible explanation is that here we are dealing with bad diversity [48]. For example, a classifier that is 100% wrong is very diverse with respect to a classifier that is 100% correct, but not beneficial when added to an ensemble. We showed in Fig. 3 that in D^{BS}, small bags often result in inaccurate classifiers, which are indeed responsible for higher diversity, but worsen the ensemble performance.

In the experiments, the Newsgroups data show very different behavior from the other data sets. Most of the subspaces (both bag and random) have nearly random performance, and the performances are not correlated with the bag label or subspace dimensionality. A possible explanation is that in this data set, many of the dissimilarities only contain noise, and the informativeness is distributed only across a few dissimilarities. RSM is particularly suitable for problems where the informativeness is spread out over many (redundant) features [32], which could explain the worse than random performance. Indeed, examining the individual informativeness (as measured by the nearest neighbor error) of each individual dissimilarity, it turns out that more than half of the dissimilarities in *Alt.atheism* have worse than random performance, as opposed to only around 10% of dissimilarities for the other data sets.

We have noticed previously [13] that positive bags in the Newsgroups data consist of dense cluster of instances and a few outliers, while negative bags consist of the dense cluster only. This distribution is caused by the bag of words representation of the data—while the outlier instances are, in fact, all positive for the *Alt.atheism* topic, they do not consist of the same words, and are far from each other in the feature space. This situation is shown in Fig. 6. The presence or absence of such outliers is very informative for the bag class. The definition of dissimilarity in (2), however, does not succeed in extracting this information. For any training bag, the instance closest to the prototype outlier instance is in the dense cluster. In this case, the minimum function in the dissimilarity is not suitable for the problem at hand, and much better performances can be obtained, for instance, using bags and prototypes, and considering the asymmetry of D^{bag} [13].

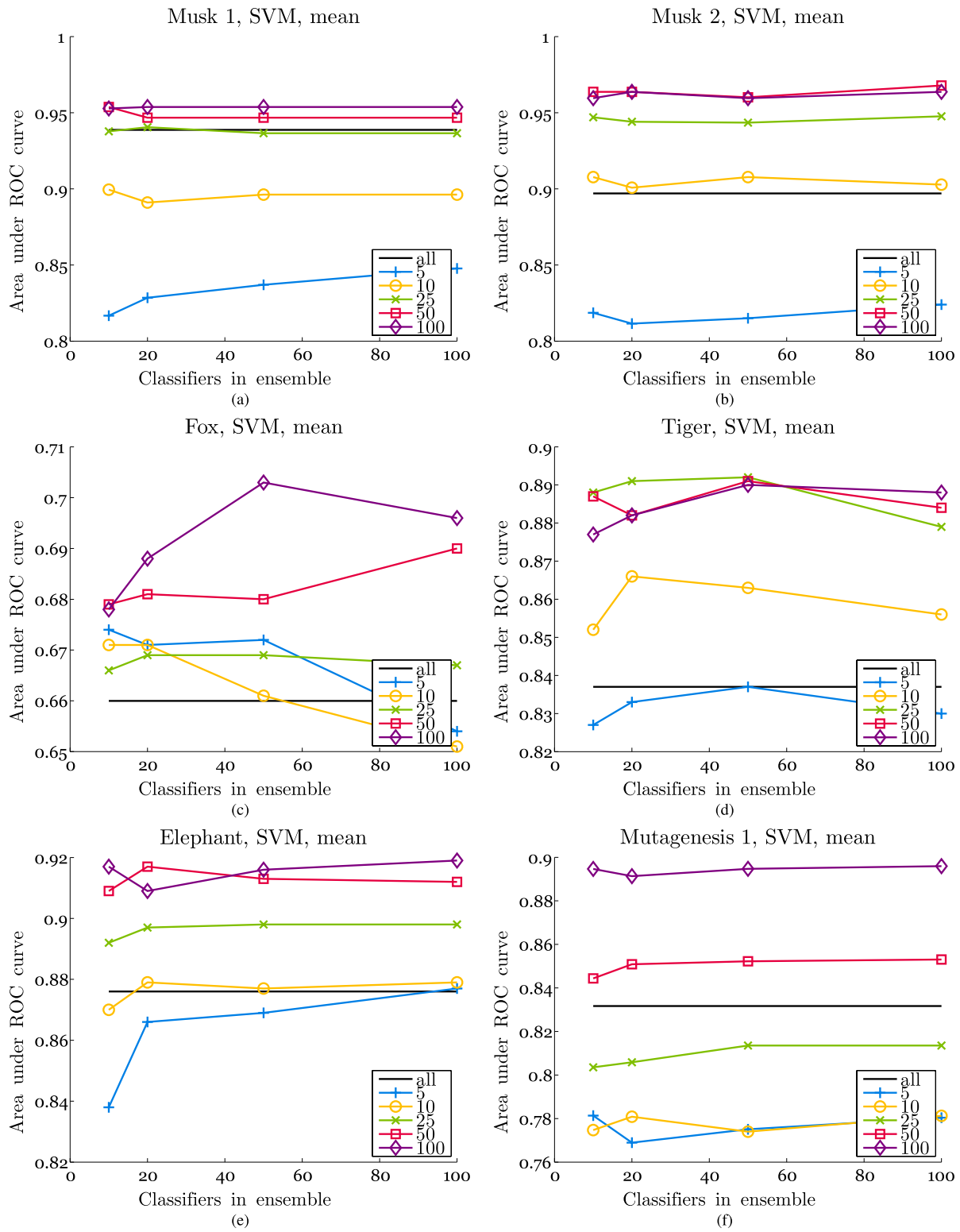


Fig. 7. AUC performances of the instance representation (black line) and the ensemble classifiers. Different lines per plot: different dimensionalities of subspace classifiers. (a) *Musk1*, SVM, mean. (b) *Musk2*, SVM, mean. (c) *Fox*, SVM, mean. (d) *Tiger*, SVM, mean. (e) *Elephant*, SVM, mean. (f) *Mutagenesis1*, SVM, mean.

C. Ensemble Experiments

With several interesting results for the individual performances of the subspace classifiers, we now investigate how the ensemble behaves when both the parameters of interest are varied. The ensembles are built in such a way that classifiers are only added (not replaced) as the ensemble size increases, i.e., an ensemble with 100 classifiers has the same classifiers as the ensemble with 50 classifiers, and 50 additional ones.

The results are shown in Fig. 7. Here, different plots show the results for different subspace dimensionalities (5, 10, 25, 50, or 100 features), and the x-axis indicates the number of classifiers used in the ensemble. The black line

TABLE III
AUC (×100), MEAN AND STANDARD ERROR OF TENFOLD CROSS VALIDATION OF THE SINGLE DISSIMILARITY-BASED REPRESENTATIONS, AND THE PROPOSED ENSEMBLE REPRESENTATION. BOLD = BEST AND ITALICS = SECOND BEST RESULT PER DATA SET

	Representation		
Dataset	D^{bag}	D^{inst}	D^{RS}
Musk1	93.7 (3.5)	*93.9 (3.6)*	**95.4 (2.4)**
Musk2	**95.7 (1.4)**	89.7 (4.7)	*93.2 (3.2)*
Fox	*67.9 (2.5)*	66.0 (3.9)	**70.2 (1.8)**
Tiger	*86.8 (5.2)*	83.7 (3.9)	**87.8 (4.2)**
Elephant	*90.9 (2.5)*	87.6 (3.3)	**92.3 (2.7)**
Mutagenesis	*84.3 (2.9)*	83.2 (3.2)	**87.4 (3.5)**
Brown Creeper	**94.7 (1.0)**	93.9 (0.8)	*94.2 (0.8)*
Winter Wren	**99.5 (0.2)**	98.4 (0.5)	*99.0 (0.3)*
African	*92.5 (1.1)*	91.6 (1.4)	**92.8 (1.2)**
Beach	**88.3 (1.2)**	85.6 (1.2)	*87.9 (1.2)*
alt.atheism	**62.4 (8.3)**	46.4 (5.9)	*46.4 (5.2)*

shows the baseline performance of D^{inst}. The performance metric is again the AUC, and the results are averaged over tenfold cross validation.

Ensembles created with higher dimensional subspaces tend to perform better. An unsurprising result is that the fixed dimensionality values in this experiment are not suitable for all data sets. For example, in Musk, none of the ensembles outperform the single classifier. Clearly, the subspace dimensionality should depend on the dimensionality (and possibly redundancy of the dissimilarities) of the original problem.

Another interesting observation in Fig. 7 is that it is often sufficient to build the ensemble from a few base classifiers, and adding further classifiers probably would not improve performance significantly. This is in line with our earlier results for ensembles of one-class classifiers [41], even though both the data and the classifiers in question are very different. The recommendation in [33] is that, when there is no prior knowledge about how redundant the features are, L should be chosen to be relatively small, whereas s should be relatively large. Based on these observations, we settle on the following choices for D^{RS}: $L = 100$ and $s = (1/5)\sum_i^N n_i$. We emphasize that these choices are good rules of thumb and do not have to be set to these exact values, which is supported by our results in Section IV-B. The performance is quite robust to changes in L and s provided s is large enough.

The performances of the proposed ensemble against those of the single classifier representations D^{bag} and D^{inst} are shown in Table III. Contrary to our earlier results in [17], D^{RS} is now a clear competitor for the single classifiers, and has especially surprising performances on the $Musk1$, Fox, and $Mutagenesis$ data sets. The advantages of D^{RS} over the high-dimensional D^{inst} are more visible, however, there are no significant differences with D^{bag}. This suggests that many of the dissimilarities are, in fact, informative, and averaging the dissimilarities over each bag preserves sufficient information. Despite the similar performances of D^{bag} and D^{RS}, D^{RS} has an additional advantage. It is possible to recover the importance of different instances, as shown in Section IV-E.

D. Comparison With Other MIL Classifiers

We compare our method to other popular MIL classifiers, which cover a range of instance-based and bag-based methods, and are often being compared with in recent papers. EM with diverse density (EM-DD) [49], multiple instance support vector machine (mi-SVM) [50], and MILBoost [51] are instance-based methods. EM-DD is an expectation-maximization algorithm, which uses diverse density (DD), which, for a given point t in the feature space, measures the ratio between the number of positive bags, which have instances near t, and the distance of the negative instances to t. The expectation step selects the most positive instance from each bag according to t, the maximization step then finds a new concept t' by maximizing DD on the selected, most positive instances. mi-SVM is an extension of SVMs, which attempts to find hidden labels of the instances under constraints posed by the bag labels. Likewise, MILBoost is an extension of boosting and MIForest is an extension of random forests, where the standard assumption is used to reweigh or relabel the instances in each iteration of the algorithm.

The MILES [4] and the minimax kernel are bag-based methods, which convert bags to a single-instance representation. MILES is similar to the 1-norm SVM applied to the D^{inst}, except that in MILES, a Gaussian kernel is used for defining similarities, and an appropriate σ parameter is necessary. The minimax kernel [9] is obtained by representing each bag by the minimum and maximum feature values of its instances, this representation can then be used with a supervised classifier. All classifiers are implemented in PRTools [52], and the MIL toolbox [53] and default parameters are used unless stated otherwise.

Next to the standard MIL classifiers, we use D^{RS} with the guidelines in Section IV-C. The dimensionality of each subspace is the 1/5th of the total dimensionality, and 100 classifiers are used in the ensemble. The base classifier is the linear SVM. For both MI-SVM and MILES, the radial basis kernel with width 10 was used. The results are shown in Tables IV and V. Some results could not be reported; in particular, for EM-DD when one cross-validation fold lasts longer than five days, and MILBoost when features with the same value for all instances are present, as in *Alt.atheism*. Needless to say, there is no method that performs the best at all times. Some of the default parameter choices may be unsuitable for a particular data set, or the assumptions that the method is based on do not hold. However, overall the method we present is always able to provide competitive performance.

E. Instance Weights

An advantage of linear classifiers is the interpretability of the result—from the weights $\mathbf{w}$ of the dissimilarities, we can derive which dissimilarities, and therefore which instances are more important (i.e., have a larger weight) to the classifier. This property can also be used in ensembles of linear classifiers, with a procedure described in [54]. For each dissimilarity, we calculate the average absolute value of its weight over all L subspaces in which the dissimilarity was selected. We then sort the dissimilarities by this average weight, and view the position of each dissimilarity in this list as its rank. The distributions of the dissimilarities with

TABLE IV

AUC ×100, MEAN AND STANDARD ERROR OF TENFOLD CROSS VALIDATION OF DIFFERENT MIL CLASSIFIERS. BOLD = BEST AND ITALICS = SECOND BEST PER DATA SET

Dataset	Classifier EM-DD	MI-SVM	MILBoost	MILES	minimax+SVM	D^{RS} +SVM
Musk1	85.0 (5.1)	91.5 (3.7)	74.8 (6.7)	*93.2 (2.9)*	87.8 (5.0)	**95.4 (2.4)**
Musk2	88.1 (2.7)	*93.9 (2.8)*	76.4 (3.5)	**97.1 (1.6)**	91.3 (1.8)	93.2 (3.2)
Fox	67.6 (3.2)	*68.7 (2.6)*	61.3 (3.2)	66.8 (3.5)	55.8 (2.9)	**70.2 (1.8)**
Tiger	-	*87.2 (3.5)*	87.0 (3.0)	84.6 (4.5)	76.0 (4.1)	**87.8 (4.2)**
Elephant	88.5 (2.1)	*90.7 (2.3)*	88.8 (2.2)	88.4 (2.5)	88.4 (2.1)	**92.3 (2.7)**
Mutagenesis	67.4 (5.3)	60.3 (4.5)	**88.1 (3.1)**	72.1 (4.3)	63.7 (4.4)	*87.4 (3.5)*
Brown Creeper	94.5 (0.9)	92.8 (1.2)	*94.9 (0.9)*	**96.1 (0.6)**	94.2 (0.9)	94.2 (0.8)
Winter Wren	98.3 (0.5)	**99.2 (0.4)**	93.8 (5.6)	*99.1 (0.5)*	98.2 (0.3)	99.0 (0.3)
African	*91.2 (1.8)*	88.6 (1.7)	89.4 (1.7)	48.7 (2.3)	87.6 (1.4)	**92.8 (1.2)**
Beach	84.6 (2.0)	78.2 (2.5)	*85.2 (2.9)*	72.8 (5.0)	83.0 (2.3)	**87.9 (1.2)**
Alt.atheism	*52.0 (8.0)*	38.8 (5.2)	-	50.0 (5.5)	**80.0 (3.6)**	46.4 (5.2)

TABLE V

ACCURACY ×100, MEAN AND STANDARD ERROR OF TENFOLD CROSS VALIDATION OF DIFFERENT MIL CLASSIFIERS. BOLD = BEST AND ITALICS = SECOND BEST PER DATA SET

Dataset	Classifier EM-DD	MI-SVM	MILBoost	MILES	minimax+SVM	D^{RS} +SVM
Musk1	85.1 (4.1)	83.0 (4.6)	69.8 (5.6)	82.8 (4.7)	*86.3 (3.8)*	**89.3 (3.4)**
Musk2	81.5 (2.9)	76.3 (5.4)	66.0 (3.7)	**86.3 (3.4)**	82.3 (2.5)	*85.5 (4.7)*
Fox	62.0 (2.7)	*63.5 (2.2)*	63.0 (2.6)	62.5 (4.2)	58.0 (2.5)	**64.5 (2.2)**
Tiger	-	73.0 (2.9)	78.5 (2.8)	**81.0 (3.4)**	72.5 (3.9)	*81.0 (4.6)*
Elephant	*82.5 (1.5)*	76.0 (2.4)	79.5 (2.8)	79.0 (2.3)	82.5 (2.5)	**84.5 (2.8)**
Mutagenesis	61.1 (5.1)	66.5 (0.4)	*75.7 (2.7)*	71.1 (3.4)	68.9 (3.0)	**83.2 (3.4)**
Brown Creeper	85.6 (1.5)	50.5 (1.5)	*88.7 (1.2)*	**89.8 (1.4)**	87.3 (1.6)	88.3 (1.0)
Winter Wren	94.5 (1.2)	81.0 (1.5)	89.0 (7.8)	**96.7 (0.8)**	93.8 (0.8)	*96.0 (0.8)*
African	82.7 (0.9)	94.7 (0.1)	*95.2 (0.2)*	95.0 (0.0)	95.0 (0.0)	**96.0 (0.5)**
Beach	73.4 (1.1)	95.0 (0.1)	**95.2 (0.2)**	*95.0 (0.0)*	94.9 (0.1)	94.8 (0.4)
Alt.atheism	49.0 (5.7)	48.0 (2.0)	-	*50.0 (4.5)*	**76.0 (4.0)**	44.0 (4.5)

ranks 1 to 100 are shown in Fig. 8 shows the distributions of top 100 dissimilarities. These most informative dissimilarities originate from both positive and negative bags, supporting the idea that not only concept, positive instances are important for these MIL problems.

V. DISCUSSION

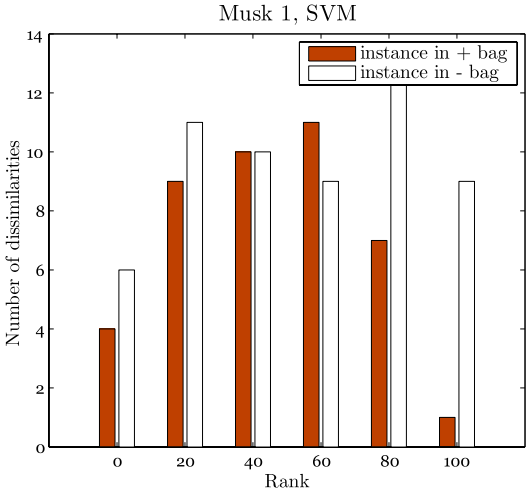
We proposed a dissimilarity-based ensemble as a novel classification method for MIL problems. When bags are represented by their dissimilarities to instances from the training set, such instances can provide redundant information about the problem. A RS inspired ensemble, where classifiers are trained on different subspaces of the dissimilarity space, is a way of dealing with this redundancy. We show that our method achieves competitive performances with other MIL algorithms, and has intuitive parameters that do not need to be set by cross validation to achieve these good results.

We investigated two choices for generating the subspaces: 1) using each training bag as a subspace and 2) using a random selection of instances (with replacement) as a subspace. The random method achieved better results, especially when the dimensionality of the subspaces was increased. We found that the subspace dimensionality is the most important factor affecting the performance of the ensemble. Overall, larger subspaces lead to more accurate classifiers. Combining subspaces of similar size and therefore accuracy as in D^{RS} therefore leads to better results than combining subspaces with high variance in size and accuracy as in D^{BS}, even though the subspaces in D^{BS} are more diverse. On the other hand, the number of subspaces does not play a very important role and just a few classifiers are sufficient for good performance. These conclusions are in line with the conclusions from other applications of the RSM, where the amount of redundancy of the features is unknown.

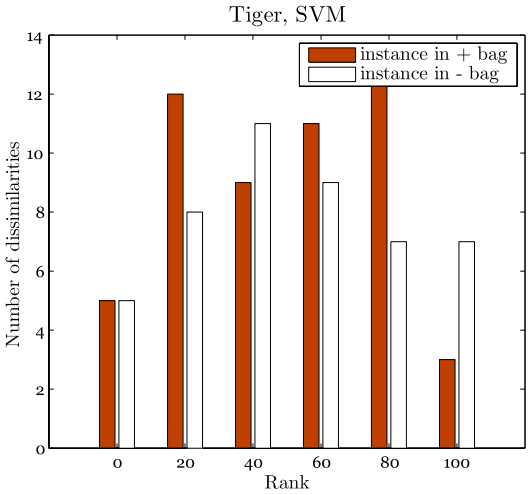
In general, the informativeness of a prototype is more related to the dimensionality of the subspace, than to the label of instances forming that subspace. Negative bags and unlabeled random sets of instances were often good prototypes, suggesting that most instances, and not only a few concept ones, are informative for these MIL problems. These results are more in line with the collective assumption for MIL, where all instances are considered to contribute to the bag label, rather than with the standard assumption, where only a few positive instances are considered important.

Based on the encouraging results concerning the effectiveness of RSs as prototypes, we also considered randomly sampling the instance space (rather than randomly selecting existing instances) to generate artificial prototype bags that are not in the training set. Although the results with artificial prototypes were slightly worse than with real prototypes, this does seem to provide opportunities for using unlabeled, or artificial bags in a semisupervised way.

We would like to conclude by emphasizing that a dissimilarity-based representation combined with a linear classifier (or an ensemble thereof) is a powerful way of classifying



(a)



(b)

Fig. 8. Top 100 ranked dissimilarities, where the rank is determined by average weight of dissimilarities across $L = 100$ subspace classifiers. (a) *Musk1*, SVM. (b) *Tiger*, SVM.

MIL bags. A question that still remains is the use of structured norms in such linear classifiers, which would enable selection of groups of dissimilarities, therefore revealing more about the relationships of the instances.

REFERENCES

[1] T. G. Dietterich, R. H. Lathrop, and T. Lozano-Pérez, "Solving the multiple instance problem with axis-parallel rectangles," *Artif. Intell.*, vol. 89, nos. 1–2, pp. 31–71, 1997.

[2] G. Fu *et al.*, "Implementation of multiple-instance learning in drug activity prediction," *BMC Bioinform.*, vol. 13, no. 15, p. S3, Sep. 2012.

[3] S. Andrews, T. Hofmann, and I. Tsochantaridis, "Multiple instance learning with generalized support vector machines," in *Proc. Nat. Conf. Artif. Intell.*, Edmonton, AB, Canada, Jul. 2002, pp. 943–944.

[4] Y. Chen, J. Bi, and J. Z. Wang, "MILES: Multiple-instance learning via embedded instance selection," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 28, no. 12, pp. 1931–1947, Dec. 2006.

[5] Z.-H. Zhou, Y.-Y. Sun, and Y.-F. Li, "Multi-instance learning by treating instances as non-I.I.D. samples," in *Proc. 26th Annu. Int. Conf. Mach. Learn.*, Montreal, QC, Canada, Jun. 2009, pp. 1249–1256.

[6] G. M. Fung, M. Dundar, B. Krishnapuram, and R. B. Rao, "Multiple instance learning for computer aided diagnosis," in *Proc. Adv. Neural Inf. Process. Syst.*, vol. 19. Vancouver, BC, Canada, Dec. 2007, pp. 425–432.

[7] J. Foulds and E. Frank, "A review of multi-instance learning assumptions," *Knowl. Eng. Rev.*, vol. 25, no. 1, pp. 1–25, 2010.

[8] J. Wang and J.-D. Zucker, "Solving the multiple-instance problem: A lazy learning approach," in *Proc. 17th Int. Conf. Mach. Learn.*, Stanford, CA, USA, Jun. 2000, pp. 1119–1126.

[9] T. Gärtner, P. A. Flach, A. Kowalczyk, and A. J. Smola, "Multi-instance kernels," in *Proc. 19th Int. Conf. Mach. Learn.*, Sydney, NSW, Australia, Jul. 2002, pp. 179–186.

[10] D. M. J. Tax, M. Loog, R. P. W. Duin, V. Cheplygina, and W.-J. Lee, "Bag dissimilarities for multiple instance learning," in *Proc. 1st Int. Workshop Similarity-Based Pattern Recognit.*, Venice, Italy, Sep. 2011, pp. 222–234.

[11] Z. Fu, A. Robles-Kelly, and J. Zhou, "MILIS: Multiple instance learning with instance selection," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 33, no. 5, pp. 958–977, May 2010.

[12] E. Pękalska and R. P. W. Duin, *The Dissimilarity Representation for Pattern Recognition: Foundations and Applications*. Singapore: World Scientific, 2005.

[13] V. Cheplygina, D. M. J. Tax, and M. Loog, "Class-dependent dissimilarity measures for multiple instance learning," in *Proc. Joint IAPR Int. Workshop Struct., Syntactic, Statist. Pattern Recognit.*, Hiroshima, Japan, Nov. 2012, pp. 602–610.

[14] E. Pękalska and R. P. W. Duin, "On combining dissimilarity representations," in *Proc. 2nd Int. Workshop Multiple Classifier Syst.*, Cambridge, U.K., Jul. 2001, pp. 359–368.

[15] J. Kittler, "Combining classifiers: A theoretical framework," *Pattern Anal. Appl.*, vol. 1, no. 1, pp. 18–27, 1998.

[16] R. P. W. Duin and D. M. J. Tax, "Experiments with classifier combining rules," in *Multiple Classifier Systems*. Berlin, Germany: Springer-Verlag, 2000, pp. 16–29.

[17] V. Cheplygina, D. M. J. Tax, and M. Loog, "Combining instance information to classify bags," in *Proc. 11th Int. Workshop Multiple Classifier Syst.*, Nanjing, China, May 2013, pp. 13–24.

[18] Z.-H. Zhou and M.-L. Zhang, "Multi-instance multi-label learning with application to scene classification," in *Proc. Adv. Neural Inf. Process. Syst.*, Vancouver, BC, Canada, Dec. 2006, pp. 1609–1616.

[19] V. Cheplygina, D. M. J. Tax, and M. Loog, "Does one rotten apple spoil the whole barrel?" in *Proc. 21st Int. Conf. Pattern Recognit.*, Tsukuba, Japan, Nov. 2012, pp. 1156–1159.

[20] A. Erdem and E. Erdem, "Multiple-instance learning with instance selection via dominant sets," in *Proc. 1st Int. Workshop Similarity-Based Pattern Recognit.*, Venice, Italy, Sep. 2011, pp. 177–191.

[21] E. Akbas, B. Ghanem, and N. Ahuja. (2011). "MIS-boost: Multiple instance selection boosting." [Online]. Available: http://arxiv.org/abs/1109.2388

[22] M.-L. Zhang and Z.-H. Zhou, "Multi-instance clustering with applications to multi-instance prediction," *Appl. Intell.*, vol. 31, no. 1, pp. 47–68, 2009.

[23] D. W. Jacobs, D. Weinshall, and Y. Gdalyahu, "Classification with nonmetric distances: Image retrieval and class representation," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 22, no. 6, pp. 583–600, Jun. 2000.

[24] I. Guyon, J. Weston, S. Barnhill, and V. Vapnik, "Gene selection for cancer classification using support vector machines," *Mach. Learn.*, vol. 46, nos. 1–3, pp. 389–422, 2002.

[25] J. Zhu, S. Rosset, T. J. Hastie, and R. Tibshirani, "1-norm support vector machines," in *Proc. Adv. Neural Inf. Process. Syst.*, vol. 16. Vancouver, BC, Canada, Dec. 2004, pp. 49–56.

[26] C. Bhattacharyya *et al.*, "Simultaneous classification and relevant feature identification in high-dimensional spaces: Application to molecular profiling data," *Signal Process.*, vol. 83, no. 4, pp. 729–743, 2003.

[27] E. Pękalska, R. P. W. Duin, and P. Paclík, "Prototype selection for dissimilarity-based classifiers," *Pattern Recognit.*, vol. 39, no. 2, pp. 189–208, 2006.

[28] Y. P. Calaña, E. G. Reyes, M. O. Alzate, and R. P. W. Duin, "Prototype selection for dissimilarity representation by a genetic algorithm," in *Proc. 20th Int. Conf. Pattern Recognit.*, Istanbul, Turkey, Aug. 2010, pp. 177–180.

[29] T. K. Ho, "The random subspace method for constructing decision forests," *IEEE Trans. Pattern Anal. Mach. Intell.*, vol. 20, no. 8, pp. 832–844, Aug. 1998.

[30] L. I. Kuncheva and C. J. Whitaker, "Measures of diversity in classifier ensembles and their relationship with the ensemble accuracy," *Mach. Learn.*, vol. 51, no. 2, pp. 181–207, 2003.

[31] G. Brown, J. Wyatt, R. Harris, and X. Yao, "Diversity creation methods: A survey and categorisation," *Inf. Fusion*, vol. 6, no. 1, pp. 5–20, 2005.

[32] M. Skurichina and R. P. W. Duin, "Bagging and the random subspace method for redundant feature spaces," in *Proc. 2nd Int. Workshop Multiple Classifier Syst.*, Cambridge, U.K., Jul. 2001, pp. 1–10.
[33] L. I. Kuncheva, J. J. Rodríguez, C. O. Plumpton, D. E. J. Linden, and S. J. Johnston, "Random subspace ensembles for fMRI classification," *IEEE Trans. Med. Imag.*, vol. 29, no. 2, pp. 531–542, Feb. 2010.
[34] A. Bertoni, R. Folgieri, and G. Valentini, "Bio-molecular cancer prediction with random subspace ensembles of support vector machines," *Neurocomputing*, vol. 63, pp. 535–539, Jan. 2005.
[35] J. Ham, Y. Chen, M. M. Crawford, and J. Ghosh, "Investigation of the random forest framework for classification of hyperspectral data," *IEEE Trans. Geosci. Remote Sens.*, vol. 43, no. 3, pp. 492–501, Mar. 2005.
[36] O. Maron and T. Lozano-Pérez, "A framework for multiple-instance learning," in *Proc. Adv. Neural Inf. Process. Syst.*, Denver, CO, USA, Nov. 1998, pp. 570–576.
[37] A. Srinivasan, S. H. Muggleton, and R. D. King, "Comparing the use of background knowledge by inductive logic programming systems," in *Proc. 5th Int. Workshop Inductive Logic Program.*, Leuven, Belgium, Sep. 1995, pp. 199–230.
[38] F. Briggs *et al.*, "Acoustic classification of multiple simultaneous bird species: A multi-instance multi-label approach," *J. Acoust. Soc. Amer.*, vol. 131, no. 6, pp. 4640–4650, 2012.
[39] O. Chapelle, "Training a support vector machine in the primal," *Neural Comput.*, vol. 19, no. 5, pp. 1155–1178, 2007.
[40] D. M. J. Tax, M. van Breukelen, R. P. W. Duin, and J. Kittler, "Combining multiple classifiers by averaging or by multiplying?" *Pattern Recognit.*, vol. 33, no. 9, pp. 1475–1485, 2000.
[41] V. Cheplygina and D. M. J. Tax, "Pruned random subspace method for one-class classifiers," in *Proc. 10th Int. Workshop Multiple Classifier Syst.*, Naples, Italy, Jun. 2011, pp. 96–105.
[42] R. P. W. Duin, "The combining classifier: To train or not to train?" in *Proc. 16th Int. Conf. Pattern Recognit.*, vol. 2. Montreal, QC, Canada, Aug. 2002, pp. 765–770.
[43] A. P. Bradley, "The use of the area under the ROC curve in the evaluation of machine learning algorithms," *Pattern Recognit.*, vol. 30, no. 7, pp. 1145–1159, 1997.
[44] J. Huang and C. X. Ling, "Using AUC and accuracy in evaluating learning algorithms," *IEEE Trans. Knowl. Data Eng.*, vol. 17, no. 3, pp. 299–310, Mar. 2005.
[45] D. M. J. Tax and R. P. W. Duin, "Learning curves for the analysis of multiple instance classifiers," in *Proc. Joint IAPR Int. Workshop Struct., Syntactic, Statist. Pattern Recognit.*, Tampa, FL, USA, Dec. 2008, pp. 724–733.
[46] C. V. Dinh, R. P. W. Duin, and M. Loog, "A study on semi-supervised dissimilarity representation," in *Proc. 21st Int. Conf. Pattern Recognit.*, Tsukuba, Japan, Nov. 2012, pp. 2861–2864.
[47] E. Pękalska, R. P. W. Duin, and M. Skurichina, "A discussion on the classifier projection space for classifier combining," in *Proc. 3rd Int. Workshop Multiple Classifier Syst.*, Cagliari, Italy, Jun. 2002, pp. 137–148.
[48] G. Brown and L. I. Kuncheva, "'Good' and 'bad' diversity in majority vote ensembles," in *Proc. 9th Int. Workshop Multiple Classifier Syst.*, Cairo, Egypt, Apr. 2010, pp. 124–133.
[49] Q. Zhang and S. A. Goldman, "EM-DD: An improved multiple-instance learning technique," in *Proc. Adv. Neural Inf. Process. Syst.*, vol. 14. Vancouver, BC, Canada, Dec. 2001, pp. 1073–1080.
[50] S. Andrews, I. Tsochantaridis, and T. Hofmann, "Support vector machines for multiple-instance learning," in *Proc. Adv. Neural Inf. Process. Syst.*, vol. 15. Vancouver, BC, Canada, Dec. 2002, pp. 561–568.
[51] P. A. Viola, J. C. Platt, and C. Zhang, "Multiple instance boosting for object detection," in *Proc. Adv. Neural Inf. Process. Syst.*, vol. 18. Vancouver, BC, Canada, Dec. 2006, pp. 1417–1426.
[52] R. P. W. Duin *et al.* (2013). *PRTools—A MATLAB Toolbox for Pattern Recognition*. [Online]. Available: http://www.prtools.org
[53] D. M. J. Tax. (2011). *MIL—A MATLAB Toolbox for Multiple Instance Learning*. [Online]. Available: http://prlab.tudelft.nl/david-tax/mil.html
[54] C. Lai, M. J. T. Reinders, and L. Wessels, "Random subspace method for multivariate feature selection," *Pattern Recognit. Lett.*, vol. 27, no. 10, pp. 1067–1076, 2006.

Veronika Cheplygina received the M.Sc. degree in media and knowledge engineering from the Delft University of Technology, Delft, the Netherlands, in 2010, where she is currently pursuing the Ph.D. degree with the Pattern Recognition Laboratory. Her thesis project "Random Subspace Method for One-Class Classifiers" about detecting outliers during automatic parcel sorting was performed in collaboration with Prime Vision.

Her current research interests include multiple instance learning, dissimilarity representation, learning in (non)-metric spaces, and structured data.

David M. J. Tax studied Physics at the University of Nijmegen, the Netherlands in 1996, and received the Masters degree with the thesis "Learning of Structure by Many-take-all Neural Networks." After that he received the Ph.D. degree with the thesis "One-class Classification" from the Delft University of Technology, The Netherlands, under the supervision of Dr. Robert P. W. Duin.

After working for two years as a Marie Curie Fellow in the Intelligent Data Analysis group in Berlin, he is currently an assistant professor in the Pattern Recognition Laboratory at the Delft University of Technology. His main research interest is in the learning and development of detection algorithms and (one-class) classifiers that optimize alternative performance criteria like ordering criteria using the Area under the ROC curve or a Precision-Recall graph. Furthermore, the problems concerning the representation of data, multiple instance learning, simple and elegant classifiers, and the fair evaluation of methods have focus.

Marco Loog received the M.Sc. degree in mathematics from Utrecht University, and the Ph.D. degree from the Image Sciences Institute, in 2004.

After the latter, joyful event, he moved to Copenhagen where he acted as assistant and, eventually, associate professor, next to which he worked as a research scientist at Nordic Bioscience. In 2008, after several splendid years in Denmark, he moved to Delft University of Technology where he now works as an assistant professor in the Pattern Recognition Laboratory. He currently is also chair of Technical Committee 1 of the IAPR and honorary full professor in pattern recognition at the University of Copenhagen. His principal research interest is with supervised pattern recognition in all sorts of shapes and sizes.