

Filter Feature Selection for One-Class Classification

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Abstract In one-class classification problems all training examples belong to a single class. The absence of counter-examples represents a challenge to traditional Machine Learning and pre-processing techniques. This is the case of various feature selection techniques for labeled data. The selection of the most relevant features from a dataset usually benefits the performance obtained by classification algorithms. Despite the relevance of this issue, few techniques have been proposed for feature selection in one-class classification problems. Moreover, most of the existent techniques are wrapper approaches, which have to rely on a specific classification algorithm for feature selection, or aggregation techniques. This paper proposes a new filter feature selection approach for one-class classification. First, five feature selection measures from different paradigms are here employed or adapted to the one-class scenario.

Next, the feature rankings produced by these measures are combined using different aggregation strategies. The proposed approach was able to reduce the size of the feature sets while maintaining or even improving the predictive performance obtained by the one-class classifier.

Keywords Filter feature selection · Rank aggregation · One-class classification

1 Introduction

In *One-class classification* (OCC) problems, also referred as anomaly or novelty detection problems, one has to induce prediction models using data from one-class only [40]. This model should be able to distinguish examples from this class, named target class, from those that do not belong to the class. Although this problem can be viewed as a standard binary classification problem, the absence of counter-examples prevents the direct use of traditional binary classification techniques, unless artificial counter-examples are provided.

Some of the current one-class classification techniques try to find a frontier that delimits the data belonging to the known class. New examples that lie within the frontier are considered positive or belonging to the known class, while examples outside the frontier are labeled as negative. In some studies, they are also named outliers [40].

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There are real various applications where negative points are absent or scarce, like the potential distribution modeling of species [13, 25]. In this application, a large number of records of the presence of a given specie is available. Nevertheless, it is not common to find records of the absence of the specie. The objective of this application is to induce models able to predict the presence of the specie in new regions, given their environmental conditions. Another application suited for one-class modeling is fault detection [35, 37, 38], where the obtainment of negative data that represent systems failures can be either costly or impossible. The prediction of protein-protein interactions in Bioinformatics can also be modeled as a OCC problem, since the set of confirmed non-interacting proteins, which correspond to negative data, is small [10, 32, 33]. Finally, one can cite the detection of intrusions in a computer network [30], where the network normal operation is modeled and it is unsafe to generate examples of intrusions or attacks.

The absence of counter-examples can lead to some difficulties in inducing accurate predictive models. The same difficulties arise when one needs to preprocess one-class datasets, as for performing feature selection. Feature selection looks for a reduced subset of features that describe a dataset. The selected features must have high relevance for data discrimination and low redundancy between each other. In classification problems, the label information is frequently used for guiding the search for a good feature subset. Adaptations can be necessary to use many of the existent feature selection techniques and feature importance measures, since in OCC problems all training data points belong to only one class.

This paper presents and investigates a feature selection technique for OCC problems. First, some feature importance measures proposed for traditional classification and clustering problems are adapted to OCC. We chose measures that take into account different characteristics from a dataset. Each of these measures produce a ranking of the most relevant features. Afterwards, these rankings are aggregated by three common rank aggregation methods: median, majority and Borda count. This ranking combination allows obtaining a consensus rank, from which the top-ranked features are selected.

The main contributions of this work can be summarized as:

- The employment, the adaptation and the creation of different feature importance measures for OCC tasks.
- The proposal and investigation of a new feature selection method for OCC problems, which only takes into account characteristics extracted from examples belonging to the positive class.

This paper extends [26], which preliminarily exposed this feature selection proposal, presenting a novel importance measure for OCC, additional rank aggregation methods and further experiments. It is structured as follows: Section 2 formalizes the basic concepts of OCC. Section 3 presents the main aspects of feature selection. Section 4 describes the feature selection technique proposed in this paper. The experiments performed to evaluate the proposal are described in Section 5, while the results achieved are presented and discussed in Section 6. Section 7 concludes this paper.

2 One-class Classification

Learning from single class data, also known as One-Class Classification (OCC), involves inducing a predictive model that distinguishes examples that belong to a given class from examples that do not belong to it [20].

While negative data may be absent in some domains, OCC can also be beneficial for problems where data distribution is uneven. When learning from such data, traditional modeling techniques tend to favor the majority class, in spite of the fact that the minority class can be the class of major interest. In this situation, OCC models can be induced for the minority class only, not favoring the majority class.

There are three basic approaches to solve OCC problems [40]. The first generates random pseudo-negative data (artificial counter-examples), also named outliers. The problem then becomes a two-class classification problem that can be solved by standard binary classification techniques. Although often used, this approach may lead to a poor predictive performance on new data, since it is necessary to assume a distribution for the unknown negative data.

The second approach requires the estimation of the distribution followed by positive data. Thereby examples that do not follow this distribution are regarded as negative. The need to assume a particular distribution for the data limits these two approaches. The third approach looks for a boundary or frontier around positive data, as shown in Fig. 1. This border must accept as many objects belonging to the modeled class as possible, while minimizing the acceptance of objects that do not belong to it [40].

Data outside the delimited boundary are considered negative examples. Machine Learning (ML) techniques can be employed for defining these boundaries nonparametrically. Among the ML techniques adapted for this purpose, one frequently used is the Support Vector Machine (SVM) [34, 40].

This paper employs a SVM version adapted to OCC, named ν -SVM [34], to evaluate the subsets of features selected. In ν -SVM, the data are first mapped into a space of higher dimension, where an hyperplane that separates positive data with maximal margin to the origin is found. Some training examples are allowed to lay outside this region, in order to avoid overfitting to training data. The parameter $\nu \in (0, 1]$ limits the proportion of these examples. The hyperplane found corresponds to a non-linear frontier delimiting positive data in the original feature space. Mapping is performed by the employment of non-linear Kernel functions [8].

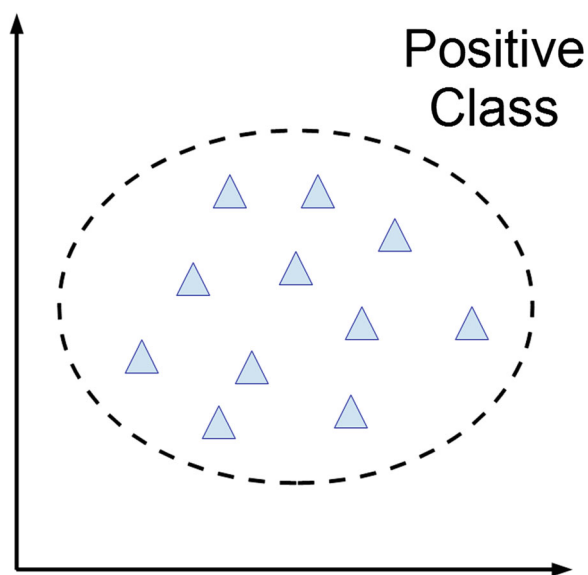


Fig. 1 Delimitation of positive data with circular boundary

3 Feature Selection

Feature Selection (FS) techniques look for a projection of a dataset using a subset of the original input attributes. The selected features should be able to adequately represent the original examples from the modeled domain [23]. This dimensional reduction is possible due to the typical presence of irrelevant and redundant features in real datasets. Irrelevant features do not contribute to the distinction of the classes and can be directly eliminated. For redundant features, whose values are correlated, it is enough to keep just one representative of the related group.

FS can be formulated as a search for subsets of features that optimize some feature importance criterion [22]. It can be performed jointly to the classification model induction, in an embedded approach. The ML algorithm can also be employed as a black box to evaluate different subsets of features and guide the search throughout, in a wrapper approach. Finally, descriptors or measures extracted from data can be used to evaluate the importance of the features. In the later case we have a filter, which can be applied to any dataset despite of the classification technique used afterwards. This is the strategy employed by the technique presented in this paper.

The filter approach is generally faster when compared to embedded and wrapper approaches. In addition, the preprocessed dataset can be used as input to any ML technique, since FS results are less biased towards a particular classification technique.

Various measures can be used to quantify the importance of the features for a classification problem. According to Liu and Motoda [22], a feature is important if its removal leads to the deterioration of a given importance measure when compared to the value obtained while using that feature. These authors propose a taxonomy for the feature importance measures, grouping them into the following categories [24]:

Consistency: tries to identify subsets of features that allow outputting a hypothesis consistent to the data. For labeled data, consistency is reflected by the presence of few similar examples with different labels in the dataset;

Dependency: also called measures of correlation or association, they quantify to which extent the value

of a feature can be predicted from the value of another feature. Thus, they verify how two features are associated with each other;

Distance: also known as measures of separability or discrimination, they consider as important those features that allow a better discrimination of the classes. Therefore, they reinforce that examples from different classes must be spatially distant;

Information: considers the information gain obtained when one or more features are used, compared to their removal. Generally some index based on the entropy or uncertainty arising from the use (or removal) of one or more features is used;

Precision: takes into account the performance achieved by a classifier when a given subset of features is selected. These measures are commonly adopted in wrapper FS.

We chose measures from all previous categories, except precision, to be combined in FS for OCC. This allows taking into account different aspects of the data for the FS. Precision measures were not considered because they are associated to wrapper FS.

Features can also be evaluated individually or jointly, in subsets. In the case each feature is evaluated isolatedly, a ranking of the features according to their importance regarding the measure adopted is output. Reduced subsets of features are obtained by selecting the top-ranked features. When features are evaluated jointly, usually some search procedure is also employed, which gradually adds or removes features from the subsets. In the experiments for this paper, we employed a set of measures for evaluating the features individually. Afterwards, their rankings are combined using different rank aggregation methods.

4 Feature Selection for OCC

There are not many studies investigating the use of FS in OCC. Most of the existing techniques are either based on wrapper [19] or use a dimensional reduction mechanism based on the aggregation of the feature values, like principal component analysis [18, 21, 44]. In [44] three filters for FS, usually adopted in data clustering, are employed in OCC tasks. The first, named $Q - \alpha$, is based on principles of group coherence [29]. $Q - \alpha$ performs FS while simultaneously grouping data. Therefore, it finds a subset of features

able to appropriately separate data into groups. Two other techniques are based on locality preservation, where the proximity in the original feature space must be preserved in the reduced feature subset. The first one is named *Locality Preserving Projections* (LPP) [17], while the second one is the *Laplacian score* (LS) [16]. All techniques employed are suited for clustering problems and where used, without further adaptations, in the OCC context. The $Q - \alpha$ technique obtained the best results in the experimental evaluations.

This paper extends [26] by including one more feature importance measure, by employing other aggregation strategy and improving the experiments. Section 4.1 presents the feature importance measures used in this work. Some of these measures were originally designed for conventional classification problems and had to be adapted to the peculiarities of the OCC scenario. Each of these measures produce a feature ranking, where the feature at the top is considered to be more important for class discrimination.

Each measure provides a different perspective of the importance of the features. Therefore, we opted to combine their outputs in order to integrate multiple views of the data. We believe that this combination makes the FS technique more robust to eventual distortions or deficiencies of the individual measures when evaluating the selected feature set. Since each measure produces a ranking of the features, we used three different rank aggregation methods for joining these feature rankings, which are described in Section 4.2.

4.1 Feature Importance Measures

When measuring the importance of features in a classification problem, the label of the examples is usually taken into account. For instance, the Correlation Based Filter (CBF) [14] employs an importance measure which considers a subset of features important if they are highly correlated to the class, while showing a low correlation to each other.

For OCC problems, all training examples have the same label. Therefore, an adaptation in the way the importance of the features is measured can be necessary. It is also possible to treat the problem as unlabeled and use FS techniques suited to unlabeled data [24]. However, adjustments may still be required, since in OCC problems it is important to choose features that enhance the characterization of only one-class, while in unsupervised learning one seeks for

subsets of features able to evidence multiple groups on data.

The following feature importance measures are adopted in this work:

Spectral score (SPEC): this measure allows the evaluation of features for both labeled and unlabeled datasets [47]. First a similarity matrix S for all pairs of data examples is built. The Radial Basis Function (RBF) can be used to compute the similarities, as shown in Equation 1 for two examples \mathbf{x}_i and \mathbf{x}_j . Based on this information, a graph G connecting the examples is obtained. The graph G has n vertices, representing n objects in the dataset, which are linked by connections weighted by the similarity between them. The concepts shown in S are reflected in the structure of G [7]. A feature consistent with the structure of the graph will have similar values for instances close to each other [47]. The spectrum of G can then be used to evaluate the features, ranking them according to their relevance. This criterion can also be used for datasets with a single class, allowing to rank the features according to their ability to maintain positive data *consistent* and *similar*.

$$S_{ij} = e^{-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}} \quad (1)$$

Information score (IS): the authors in [27] present an *information* measure for unlabeled data, shown in Equation 2. The RBF similarity matrix S is used to calculate the entropy of the data, measuring its randomness. The entropy value is low when the similarity between the examples is high, favoring low intra-group randomness. This is an important issue for OCC too, where intra-class distances must be kept low. However, in its original version, this measure also attributes low entropy values to low similarity values. This occurs because, for clustering purposes, high inter-groups distances must also be favored. This is not the case for OCC, where all data belong to the same class or, ultimately, to the same group. In this paper, we adapted this entropy measure to output low values only when the examples are very similar and high values otherwise. For such, the similarities are normalized within the interval $[0.5, 1]$ instead of $[0, 1]$. Thus, low similarities will be close to 0.5, which leads to a high entropy value. On the other hand, high similarities, next to 1, will lead to smaller entropy values, since

they indicate less randomness and a more structured dataset. To estimate the relevance of each feature according to this criterion, we measure the reduction in the entropy advent from its elimination from the dataset. If the entropy decreases, the removal of the feature makes the data more homogeneous. In this case, the feature can be considered important.

$$E = - \sum_{i=1}^n \sum_{j=1}^n S_{ij} \log_2 S_{ij} + (1 - S_{ij}) \log_2 (1 - S_{ij}) \quad (2)$$

Pearson Correlation (PC): to quantify the *association* of each feature with the others, we used the Pearson correlation measure. It allows checking whether the features are linearly related. Its values are between -1 and 1. As both limits of the scale indicate high correlations, the absolute values of this measure were taken. Next, for each feature in the data, we measured its Pearson correlation to each of the other features and summed the absolute values calculated, as shown in Equation 3. Features with high values for this index are very correlated to others. To favor the maintenance of features that represent more exclusive concepts, lower values are preferred.

$$\text{corr}(f_i) = \sum_{j=1}^m |\text{pearson}(f_i, f_j)| \quad (3)$$

Intra-class distance (ICD): given by Equation 4, where n is the number of data instances and $\bar{\mathbf{x}}$ is the centroid of the class, this measure quantifies the distance from all examples of a class to the centroid of the class. Lower intra-class distances must be favored in OCC, in order to make positive data closer to each other. Like in IS, we measure the reduction in intra-class distance arising from the elimination of each individual feature. The features are then ranked such that those that approximate more the data are considered better. We employed the standard Euclidean distance measure in the computations.

$$IE = \frac{1}{n} \sum_{i=1}^n d(\mathbf{x}_i, \bar{\mathbf{x}}) \quad (4)$$

Interquartile range (IQR): this measure takes into account the distribution of the feature values through their interquartiles. Its use is motivated by

the principle that if a feature is characteristic from a particular class, its values tend to be more concentrated, which is reflected in the interquartile ranges. As an example, Fig. 2 shows box-plots of the feature values in the *iris* dataset from the UCI repository [2]. It is possible to notice that the class *iris setosa*, in the top, can be easily distinguished from the other classes by considering the values of the features petal length and petal width, which show more concentrated distributions. Although two features may have the same interquartile while their values overlap, this overlapping is more likely to occur if the values are widely dispersed.

Among the presented measures, only SPEC was employed without any adaptation. IS and ICD were adapted for OCC, while PC and IQR were proposed by the authors.

All measures allow to rank the features individually. Nonetheless, each criterion gives a different emphasis to a particular aspect of the one-class dataset and has its deficiencies. For instance, IQR may attribute high rankings to features whose values may overlap to those from other classes. In fact, it is difficult to take into account whether a feature is indeed discriminative when only information from a single class is available.

4.2 Rank Aggregation

The objective of rank aggregation is to combine the results produced by multiple rankings, generating a consensus ranking. In our case, as a result, a new order of importance for the features is produced. The proposed approach can also be regarded as a committee or ensemble of FS techniques [28, 36, 41, 43, 46].

Each importance measure produces a ranking of the features based on some data characteristic. For instance, the PC measure focus on poorly correlated features, while IQR ranks higher the features with more concentrated values. These criteria represent suboptimal evidence of the importance of the features and they have associated shortcomings. To incorporate the distinct aspects of the data considered by the different importance measures, we decided to combine the rankings produced by them.

Combining multiple feature rankings also enables us to explore complementaries of the different measures and enhance FS by minimizing specific

influences of a single univariate measure in the results [45]. Thereby, multiple views of the importance of the features can be taken into account.

An important aspect to be considered is how to combine the rankings produced by the different measures. There are different techniques proposed in the literature for ranking aggregation. The choice of a particular ranking technique can be based on the predictive performance achieved when using the selected subset of features or on its computational cost.

One simple way to combine rankings is to average the positions of the features in the ranking lists [45]. Another alternative is to apply a majority voting rule for the positions attributed to each feature in the lists [3, 42]. There are also methods to aggregate voting results from the areas of politics and social science [12]. This is the case of the Borda method [4], a positional voting system proposed in 1784. In this method, each feature gets points according to its position in the rankings. These points increase from the first to the last place of a ranking. The feature with the smallest accumulated sum of points is ranked better.

Table 1 presents the order of the features for the *iris-setosa* class [2], obtained using the importance measures described in Section 4.1 and aggregating them according to the different rank aggregation methods presented in this section. PL refers to the *petal-length* feature, PW to the *petal-width* feature, SL to *sepal-length* and SW to *sepal-width*. We can observe how the rankings vary for different measures, since they consider distinct aspects of the data. For instance, for the SPEC importance measure, the following ranking of features is produced: SW, PW, PL and SL. After combining the different rankings of the features by the Mean (average) criterion, the result is: PW, PL, SL and SW. We deal with ties in the aggregation results by positioning the tied features according to their original ordering in the dataset.

Figure 3 represents the aggregation results from Table 1 graphically. The best (highest ranked) features are represented by darker shades of gray. Although there are some disagreements between ranking results, in general, we can observe that the features PL and PW assume higher positions.

There are many other rank aggregation methods in the literature and also empirical studies comparing some of them [3, 12, 41, 45]. In general, there is no consensus on the best method to use. In [11], for example, the Mean is recommended, while in [31]

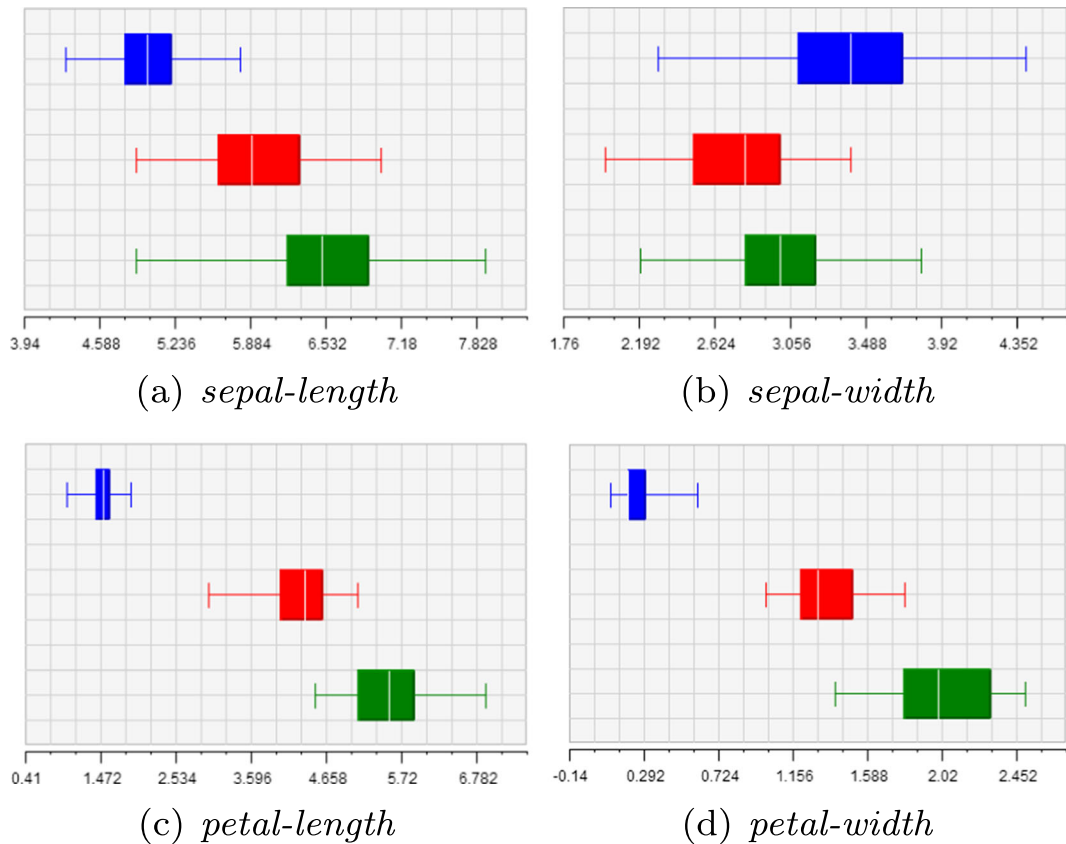


Fig. 2 Box-plots of the feature values in the *iris* dataset. The top bars designate class *Iris-setosa*, middle bars are from class *Iris-versicolor* and bottom bars are from class *Iris-virginica*

a method named Schulze is considered better. In this study, three of the most common aggregation meth-

ods employed in the related literature, namely Mean, Majority and Borda, were investigated.

Table 1 Results of applying different feature aggregation measures for *iris-setosa* class

		Features			
		SL	SW	PL	PW
Feature Importance Measures	SPEC	4	1	3	2
	Inter-quartile	4	3	1	2
	Pearson	3	4	2	1
	Entropy	2	4	1	3
	Intra-Class	1	4	3	2
Aggregation Methods	Mean	3	4	2	1
	Majority	4	3	1	2
	Borda	4	1	3	2

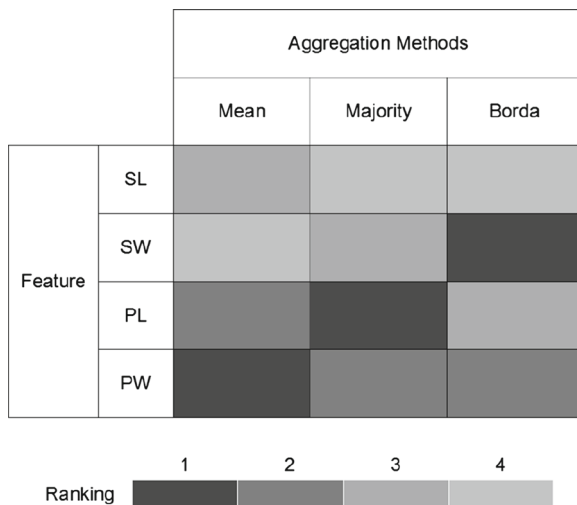


Fig. 3 Aggregation results for *iris-setosa* class

5 Experiments

This section presents the experiments performed in this work for the evaluation of the proposed FS technique for OCC. All experiments were coded in Matlab using Weka [15] and LibSVM [5].

5.1 Datasets

Fourteen datasets from the UCI [2] and Keel [1] repositories were used in the experiments. The main

characteristics of these datasets are illustrated in Table 2, which presents, for each dataset: number of classes ($\#$ Classes), number of examples ($\#$ Examples), number of examples per class ($\#$ Examples/Classes), number of features ($\#$ Features) and number of examples per feature ($\#$ Examples/ $\#$ Features) for each class. For the later information, low ratios designate more sparse data. All features are continuous or integer valued, since some measures can only be calculated for numerical values. This does not prevent the use of nominal features, which have to be previously mapped into a numerical value.

One-class versions from these datasets were generated by separating data from each of their classes. For instance, the *blood* dataset originates two one-class datasets: one for the class *yes* and another for the class *no*. On the other hand, the *iris* dataset generates three one-class datasets: *setosa*, *versicolor* and *virginica*. The same reasoning applies to the *wine* dataset, giving rise to three one-class datasets, totalizing 30 one-class datasets for the experiments. This strategy is the same employed in related works regarding one-class datasets [39].

5.2 Methodology

Initially, all one-class datasets were divided according to the ten-fold cross-validation methodology. For each dataset, the training folds will have only the examples from one of the classes, 90 % of them. The test fold

Table 2 Summary of the characteristics of the datasets

Dataset	$\#$ Classes	$\#$ Examples	$\#$ Examples/Classes	$\#$ Features	$\#$ Examples/ $\#$ Features
<i>appendicitis</i>	2	106	85-21	7	12.14-3.00
<i>blood</i>	2	748	178-570	4	44.50-142.50
<i>bupa</i>	2	345	145-200	6	24.17-33.33
<i>fertility</i>	2	100	88-12	9	9.78-1.33
<i>indian</i>	2	579	414-165	10	41.40-16.50
<i>ionosphere</i>	2	351	225-126	33	6.82-3.52
<i>iris</i>	3	150	50-50-50	4	12.50-12.50-12.50
<i>phoneme</i>	2	5404	3818-1586	5	763.60-317.20
<i>pima</i>	2	768	500-268	8	62.50-33.50
<i>sonar</i>	2	208	97-111	60	1.62-1.85
<i>spambase</i>	2	4601	1813-2788	57	31.79-48.86
<i>spectheart</i>	2	267	55-212	44	1.25-4.82
<i>wdbc</i>	2	569	212-357	30	7.07-11.90
<i>wine</i>	3	178	59-71-48	13	4.54-5.46-3.69

has all the examples from the other classes, to simulate the presence of negative data, plus 10 % of the examples from the training class.

For instance, in the *iris-setosa* dataset, we will have ten test folds of size 105, where 5 examples are from the *iris-setosa* class and the remaining 100 examples come from the other two classes (*iris-virginica* and *iris-versicolor*). We highlight that all test data are not seen by any of the classification algorithms during induction nor by the feature selection techniques, which use only training data information.

The feature importance measures from Section 4.1 are calculated for each training set partition. The feature rankings produced are then aggregated using the Mean, Majority and Borda methods. We then systematically remove the least important feature according to these methods from the training and test folds, until only the most important feature remains. ν -SVM classifiers, with varying ν values and Kernel functions, are induced for the original datasets (with all features) and all of their reduced counterparts. The objective of this procedure is to monitor whether the number of features can be reduced while maintaining the predictive performance achieved when all features are used. The following ν values were tested: 0.01, 0.1, 0.5, 0.7 and 0.9. The Kernel functions tested were the RBF and the Linear, with the default parameters from the LibSVM tool [6]. This totalizes 10 combinations of parameter values for the ν -SVM classifiers.

The F1 measure was used to evaluate the predictive performance of the classifiers for the different experimental setups investigated in this study (5). It measures the ability to correctly retrieve the positive data by combining the precision (P, defined by Equation 6) and recall (R, defined by Equation 7) obtained for the positive class.

$$F1 = 2 \frac{(P * R)}{(P + R)} \quad (5)$$

$$P = \frac{TP}{TP + FP} \quad (6)$$

$$R = \frac{TP}{TP + FN} \quad (7)$$

In the Equations 6 and 7, TP refers to the number of true positive examples in test data, FP is the number of false positive examples and FN stands for the number of false negative examples. Therefore, while the precision measures whether the examples predicted

as positive are indeed positive, recall represents the positive data fraction that was correctly retrieved.

The overall methodology employed is outlined in Fig. 4. For each training partition i of a one-class dataset, we apply the five feature importance measures, aggregate their results and induce ν -SVMs using decreasing numbers of features. The F1 performance achieved on the test fold i is then recorded. Since all datasets were divided with ten-fold cross-validation, average and standard-deviation of the F1 results are calculated.

6 Experimental Results

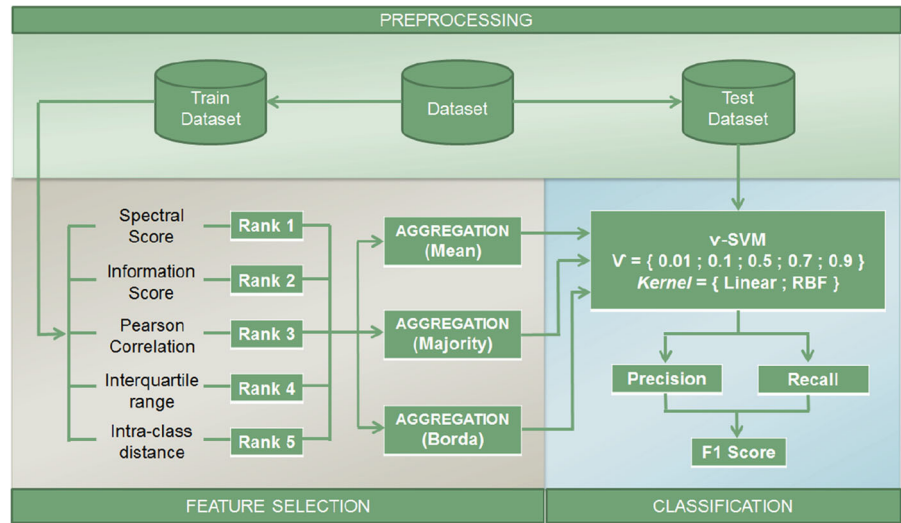
Several experiments were performed to evaluate FS for OCC using the previously mentioned datasets. Table 3 presents the best F1 results obtained in the experiments for each one-class dataset. It shows the F1 average performance and standard deviation, obtained by following the cross-validation methodology, for both original data (with all features) and the data obtained after FS (using the format average F1 \pm standard-deviation). The FS results correspond to the best configuration among all tested combinations of aggregation methods and ν -SVM parameter values. Table 3 also shows the ν values and Kernel function associated with the reported results. For the results after FS, we also present the rank aggregation method employed and the percentage of reduction (PR) in the number of features after FS. The best F1 in each dataset is highlighted in boldface. When the results after FS are significantly different from those obtained for the original data, they are highlighted in boldface and italics. The statistical test employed was the paired Wilcoxon signed-ranks test [9], with 95 % of confidence level.

Next we discuss the results concerning: the F1 values obtained; the reduction in the number of features; the aggregation strategies employed; the ν -SVM parameter values; the precision and recall of the classifiers; and a trade-off between the F1 values achieved and the percentage of reduction in the number of features.

6.1 F1 Measure Values

It is possible to notice in Table 3 that the use of FS either maintained or improved the F1 rates for most of

Fig. 4 Methodology employed in the experiments for each data fold



the datasets. Employing the paired Wilcoxon signed-ranks statistical test [9] with a 95 % of confidence value, it is possible to observe that:

1. The F1 performance was significantly improved after FS for the datasets: *appendicitis1*, *bupa2*, *indian2*, *phoneme1*, *phoneme2*, *spambase1*, *spambase2*, *wdbc2* and *wine3*.
2. For all other datasets, the F1 performance was maintained after FS, when compared to the original F1 values.

Therefore, FS was always capable to either maintain (in 21 datasets) or significantly improve (in nine datasets) the predictive performance of the one-class classifiers, while using less predictive features. It is interesting to notice that some of the major performance gains occurred for some of the datasets with more features, like *phoneme1*, *phoneme2*, *spambase1*, *spambase2* and *wdbc2*. Overall, there were more predictive performance gains for datasets with more examples. Since we adopt a filter approach, which consider aspects from data, this is a somewhat expected result.

Taking each dataset paired according to its original domain, some interesting results can be seen. For example, class *appendicitis1* was more accurately identified than class *appendicitis2*, according to the F1 measure. The same happens for the pairs *blood1-blood2*, *fertility1-fertility2*, *indian1-indian2*, *phoneme1-phoneme2* and *specheart1-specheart2*. In all these pairs, the class with lowest predictive

performance is the one with the smallest number of examples.

6.2 Reduction in the Number of Features

The reductions in the number of features were mostly large. There are several cases (19 out of 30 datasets) where the reduction in the number of features was higher than or equal to 50 %, which can be considered a sharp decrease. Smaller reductions occurred in the datasets *sonar1* and *spambase2*. In absolute numbers, three features were removed from the *sonar1* dataset, while five features were removed from the *spambase2* dataset. As these datasets have a high number of features, their percentage of feature reduction was low.

Finally, reductions of 90 % or more in the number of features were obtained for the *indian1*, *ionosphere2* and *specheart2* datasets. The *ionosphere2* and *specheart2* datasets, particularly, are originally sparse datasets, which may have benefited more from the dimensional reduction promoted by FS.

6.3 Aggregation Strategies

The results obtained by the three aggregation strategies employed were similar, although the Borda method had the best predictive performance in a larger number of datasets. While Borda was the best in 14 cases, Majority figured as the best in 9 datasets and Mean outperformed Borda and Majority in 7 of

Table 3 Best results achieved for original data and for the feature selectors

Dataset	Original			After FS				
	F1	ν	Kernel	F1 _{FS}	ν	Aggregation	PR	Kernel
<i>appendicitis1</i>	0.64±0.10	0.1	Linear	0.71±0.09	0.1	Borda	42.86	Linear
<i>appendicitis2</i>	0.17±0.27	0.9	RBF	0.16±0.26	0.9	Borda	14.29	RBF
<i>blood1</i>	0.09±0.02	0.5	Linear	0.09±0.04	0.9	Mean	50.00	Linear
<i>blood2</i>	0.39±0.00	0.01	Linear	0.41±0.02	0.01	Majority	50.00	RBF
<i>bupa1</i>	0.14±0.01	0.1	Linear	0.17±0.07	0.01	Borda	66.67	RBF
<i>bupa2</i>	0.21±0.00	0.01	Linear	0.27±0.03	0.5	Mean	50.00	Linear
<i>fertility1</i>	0.60±0.02	0.01	Linear	0.60±0.03	0.01	Mean	55.56	Linear
<i>fertility2</i>	0.03±0.03	0.01	RBF	0.10±0.14	0.9	Majority	22.22	RBF
<i>indian1</i>	0.44±0.05	0.5	Linear	0.45±0.05	0.5	Majority	90.00	Linear
<i>indian2</i>	0.07±0.00	0.01	Linear	0.13±0.04	0.01	Mean	60.00	RBF
<i>ionosphere1</i>	0.56±0.03	0.1	Linear	0.60±0.09	0.1	Borda	66.67	RBF
<i>ionosphere2</i>	0.09±0.01	0.01	Linear	0.38±0.29	0.01	Majority	96.97	Linear
<i>iris1</i>	0.95±0.14	0.01	RBF	0.96±0.08	0.01	Mean	50.00	RBF
<i>iris2</i>	0.65±0.21	0.5	RBF	0.64±0.18	0.1	Majority	75.00	RBF
<i>iris3</i>	0.69±0.15	0.01	RBF	0.73±0.29	0.1	Majority	75.00	Linear
<i>phoneme1</i>	0.34±0.01	0.1	RBF	0.59±0.03	0.5	Borda	80.00	RBF
<i>phoneme2</i>	0.15±0.01	0.7	Ambos	0.18±0.02	0.7	Mean	20.00	Linear
<i>pima1</i>	0.27±0.00	0.01	Linear	0.27±0.00	0.01	Majority	12.50	Linear
<i>pima2</i>	0.23±0.04	0.5	Linear	0.23±0.03	0.5	Majority	12.50	Linear
<i>sonar1</i>	0.18±0.08	0.7	RBF	0.20±0.07	0.7	Majority	5.00	RBF
<i>sonar2</i>	0.25±0.09	0.5	Linear	0.28±0.07	0.5	Borda	88.33	Linear
<i>spambase1</i>	0.43±0.02	0.01	RBF	0.47±0.03	0.9	Borda	81.00	RBF
<i>spambase2</i>	0.23±0.01	0.5	Linear	0.35±0.07	0.5	Borda	8.77	Linear
<i>spectfheart1</i>	0.16±0.12	0.7	Linear	0.20±0.17	0.9	Mean	49.12	Linear
<i>spectfheart2</i>	0.44±0.05	0.01	Linear	0.44±0.00	0.01	Borda	97.73	Linear
<i>wdbc1</i>	0.65±0.14	0.5	Linear	0.65±0.14	0.5	Borda	16.67	Linear
<i>wdbc2</i>	0.25±0.01	0.01	Linear	0.63±0.04	0.1	Borda	50.00	RBF
<i>wine1</i>	0.64±0.18	0.5	Linear	0.64±0.18	0.5	Majority	23.08	Linear
<i>wine2</i>	0.12±0.01	0.01	Linear	0.27±0.23	0.01	Borda	76.92	RBF
<i>wine3</i>	0.08±0.01	0.1	Linear	0.44±0.28	0.1	Borda	76.92	RBF

the datasets. The Borda aggregation method is somewhat costly, and this can be taken into account when choosing a particular aggregation method. Mean and Majority are computed in $O(n)$ while Borda $O(n^2)$. Nonetheless, it is advisable to test all strategies experimentally before choosing an aggregation method for a given dataset.

The percentage of reduction (PR) in the number of features obtained by the aggregation strategies were: 55.76 ± 28.72 for Borda; 46.23 ± 35.35 for Majority; and 54.05 ± 21.31 for Mean. Therefore,

similar PR values were also obtained by the aggregation strategies.

6.4 SVM Parameter Values

Concerning the ν -SVM parameter values, it is possible to notice in Table 3 that the *Linear* Kernel excelled for the original datasets. However, after FS, there were cases where a non-linear boundary became necessary and the *RBF* Kernel showed better results. The ν values remained similar in most of the cases, increasing

Fig. 5 Plots of the F1, precision and recall values per dataset - part 1. Gray columns correspond to original results, while black columns show results after FS

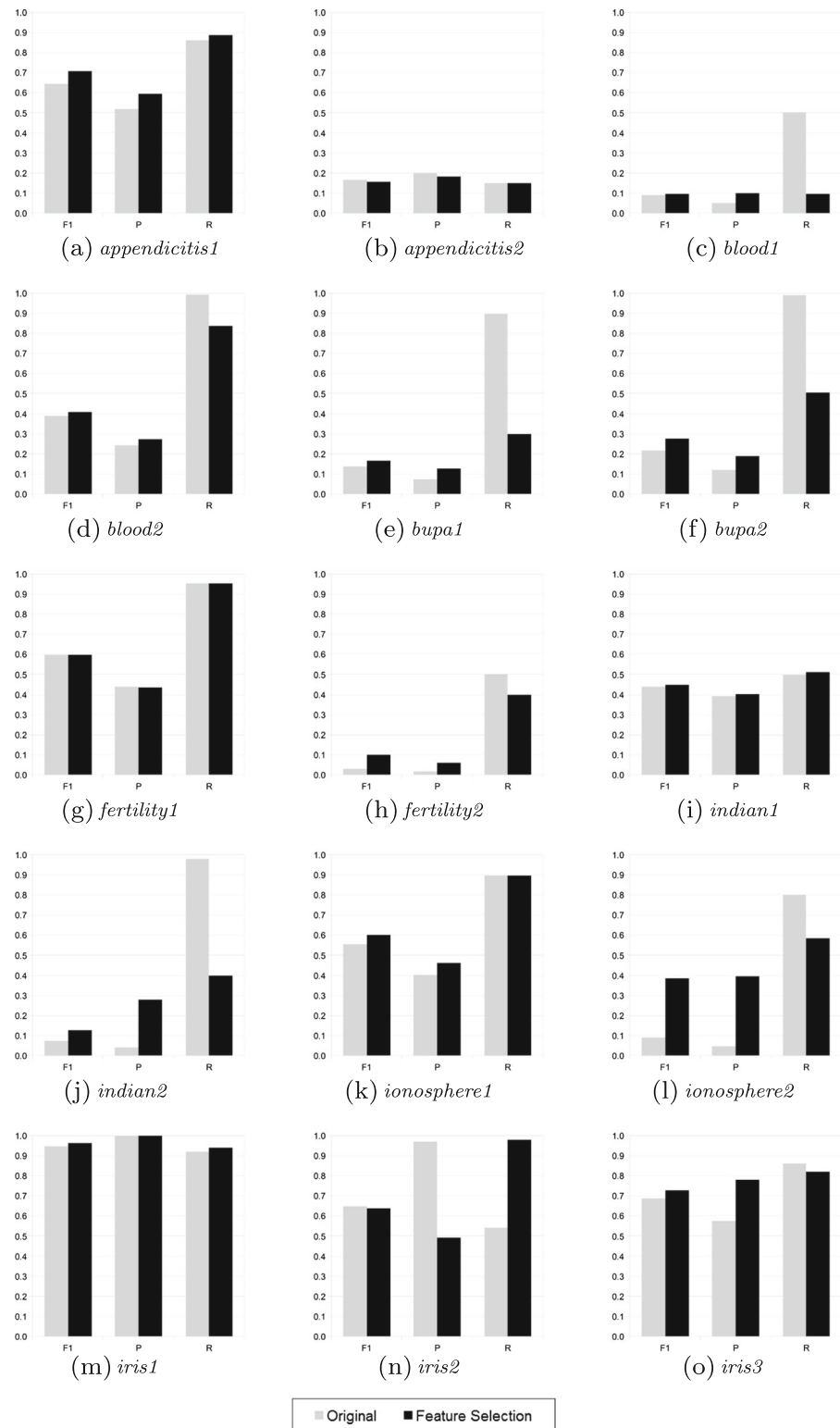
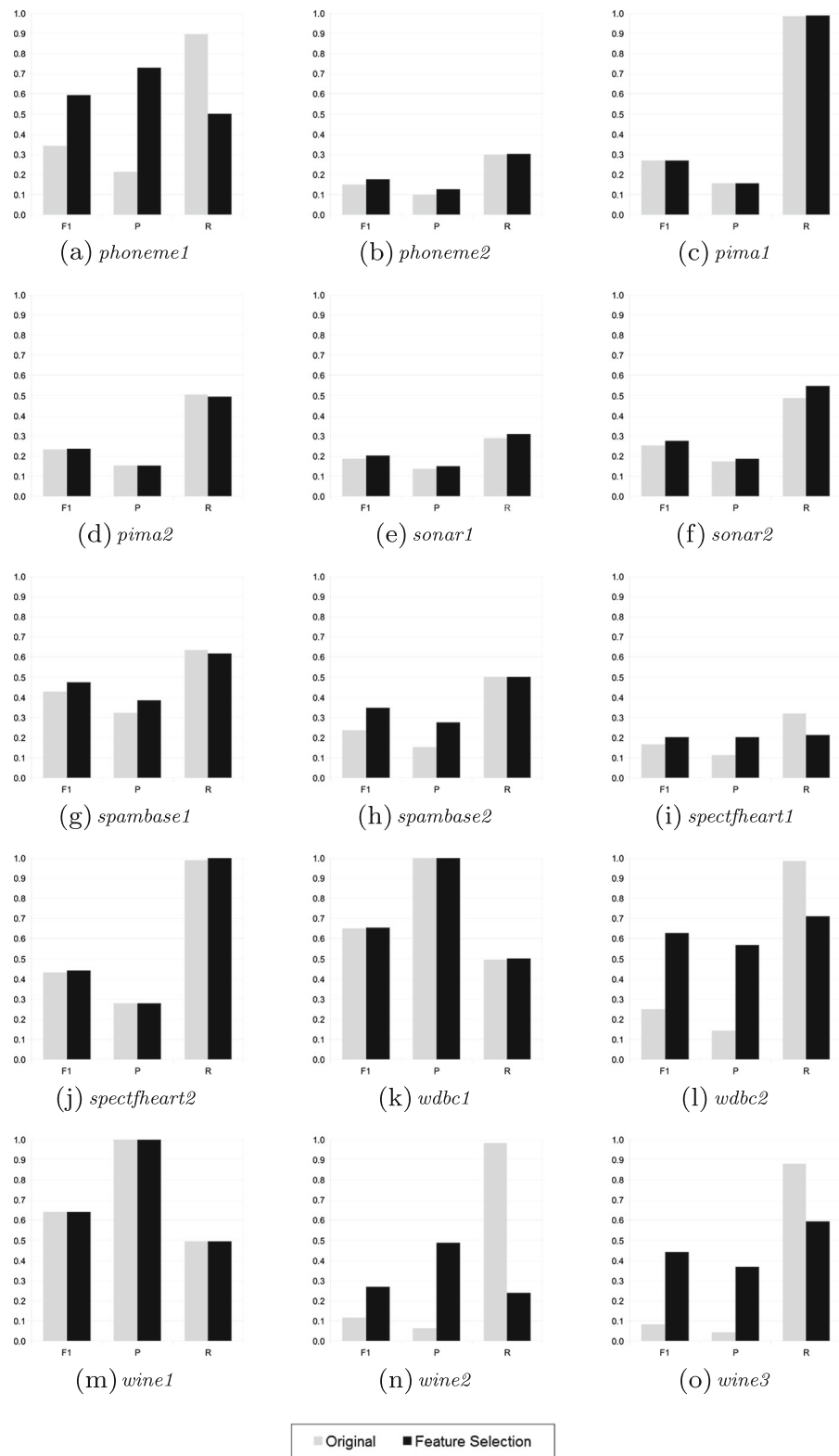


Fig. 6 Plots of the F1, precision and recall values per dataset - part 2. Gray columns correspond to original results, while black columns show results after FS



in several others. This implies in the need for frontiers less restricted to the positive training data after the application of FS.

6.5 Precision and Recall

For better assessing whether the F1 variations are due to changes in precision or recall, in the Figs. 5 and 6 we present plots of the F1, precision and recall average values achieved for each dataset. Two columns are drawn per performance metric, one for the results in the original data (light gray), and the other for the results achieved after the FS procedure (black).

It is possible to notice from these figures that, after the FS, an increase in the precision values often occurs. Precision accounts for the correct positive predictions, i.e., it is larger when more data predicted as positive are indeed from the target class. This result is interesting, since the false positive rate cannot be directly minimized when training one-class classifiers, because counterexamples are absent at this stage. FS seems to have minimized this effect.

There were cases where the increase in precision was obtained at the cost of a reduction in recall, namely the occurrence of more false negatives. There is usually a trade-off between precision and recall rates, so that if one increases the other decreases. But there are also cases where both precision and recall values increased after the FS. This is the case, for example, of the datasets *appendicitis1*, *indian1* and *sonar2*, which showed room for improvement in the predictions for both positive and negative classes, which was exploited by the FS.

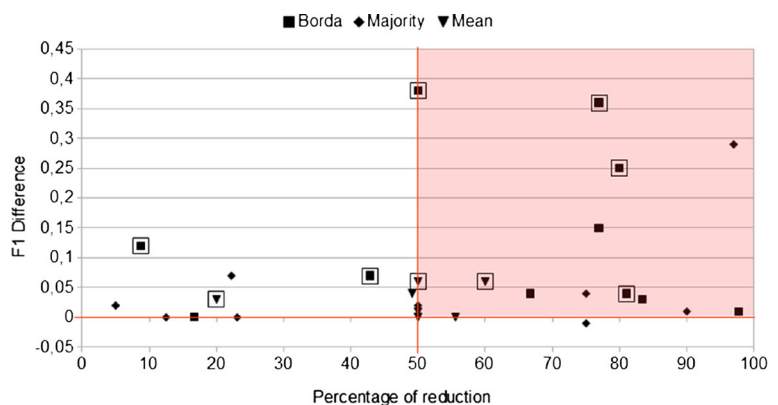
6.6 Trade-off F1 Versus PR

Figure 7 presents an overview of the FS results for all datasets, associating the percentage of reduction in the number of features (x axis) with the difference between the F1 value before and after the FS (y axis). The closer the point is to the extreme right of the graph, the better is the corresponding result, since it represents higher gains in F1 while using less features. The region representing gains in F1 and large reductions in the number of features (higher or equal to 50 %) is shaded. Datasets for which the F1 gains were statistically significant are highlighted with a square. It is worth noting that many of the statistically significant predictive results were obtained using less than 50 % of the original features.

It is possible to observe, in many cases, improvements of predictive results with large reductions in the number of features. In several datasets the reductions in the number of features was higher than 50 %, a significant dimensional reduction. The Borda aggregation method showed more F1 gains and larger reductions in the number of features, when compared to the other aggregation methods.

Overall, we should also observe that many of the single class results observed in this work can be considered poor if compared with the performance that can be obtained when treating the same data by standard binary or multi-class techniques. This may be due to the inherent difficulty of OCC when compared to standard classification scenarios, but also to the fact that the datasets used are not naturally one-class. Future work shall investigate the performance of the proposed FS technique for real one-class applications.

Fig. 7 Feature reduction percentage versus F1 gains after the FS



7 Conclusion

This paper presented a new filter approach for feature selection in one-class classification problems. The proposed method combines rankings of the features selected by different feature importance measures. The chosen measures are able to capture distinct aspects from the data. Thereby, their combination allow exploring multiple and complementary views of the data.

Each importance measure combined belongs to one or more categories among those listed in [24]: the spectral score measures the *consistency* relative to data structure; the information score calculation has been adapted to the one-class context in this work and focuses on features that bring a higher *information* gain for the target class; the correlation between the features considers the *association* between them, allowing the removal of redundant features; the intra-class *distance* focuses on preserving the locality of the data from the target class; and the inter-quartile range, introduced in this paper, is based on the *distribution* of the features in the target class. Each of these measures provides evidence of the importance of the features that can be complemented by their combination. To combine their results, three different ranking aggregation strategies were employed: Mean, Majority and Borda.

Experiments were performed on 30 artificial one-class datasets generated from binary and multiclass datasets obtained from public repositories. It was possible to reduce data dimension while maintaining or even improving one-class classification predictive performance, especially regarding the precision in the recognition of the target class. We thereby proved the hypothesis of the work that it is possible to perform FS in OCC tasks using only descriptors extracted from the target class data.

It is worth mentioning that, in many cases, the use of FS also reduced the number of false positives. As the false positive rate cannot be minimized directly during the induction of one-class classifiers, this result is important and reinforces that this deficiency can be reduced if data are properly preprocessed.

As future work, we plan to employ the investigated technique in one-class real applications and datasets. Other one-class classification techniques can also be employed for evaluating the subsets of features selected, since, in the filter approach, the results are

independent of the classification technique employed. This can also provide the achievement of more general experimental results. It would also be interesting to investigate and highlight which are the characteristics of the datasets for which FS was more beneficial.

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References

1. Alcalá-Fdez, J., Fernandez, A., Luengo, J., Derrac, J., García, S., Sánchez, L., Herrera, F.: Keel data-mining software tool: Data set repository, integration of algorithms and experimental analysis framework. *J. Multiple-Valued Logic Soft Comput.* **17**(2-3), 255–287 (2011)
2. Bache, K., Lichman, M.: UCI machine learning repository (2014). <http://archive.ics.uci.edu/ml>
3. Bauer, E., Kohavi, R.: An empirical comparison of voting classification algorithms: Bagging, boosting, and variants. *Mach. learn.* **36**(1-2), 105–139 (1999)
4. De Borda, J.C.: Mémoire sur les élections au scrutin. *Histoire de l'Académie Royale des Sciences* (1784)
5. Chang, C.C., Lin, C.J.: Libsvm: a library for support vector machines. *ACM Trans. Intell. Syst. Technol.* **2**(3), 1–30 (2011)
6. Chang, C.C., Lin, C.J.: Libsvm: a library for support vector machines. *ACM Trans. Intell. Syst. Technol.* **2**(3), 1–30 (2011)
7. Chapelle, O., Scholkopf, B., Zien, A.: Semi-supervised Learning, Chap. Graph-Based Methods. The MIT Press (2006)
8. Cristianini, N., Shawe-Taylor, J.: An Introduction to Support Vector Machines and other kernel-based learning methods. Cambridge University Press (2000)
9. Demšar, J.: Statistical comparisons of classifiers over multiple data sets. *J. Mach. Learn. Res.* **7**, 1–30 (2006)
10. Deris, S., Alashwal, H., Othman, M.: One-class support vector machines for protein-protein interactions prediction. *Int. J. Biol. Med. Sci.* **1**(2), 120–127 (2006)
11. Dittman, D.J., Khoshgoftaar, T.M., Wald, R., Napolitano, A.: Classification performance of rank aggregation techniques for ensemble gene selection. In: The Twenty-Sixth International FLAIRS Conference (2013)
12. Dwork, C., Kumar, R., Naor, M., Sivakumar, D.: Rank aggregation methods for the web. In: Proceedings of the 10th international conference on World Wide Web, pp. 613–622. ACM (2001)
13. Elith*, J., H. Graham*, C., P. Anderson, R., Dudík, M., Ferrier, S., Guisan, A., J. Hijmans, R., Huettmann, F., R. Leathwick, J., Lehmann, A., Li, J., G. Lohmann, L., A. Loiselle,

- B., Manion, G., Moritz, C., Nakamura, M., Nakazawa, Y., McC. M. Overton, J., Townsend Peterson, A., J. Phillips, S., Richardson, K., Scachetti-Pereira, R., E. Schapire, R., Sober?n, J., Williams, S., S. Wisz, M., E. Zimmermann, N.: Novel methods improve prediction of species? distributions from occurrence data. *Ecography* **29**(2), 129–151 (2006). doi:[10.1111/j.2006.0906-7590.04596.x](https://doi.org/10.1111/j.2006.0906-7590.04596.x)
14. Hall, M.: Correlation-based feature selection for discrete and numeric class machine learning. In: *Proceedings 17th International Conference Machine Learning*, pp. 359–366 (2000)
15. Hall, M., Frank, E., Holmes, G., Pfahringer, B., Reutemann, P., Witten, I.H.: The weka data mining software: an update. *SIGKDD Explor. Newsl.* **11**(1), 10–18 (2009). doi:[10.1145/1656274.1656278](https://doi.org/10.1145/1656274.1656278)
16. He, X., Cai, D., Niyogi, P.: Laplacian score for feature selection. In: *NIPS*, Vol. 186, p. 189 (2005)
17. He, X., Niyogi, P.: Locality preserving projections. In: *NIPS*, Vol. 16, pp. 234–241 (2003)
18. Hoffmann, H.: Kernel pca for novelty detection. *Pattern Recogn.* **40**(3), 863–874 (2007)
19. Jeong, Y.S., Kang, I.H., Jeong, M.K., Kong, D.: A new feature selection method for one-class classification problems. *Systems, Man, and Cybernetics, Part C: Applications and Reviews. IEEE Trans.* **42**(6), 1500–1509 (2012)
20. Khan, S.S., Madden, M.G.: A survey of recent trends in one class classification. *Artif. Intell. Cogn. Sci.* **6206**, 188–197 (2010)
21. Lian, H.: On feature selection with principal component analysis for one-class svm. *Pattern Recogn. Lett.* **33**(9), 1027–1031 (2012)
22. Liu, H., Motoda, H.: *Feature Extraction, Construction and Selection - A Data Mining Perspective*. Kluwer Academic Publishers (1998)
23. Liu, H., Motoda, H., Setiono, R., Zhao, Z.: Feature selection : An ever evolving frontier in data mining. *Knowl. Creat. Diffus. Utilization* **4**, 4–13 (2010)
24. Liu, H., Yu, L.: Toward integrating feature selection algorithms for classification and clustering. *IEEE Trans. Knowl. Data Eng.* **17**(4), 491–502 (2005)
25. Lorena, A.C., Jacintho, L.F.O., Siqueira, M.F., Giovanni, R., Lohmann, L.G., Carvalho, A.C.P.L.F., Yamamoto, M.: Comparing machine learning classifiers in potential distribution modelling. *Expert Syst. Appl.* **38**, 5268–5275 (2011)
26. Lorena, L.H.N., De Carvalho, A.C.P.L.F., Lorena, A.C.: Seleção de atributos em problemas de classificação com uma única classe [in portuguese]. In: *X Encontro Nacional de Inteligência Artificial e Computacional (ENIAC)*, pp. 1–11 (2013)
27. Mitra, P., Murthy, C.A., Pal, S.: Unsupervised feature selection using feature similarity. *IEEE Trans. Pattern Anal. Mach. Intell.* **24**(3), 301–312 (2002)
28. Namsrai, E., Munkhdalai, T., Li, M., Shin, J.H., Namsrai, O.E., Ryu, K.H.: A feature selection-based ensemble method for arrhythmia classification. *JIPS* **9**(1), 31–40 (2013)
29. Ng, A.Y., Jordan, M.I., Weiss, Y.: On spectral clustering analysis and an algorithm. *Proceedings of Advances in Neural Information Processing Systems*. Cambridge, MA: MIT Press **14**, 849–856 (2001)
30. Pimentel, M.A., Clifton, D.A., Clifton, L., Tarassenko, L.: A review of novelty detection. *Sig. Process.* **99**(0), 215–249 (2014)
31. Prati, R.C.: Combining feature ranking algorithms through rank aggregation. In: *Neural Networks (IJCNN), The 2012 International Joint Conference on*, pp. 1–8. IEEE (2012)
32. Reyes, J., Gilbert, D.: Combining one-class classification models based on diverse biological data for prediction of protein-protein interactions. In: *Data Integration in the Life Sciences, Lecture Notes in Computer Science*, Vol. 5109, pp. 177–191. Springer Berlin Heidelberg (2008)
33. Reyes, J.A., Gilbert, D.: Prediction of protein-protein interactions using one-class classification methods and integrating diverse data. *J. Integr. Bioinforma.* **4**(3), 77 (2007)
34. Scholkopf, B., Platt, J.C., Shawe-Taylor, J., Smolax, A.J., Williamson, R.C.: Estimating the support of a high-dimensional distribution. *Neural Comput.* **13**(7), 1443–1471 (2001)
35. Shahid, N., Aleem, S., Naqvi, I.H., Zaffar, N.: Support vector machine based fault detection & classification in smart grids. In: *Globecom Workshops (GC Wkshps), 2012 IEEE*, pp. 1526–1531. IEEE (2012)
36. Shen, Q., Diao, R., Su, P.: Feature selection ensemble. In: A. Voronkov (ed.) *Turing-100, EPIc Series*, Vol. 10, pp. 289–306. EasyChair (2012)
37. Shin, H.J., Eom, D.H., Kim, S.S.: One-class support vector machines—an application in machine fault detection and classification. *Comput. Ind. Eng.* **48**(2), 395–408 (2005). doi:[10.1016/j.cie.2005.01.009](https://doi.org/10.1016/j.cie.2005.01.009)
38. Smart, E., Brown, D.J., Axel-Berg, L.: Comparing one and two class classification methods for multiple fault detection on an induction motor. In: *ISIEA, 2013 IEEE Symposium on* (2013)
39. Tax, D.M., Duin, R.P.: Characterizing one-class datasets. In: *Proceedings of the Sixteenth Annual Symposium of the Pattern Recognition Association of South Africa*, pp. 21–26 (2005)
40. Tax, D.M.J.: One-class classification: Concept-learning in the absence of counter-examples. PhD dissertation, Delft University of Technology (2001)
41. Tsymbal, A., Cunningham, P.: Diversity in ensemble feature selection. *Tech. rep.*, Department of Computer Science, Trinity College Dublin (2003). URL <http://www.cs.tcd.ie/publications/tech-reports/reports.03/TCD-CS-2003-44.pdf>
42. Tsymbal, A., Pechenizkiy, M., Cunningham, P.: Diversity in search strategies for ensemble feature selection. *Inf. fusion* **6**(1), 83–98 (2005)
43. Tsymbal, A., Puuronen, S., Patterson, D.W.: Ensemble feature selection with the simple bayesian classification. *Information Fusion* **4**(2), 87–100 (2003)
44. Villalba, S.D., Cunningham, P.: An evaluation of dimension reduction techniques for one-class classification. *Artif. Intell. Rev.* **27**(4), 273–294 (2007)
45. Wald, R., Khoshgoftaar, T.M., Dittman, D., Awada, W., Napolitano, A.: An extensive comparison of feature ranking aggregation techniques in bioinformatics. In: *Information Reuse and Integration (IRI), 2012 IEEE 13th International Conference on*, pp. 377–384. IEEE (2012)

46. Zhang, D., Wang, Y.: A new ensemble feature selection and its application to pattern classification. *J. Control Theory Appl.* **7**(4), 419–426 (2009)
47. Zhao, Z., Liu, H.: Spectral feature selection for supervised and unsupervised learning. In: *Proceedings 24th International Conference on Machine Learning*, pp. 1151–1157 (2007)