Feature construction based on class outliers

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Report CW 648, November 2013

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Abstract

Data for training a classification model can be considered to consist of two types of points: easy to classify ones typical for a class and difficult to classify ones atypical for a class and often lying on class boundaries. Most existing techniques deal with atypical points in later stages of model building, after typical points have been modeled. This means that atypical points are often modeled only if doing so results in an improvement in comparison to the model of typical points. An alternative way of viewing atypical points is as outliers w.r.t. the class to which they supposedly belong. Based on this realization, we introduce the concept of class outliers, whose immediate neighborhoods we use to construct discriminative features. We investigate ways of employing the newly derived features and compare the quality of resulting models with results on un-augmented data for a variety of UCI benchmarks sets. We find that while some overfitting control can be necessary, the newly derived features improve the classification accuracy of SVM, Naive Bayes, and C4.5 classifiers.

CR Subject Classification : I.2, H.2.8

Feature Construction based on Class Outliers

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Abstract. Data for training a classification model can be considered to consist of two types of points: easy to classify ones – *typical* for a class – and difficult to classify ones – *atypical* for a class and often lying on class boundaries. Most existing techniques deal with atypical points in later stages of model building, after typical points have been modeled. This means that atypical points are often modeled *only* if doing so results in an improvement in comparison to the model of typical points. An alternative way of viewing atypical points is as *outliers* w.r.t. the class to which they supposedly belong. Based on this realization, we introduce the concept of class outliers, whose immediate neighborhoods we use to construct discriminative features. We investigate ways of employing the newly derived features and compare the quality of resulting models with results on un-augmented data for a variety of UCI benchmarks sets.
We find that while some overfitting control can be necessary, the newly derived features improve the classification accuracy of SVM, Naive Bayes, and C4.5 classifiers.
Keywords: feature construction, classification, outlier detection

1 Introduction

Supervised learning, the other contender being clustering, is arguably the oldest sub-discipline of machine learning. Especially in real-life data one can often consider a class to consist of two types of instances. There are typical ones, i.e. representatives of the generating process, that are easy to classify since they make up the majority of a class which allows for good generalization. On the other hand there can be atypical instances, a minority that is structurally dissimilar to the majority of the class and often prove more difficult to classify. The latter is especially then the case if these atypical instances occupy similar regions as, i.e. are similar to, instances from other classes.

The problem is well-known and has for instance been used to characterize data sets' learnability [9, 12] or make analytic statements about learners' ability to generalize from data. Additionally, all successful learning paradigms have a mechanism for addressing this problem, whether by first learning the majority model and modeling atypical instances if need be [4, 10, 11] or by using atypical instances to delineate class boundaries, modeling typical instances along the way [5].

A different way of describing atypical instances is as *outliers* within their assigned class. Clustering, the "other" well-established sub-field of machine learning, has had need to address outliers that cannot be assigned to any clusters easily, eventually giving rise to *outlier detection* [2]. It seems therefore plausible to employ outlier detection for identifying atypical instances and it is surprising how little attention has been given to *exploiting* the aforementioned structural differences among instances of the same class. A notable exception is [13] which used clustering to partition classes into clearly delineated sub-classes. Clustering is concerned with uncovering the underlying structure of a data set, an aspect that Vilalta *et al.*'s work exploited to create classes that are easier to model.

Our contribution is two-fold:

1. Based on this observation, we propose the concept of *class outliers*, i.e. instances of a given class that do not belong to any cluster within this class.
2. By mining discriminative patterns from the neighborhoods of such outliers we can construct features that add additional dimensions to the description of the data and improve class separation and hence learnability and classification accuracy, as show experimentally

The paper is structured as follows: in the next section we introduce our notion of class outliers and discuss how to leverage them for feature generation. In Section 3, we discuss existing techniques that address atypical instances to place our approach in context. In Section 4 we evaluate our framework experimentally on a variety of UCI data sets, discussing resulting classification accuracies in detail, before we conclude.

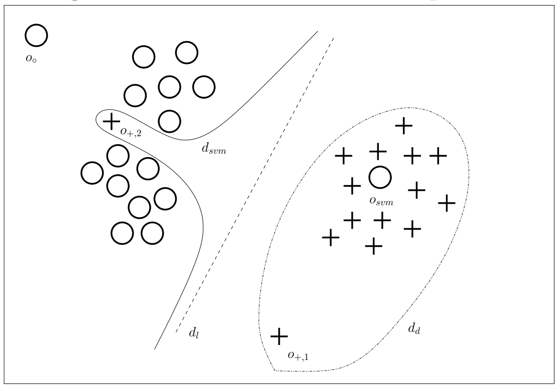
2 Problem Setting and Proposed Solution

As a motivation of the problem addressed in our work, consider Figure 1. Both classes are characterized by large clusters of typical instances, as well as several outlying points. There can be different reasons for such a distribution: the training set could, e.g., *not* be a representative sample – this could be an explanation for $o_\circ$ or o_{+_1}. An instance like o_{+_2}, however, either is mis-labeled or has incorrect attribute values (in other words, it is noise), or indicates that the description space does not allow to represent the underlying concepts correctly.

If the latter is the case, there are decision surfaces induced by the clusters of typical instances that will be unable to classify outlying instances correctly, i.e. in the case of surfaces denoted by d_l and d_d. While a decision surface such as d_{svm} would be capable of classifying the outliers mentioned so far, o_{svm} would even defeat a learner capable of inducing a decision surface such as this one. From a pattern miner's perspective a solution to this problem seems straight-forward:

1. Identify atypical points.
2. Identify their nearest neighbors (belonging to (a) different classe(s)).
3. Use a pattern miner to find patterns discriminating among instances of different classes in this neighborhood.

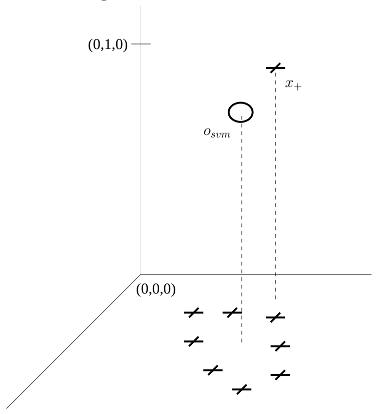
Fig. 1. Class outliers in a two-class problem



4. Enrich the data with those patterns, using them as binary features.

If o_{svm} and surrounding instances were enriched by an additional feature that has e.g. value 1 for o_{svm} as opposed to 0 for its neighborhood (see Figure 2), correct modeling would become possible. Such a feature cannot be expected to be found *globally*, since this would correspond to a (simple) decision surface. In fact, already outside the immediate neighborhood it might not be enough to discriminate between classes, as is the case for x_+, so that additional model induction by a learner is necessary.

Fig. 2. Enriching data with an additional feature



In this study, we work in the usual space of data described by a vector of attribute values: given a set of attributes $\mathcal{A} = \{A_1, \ldots, A_d\}$, having domains $dom(A_i)$, each instance d is a tuple $(\boldsymbol{x}, y)$ with $\boldsymbol{x} = \langle x_1, \ldots, x_d \rangle, x_i \in dom(A_i)$, $y \in dom(C) = \{c_1, \ldots, c_m\}$ a class label. A set of data is denoted by $\mathcal{D} =$

$\{d_1, \ldots, d_n\}$ and each class within this data set by $\mathcal{D}_c = \{d = (\boldsymbol{x}, y) \mid y = c\}$. A natural choice for the kind of binary feature with which to enrich the data is the class of conjunctive patterns.[1]

Assuming an *outlier oracle* $OO(d, \mathcal{D}') \mapsto \{\text{true}, \text{false}\}$ that can decide whether a instance d is an outlier w.r.t. $\mathcal{D}'$, we can define the set of class outliers:

Definition 1 *Given a set of labeled data $\mathcal{D} = \{(\boldsymbol{x}, y)\}$, the set of outliers of class c in $\mathcal{D}$ is defined as $\mathcal{O}_{c,\mathcal{D}} = \{d \in \mathcal{D}_c \mid OO(d, \mathcal{D}_c) = true\}$. The union over all the outliers of all classes $\mathcal{O}_{C,\mathcal{D}} = \bigcup_c \mathcal{O}_{c,\mathcal{D}}$ is called the set of* class outliers.

For each instance d, we can define its *k-neighborhood*, i.e. the k instances in $\mathcal{D}$ that are closest to d:

Definition 2 *Given an instance d and a distance measure $\delta : \mathcal{D} \times \mathcal{D} \mapsto \mathbb{R}$, its k-*neighborhood *is defined as: $\mathcal{N}_k(d) = \{d' \in \mathcal{D} \setminus \{d\}$ s.t. $|\{d'' \mid \delta(d'', d) \leq \delta(d', d)\}| \leq k - 1\}$*

By assembling the k-neighborhoods of all class outliers in $\mathcal{D}$, we are selecting small subsets where local decision boundaries can be expected to occur. We furthermore assume a pattern miner $PM(\mathcal{D})$ capable of constructing *discriminative* patterns from a multi-class data set. Such a pattern miner can take the form of a class-association rule miner but also a regular learner for classification rules or a decision tree learner. Using it we construct patterns from the respective $\mathcal{N}_k(o)$, e.g. the left-hand sides of predictive rules, which we can then use to enrich the data. A high-level algorithm summarizing the steps involved in our feature construction approach is given as Algorithm 1.

If all instances in a k-neighborhood belong to the same class as the outlier itself, the outlier that gave rise to it was atypical but not hard to classify, and we therefore ignore the subset for the purpose of feature construction (line 9). Furthermore, it is possible that the k-neighborhood of a class outlier includes one (or several) other class outlier(s). Since using these subsets separately would probably give rise to a number of redundant features, we instead merge any pair of k-neighborhoods of class outliers whose intersection includes at least 50% of the instances of the smaller neighborhood (lines 12/13). Note, that this is a transitive relationship. Once all such neighborhoods have been identified, we can use the pattern miner to derive features for augmenting the data.

This augmentation takes the form that we add one binary attribute per pattern to each instance, with the value 1 if the pattern matches the instance and the value 0 if it does not.

[1] While we limit ourselves to the space of attribute-valued data herein, this is w.l.o.g. Any instance space in which a distance measure between instances is defined allows for the identification of outliers, as well as each instance space that allows for pattern mining operations allows to derive features from these outliers.

Algorithm 1 High-level algorithm for class outlier-based feature construction

```
 1: Given: data set $\mathcal{D}$, set of class labels $C$
 2: Return: set of discriminative patterns $\mathbb{F}$
 3:
 4: $\mathcal{O}_{C,\mathcal{D}} = \emptyset$
 5: **for** $c \in C$ **do**
 6:     $\mathcal{O}_{C,\mathcal{D}} = \mathcal{O}_{C,\mathcal{D}} \cup \mathcal{O}_{c,\mathcal{D}}$
 7: $\mathbb{N} = \emptyset$
 8: **for** $o \in \mathcal{O}_{C,\mathcal{D}}$ **do**
 9:     **if** $\exists d_i = (\boldsymbol{x}_i, y_i), d_j = (\boldsymbol{x}_j, y_j) \in \mathcal{N}_k(o) : y_i \neq y_j$ **then**
10:         $\mathbb{N} = \mathbb{N} \cup \{\mathcal{N}_k(o)\}$
11: **while** $\exists \mathcal{N}_k(o), \mathcal{N}_k(o') \in \mathbb{N} : (o \in \mathcal{N}_k(o') \vee o' \in \mathcal{N}_k(o)) \wedge \frac{|\mathcal{N}_k(o') \cap \mathcal{N}_k(o)|}{\min\{|\mathcal{N}_k(o')|, |\mathcal{N}_k(o)|\}} \geq 0.5$
    **do**
12:     $\mathcal{N}_k(o') = \mathcal{N}_k(o') \cup \mathcal{N}_k(o)$
13: **for** $\mathcal{N}_k(o) \in \mathbb{N}$ **do**
14:     $\mathbb{F} = \mathbb{F} \cup \{\mathrm{PM}(\mathcal{N}_k(o))\}$
15: **return** $\mathbb{F}$
```

3 Related Work

The problem of atypical instances has of course been identified early on in classification learning and some way of dealing with it is included in most learning techniques.

Decision trees [10], are induced in such a manner that subsets with low class-entropy are split off while deepening the tree, ideally ones that have high cardinality. Deeper nodes in the tree then consist of hard-to-separate, i.e. atypical, instances of which smaller subsets are split off. In the case of *sequential rule learning* [4], on the other hand, this is achieved by sequential covering techniques that typically learn rules of high accuracy early on, remove the covered instances, which are typical of one of the classes, until only data from boundary regions remains for which then rules are learned that often have lower accuracy. Rule learning can also be employed in a second mode, in which rules do not form a sequential list derived by sequential covering, but an unordered set. For unseen instances, all rules are selected that match the instances and called upon to make a decision. For atypical instances, this can lead to conflicting predictions which are then integrated using a voting mechanism. The authors of [8] go beyond this by collecting all instances covered by conflicting rules, i.e. atypical instances, and reinducing classification rules on this subset. *Boosting* [11] also follows a strategy of modeling typical instances first. After inducing a first model, misclassified instances are given larger weight for the next modeling step. Depending on the choice of weak learner, this can lead to modeling of typical instances from different classes in turn, before atypical instances are modeled.

All those techniques work by modeling typical instances first and then modeling atypical instances in the context of these prior models. Therefore, partial models for typical instances may include some misclassified atypical instances whose error is marginalized by the correct prediction on the typical ones. Additionally, attempts to avoid over-fitting can lead to pruning of the rules and tests referring to atypical instances, losing the ability to classify them correctly. Our proposed approach instead treats atypical instances first and augments typical instances in terms of found patterns.

In contrast, *Support Vector Machines* (SVM) [5] in a sense focus on atypical instances: in SVM learning, a separating hyperplane between two classes is found that maximizes the distance to the closest instances (support vectors) of each class. Support vectors, lying on class boundaries, may be atypical instances that, if modeled correctly, enable the classification of typical ones. Since the separating hyperplane is constructed globally, however, atypical points have to be accommodated *globally* as well, potentially leading to rather complex hyperplanes, e.g. for $o_{+,2}$ in Figure 1. To control over-fitting, the complexity of the hyperplane is typically traded off against the errors committed in classification, meaning that modeling of atypical instances may be sacrificed again if enough typical ones are modeled correctly. Contrary to this, our proposed approach treats atypical instances in a local context, reducing the strain on the global model.

Additionally, there are k-NN classifiers [6] and related techniques such as *locally weighted regression* [3] that use the k-neighborhood of an instance for classification. An obvious difference to our approach lies in that k-nearest neighbor techniques use the neighborhood to assign a label to the instance, therefore potentially exacerbating the situation in the case of class outliers, while we use it to construct discriminating features.

There have been works characterizing the difficulty of learning problems in terms of direct neighbors in the description space having differing class labels, via class variation [9]. Since the original definition of class variation was limited to binary vectors and neighbors that differ in at most one attribute value, it was generalized in [12] to a distance-based notion that compares the class labels of instances within a certain *radius* around a given instance. Both of these works, however, do not attempt to *exploit* knowledge about neighbors with differing class labels to aid classification. Such a step was taken in [13], in which clustering is used to explain Naïve Bayes well-known good performance, and to partition classes with difficult structure into subclusters to improve classification accuracy.

Generally speaking, the treatment of atypical instances has been somewhat different in the context of *clustering* and *outlier detection*. In clustering, instances that do not fit any of the formed clusters are often removed from the data with the goal of producing well-described clusters. Those *outliers* are usually either considered noise or to form their own (minority) clusters. Outlier detection, e.g. [2], finally, assumes that outliers are abnormalities that carry important information and treats them not as an unwanted side-product but as the main target of data mining.

4 Experimental Setup

We expect the class outlier-derived features to help improve the modeling of classification problems and therefore the estimated classification accuracy. To evaluate classification performance, we perform a ten-fold cross-validation on a number of UCI data sets [1]. We aimed at data sets of different dimensionality, different size, and different distribution and number of classes to allow us to evaluate the behavior of class outlier detection and the effects of derived features thoroughly.[2] For each fold, class outliers and their k-neighborhoods are extracted from the combined training folds, and conjunctive patterns mined on these subsets. As learners we used the SVM implementation contained in the WEKA workbench [7], as well as the J48 decision tree and the Naïve Bayes classifiers. As to the two components of our approach, the outlier oracle and the pattern miner:

- To identify class outliers, we use the LOF algorithm proposed in [2] in the version available for download by the authors as part of the ELKI package.[3]
- To mine conjunctive patterns, we use the C4.5 implementation of WEKA, with pruning turned off and minimum number of instances set to 1. We transform the resulting tree into conjunctive rules and use the left-hand side of these rules as features for augmentation.

4.1 Outlier Detection

LOF is a distance-based approach that calculates a *local outlier factor* (*lof*) by comparing the distance of an instance d to points in its k-neighborhood to the average distance of points within $\mathcal{N}_k(d)$. The local outlier factor is therefore strongly dependent on k: $lof_k(d)$ (and the data set on which it is derived, omitted from the notation). In combination with a threshold l_{min}, the outlier oracle takes the form: $OO(d, \mathcal{D}_c) := lof_k(d) \geq l_{min}$

We chose *Euclidean* distance for data with numerical attributes and *Manhattan* distance for nominally valued data. To use the Manhattan distance, nominal attributes were binarized into a number of binary-valued attributes.

The decision on the size of the k-neighborhood is not straight-forward. To get a reliable estimate, the authors of LOF recommend to calculate a number of *lof* over an interval $[k_{min}, k_{max}]$. An additional recommendation is to set $k \geq 10$ to remove statistical fluctuations. Since this is not always possible, especially for small classes, we instead based our choice of the minimum k-value on the following considerations:

- We assume that the minimum size k-neighborhood for a point can be 10% of the class.
- If these 10% are larger than ten, we follow the advice of the authors of LOF and set k_{min} to ten.
- The minimum number of k needed to derive a meaningful outlier is two, so this is set as a hard minimum and if a class does not support a 2-neighborhood for a given point, no outlier calculation is performed.

[2] We do not list their characteristics since those can be accessed at the UCI repository.
[3] At: `http://www.dbs.ifi.lmu.de/research/KDD/ELKI/`

To summarize: $k_{min}(\mathcal{D}_c) = \max\{2, \min\{10, \frac{|\mathcal{D}_c|}{10}\}\}$. Second, the authors of [2] state that maximum k should be "...the maximum number of 'close' by objects that can potentially be local outliers." We use the following heuristics for selecting a maximum k:

– At most 50% of the class can be local outliers since otherwise the concept of a distinct "class" becomes questionable.
– To facilitate termination, we initially limit k_{max} to twenty.
– It turns out, however, that for $k = 20$ occasionally points receive an outlier factor of "NaN" or ∞. We therefore increment k_{max} until there is at least one numeric *lof* value for each point of a class.

Thus: $k_{max}(\mathcal{D}_c) = \max\{\{k \text{ s.t. } \forall d \in \mathcal{D}_c : lof_k(d) \in \mathrm{R}\}, \min\{20, \frac{|\mathcal{D}_c|}{2}\}\}$. Table 1 gives an impression of the range of k-values for different data sets and classes. It reports all $[k_{min}, k_{max}]$ intervals used for different classes of a data set, annotated with the number of classes for which this interval was used. The table shows that many classes are not large enough to allow for 10 instances involved in the *lof*-calculation but also that 20 is often a sufficiently large k_{max}-value to derive a *lof*-value for all instances of a class.

This procedure gives rise to a set of local outlier factors for each point and the question remains how to interpret those. Generally speaking, a local outlier factor larger than 1 indicates an outlier. According to [2], the best way to decide whether a point is in fact an outlier consists of taking the *maximum lof* value over the entire range of k. The rationale for this is that using the *average* outlier factor might lead to its being an outlier being overridden by the effects of having another local outlier in the neighborhood.

As illustration, consider Figure 3. In the case of $k = 2$, the two neighbors of the instance in question are much easier to reach, and the instance is assigned a high *lof*. If k is increased to 3, however, the third neighbor is a local outlier itself, harder to reach and therefore makes the instance in question appear more "normal". Using the maximum outlier factor and a threshold of 1 to decide on whether instances are outliers leads to an excessive amount of instances per class tagged as outliers, as Figure 4 shows. The values reported are the weighted average over all classes, i.e. each class' contribution to the overall average value is weighted by its proportional size.

In fact, even using the average outlier factor and threshold 1, i.e. using an oracle of the form:

$$OO_{avg}(d, \mathcal{D}_c) := \frac{\sum_{k=k_{min}(\mathcal{D}_c)}^{k_{max}(\mathcal{D}_c)} lof_k(d)}{k_{max}(\mathcal{D}_c) - k_{min}(\mathcal{D}_c)} > 1,$$

leads to more than half of all instances being tagged as outliers (cf. Figure 4). Clearly, using a threshold of 1 to identify class outliers is overly strict. In reaction to this, we evaluated a number of different thresholds in the range $[1, 3]$ with increments of 0.0625. Thresholds and selection methods have been chosen for each class separately since differing underlying distributions can lead to differing outlier behavior. The goal was to find the largest set of outliers that

Table 1. Overview of minimum/maximum k-values

Data set	$[k_{min}(\mathcal{D}_c), k_{max}(\mathcal{D}_c)]$ intervals (number of classes with these values)
BUPA Liver Disorders	$[10, 20]$ (2)
Ecoli Protein Localization	$[2, 2]$ (3), $[2, 9]$ (1), $[3, 16]$ (1), $[4, 20]$ (1), $[6, 20]$ (1), $[10, 20]$ (1)
Glass Identification	$[2, 2]$ (1), $[2, 4]$ (1), $[2, 6]$ (1), $[2, 8]$ (1), $[2, 13]$ (1), $[6, 20]$ (2)
Heart Statlog-statlog	$[10, 20]$ (2)
Ionosphere	$[10, 20]$ (2)
Iris	$[4, 20]$ (3)
Letter Image Recognition	$[10, 20]$ (25), $[10, 24]$ (1)
opdigits	$[10, 20]$ (10)
Page Blocks	$[2, 13]$ (1), $[7, 20]$ (1), $[10, 20]$ (3)
Pendigits	$[10, 20]$ (10)
Pima Diabetes	$[10, 20]$ (2)
Segment	$[10, 20]$ (7)
Segnoise	$[10, 20]$ (7)
Sonar, Mines vs Rocks	$[8, 20]$ (1), $[9, 20]$ (1)
Spambase	$[10, 20]$ (1), $[10, 63]$ (1)
Spectrometer	$[2, 2]$ (27), $[2, 3]$ (1), $[2, 4]$ (4), $[2, 5]$ (1), $[2, 6]$ (1), $[2, 7]$ (1), $[2, 8]$ (1), $[2, 9]$ (3), $[2, 11]$ (1), $[2, 12]$ (2), $[2, 13]$ (1), $[2, 14]$ (1), $[3, 16]$ (1), $[3, 19]$ (1), $[4, 20]$ (2)
Vehicle	$[10, 20]$ (4)
Wisconsin Breast Cancer	$[10, 30]$ (1), $[10, 33]$ (1)
Audiology	$[2, 2]$ (16), $[2, 3]$ (1), $[2, 4]$ (2), $[2, 9]$ (1), $[2, 10]$ (2), $[4, 20]$ (1), $[5, 20]$ (1)
Breast Cancer	$[7, 20]$ (1), $[10, 20]$ (1)
Car Evaluation	$[5, 20]$ (1), $[6, 20]$ (1), $[10, 20]$ (2)
Chess (KP vs KP)	$[10, 20]$ (2)
Congressional Voting Records	$[10, 25]$ (1), $[10, 26]$ (1)
Dermatology	$[2, 9]$ (1), $[4, 20]$ (2), $[5, 20]$ (1), $[6, 20]$ (1), $[10, 20]$ (1)
Lung Cancer	$[2, 4]$ (2), $[2, 6]$ (1)
Lymphography	$[2, 2]$ (2), $[5, 20]$ (1), $[7, 20]$ (1)
Molecular Biology (Promoters)	$[4, 20]$ (2)
Molecular Biology (Splice-junction Gene Sequences)	$[10, 20]$ (3)
Nursery	$[2, 2]$ (1), $[10, 20]$ (4)
Postoperative Patient Data	$[2, 2]$ (1), $[2, 11]$ (1), $[5, 20]$ (1)
Primary Tumor	$[2, 2]$ (6), $[2, 3]$ (3), $[2, 4]$ (2), $[2, 6]$ (2), $[2, 7]$ (1), $[2, 9]$ (1), $[2, 11]$ (2), $[2, 13]$ (2), $[3, 18]$ (1), $[7, 20]$ (1)
Soybean	$[2, 4]$ (1), $[2, 6]$ (1), $[2, 7]$ (2), $[2, 9]$ (9), $[3, 20]$ (2), $[7, 20]$ (1), $[8, 20]$ (3)
Tic Tac Toe	$[10, 20]$ (2)

Fig. 3. Effects of increasing k/occurrence of max-value for small k

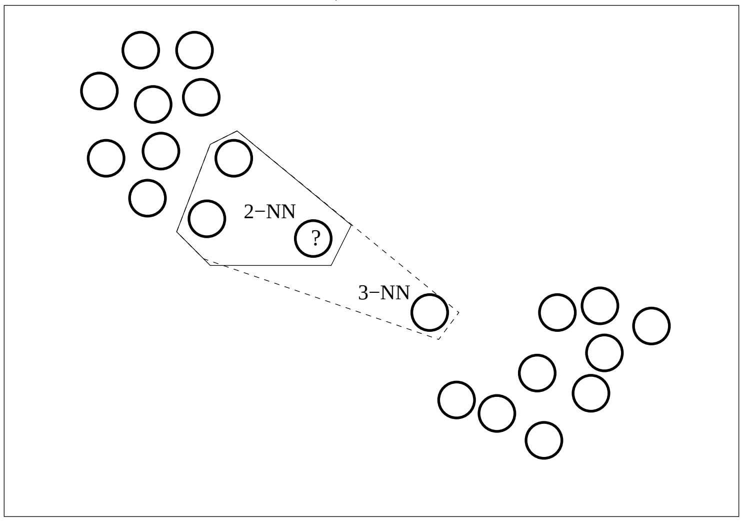
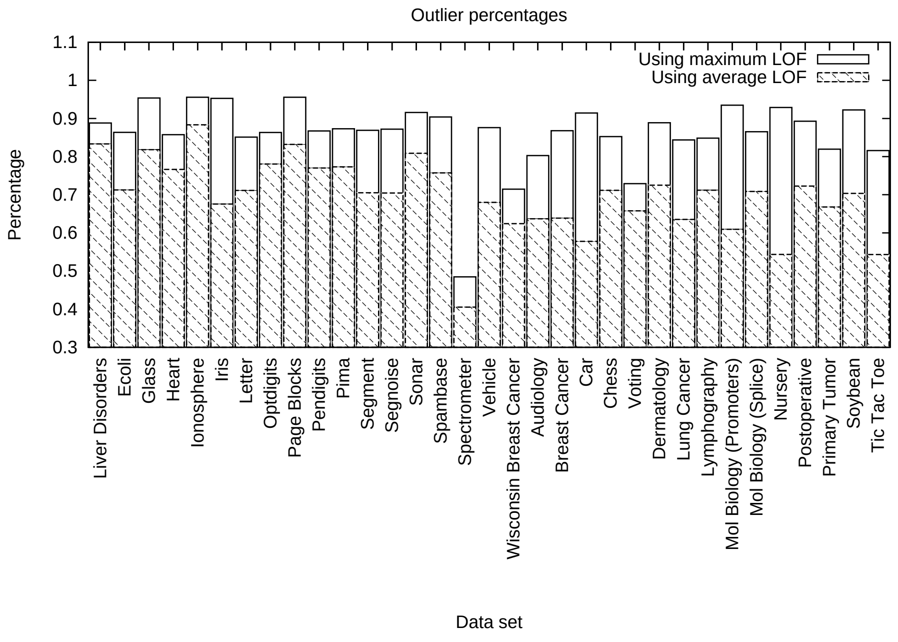


Fig. 4. Outlier percentages for OO_{max} and OO_{avg}, $l_{min} = 1$



did not exceed 10% of a class' instances. A summary of the chosen threshold-values and selection methods for different classes and data sets is given in Table 2. Averaging thresholds over different classes does not give a comprehensible picture so we chose the same presentation as in the case of $[k_{min}, k_{max}]$ intervals.

The results show that there is no one setting that can be applied to all classes in a data set, let alone across different data sets. Due to different underlying distributions instances whose *lof* would tag them as outliers in one class might be considered average instances in another class.

4.2 Feature Construction

Once the class outliers are identified, it is necessary to decide on the k parameter used to assemble each outliers' k-neighborhood. Given the results of selecting k-values for calculating the *lof*-score, we decided against setting a single k for all classes of a data set. Instead, we use the information about the selection method used to decide that an instance is an outlier for guidance:

– If o was tagged as an outlier using OO_{max}, we use the k for which $lof_k(o)$ is maximal
– If o was tagged as an outlier using OO_{avg}, we use the average over all k for which $lof_k(o) \in \mathbb{R}$

The important difference to the outlier detection step lies in the fact that during outlier detection k instances from the *same* class as o are used while for feature construction all classes are involved in selecting the k nearest neighbors.

We use the WEKA-implementation of C4.5 to derive the conjunctive patterns. Since the subsets are relatively small and not representative of the distribution of the entire data set, we do not perform any pruning of the resulting decision trees and set the minimum number of instances per leaf to 1. We do not attempt to address over-fitting in this step but instead rely on the learner's regularization mechanism.

When gathering the features derived from each subset into a complete feature set, it is possible that a single pattern might predict different classes, depending on the subset from which they were constructed. Since this indicates that these features lack the ability to discriminate classes, we remove them from the set.

4.3 Experimental Evaluation: Classification Accuracy

We chose the RBF kernel (with standard WEKA settings) for the SVM classifier and selected the C-parameter by internal five-fold cross-validation from the range $[1, 128]$, doubling the value in each step. The SVM-implementation contained in WEKA took more than 24 hours for a single fold of the *Letter* data set, leading us to remove it from the SVM's evaluation. J48 and Naïve Bayes were run using the standard settings predefined in WEKA. We show the resulting accuracies for the SVM in table 3, and the results for J48 and Naïve Bayes in 4. The tables always list both the training and testing accuracy for the original representation and

Table 2. Overview of threshold values and selection methods

Data set	Threshold values (# classes)	Methods (# classes)
BUPA Liver Disorders	1.5 (2)	OO_{avg} (1), OO_{max} (1)
Ecoli Protein Localization	1 (2), 1.5 (2), 1.75 (1), 1.875 (2), 2.5 (1)	OO_{avg} (1), OO_{max} (7)
Glass Identification	1 (3), 1.5 (1), 1.75 (1), 2.5 (2)	OO_{avg} (4), OO_{max} (3)
Heart Statlog-statlog	1.25 (1), 1.5 (1)	OO_{avg} (1), OO_{max} (1)
Ionosphere	1.75 (1), 2.25 (1)	OO_{avg} (2)
Iris	1.375 (2), 1.5 (1)	OO_{avg} (3)
Letter Image Recognition	1.125 (2), 1.25 (23), 1.375 (1)	OO_{avg} (3), OO_{max} (23)
Optdigits	1.125 (1), 1.25 (9)	OO_{avg} (1), OO_{max} (9)
Page Blocks	1 (2), 1.375 (1), 2.25 (1), 3 (1)	OO_{avg} (1), OO_{max} (4)
Pendigits	1.25 (8), 1.375 (2)	OO_{avg} (2), OO_{max} (8)
Pima Diabetes	1.375 (2)	OO_{avg} (2)
Segment	1.25 (4), 1.375 (1), 1.5 (1), 2.25 (1)	OO_{avg} (1), OO_{max} (6)
Segnoise	1.125 (2), 1.25 (2), 1.375 (1), 1.625 (1), 2.25 (1)	OO_{avg} (5), OO_{max} (2)
Sonar, Mines vs Rocks	1.25 (1), 1.375 (1)	OO_{max} (2)
Spambase	1.5 (1), 1.625 (1)	OO_{avg} (1), OO_{max} (1)
Spectrometer	1 (17), 1.0625 (4), 1.125 (2), 1.25 (5), 1.375 (5), 1.5 (4), 1.5625 (2), 1.625 (2), 1.75 (2), 1.875 (3), 2.5 (1), 3 (1)	OO_{avg} (7), OO_{max} (41)
Vehicle	1.125 (3), 1.25 (1)	OO_{avg} (2), OO_{max} (2)
Wisconsin Breast Cancer	1.25 (1), 1.875 (1)	OO_{avg} (1), OO_{max} (1)
Audiology	1 (15), 1.0625 (1), 1.125 (1), 1.375 (1), 1.625 (1), 1.75 (1), 1.875 (2), 2.25 (1), 3 (1)	OO_{avg} (3), OO_{max} (21)
Breast-Cancer	1.125 (1), 1.375 (1)	OO_{avg} (1), OO_{max} (1)
Car Evaluation	1.0625 (3), 1.5 (1)	OO_{avg} (3), OO_{max} (1)
Chess (KP vs KP)	1.375 (1), 1.5 (1)	OO_{max} (2)
Congressional Voting Records	1.75 (1), 2.5 (1)	OO_{avg} (1), OO_{max} (1)
Dermatology	1.25 (4), 1.375 (2)	OO_{avg} (3), OO_{max} (3)
Lung Cancer	1.0625 (1), 1.25 (2)	OO_{avg} (1), OO_{max} (2)
Lymphography	1 (1), 1.125 (2), 1.25 (1)	OO_{avg} (1), OO_{max} (3)
Molecular Biology (Promoters)	1.0625 (1), 1.125 (1)	OO_{max} (2)
Molecular Biology (Splice-junction Gene Sequences)	1.0625 (1), 1.125 (2)	OO_{max} (3)
Nursery	1 (1), 1.0625 (2), 1.25 (2)	OO_{avg} (2), OO_{max} (3)
Postoperative Patient Data	1 (1), 1.625 (1), 1.75 (1)	OO_{max} (3)
Primary Tumor	1 (7), 1.125 (1), 1.25 (1), 1.375 (3), 1.5 (1), 1.5625 (1), 1.625 (1), 1.75 (2), 2 (1), 2.5 (2), 3 (2)	OO_{avg} (6), OO_{max} (16)
Soybean	1 (1), 1.125 (1), 1.25 (3), 1.375 (5), 1.5 (3), 1.5625 (2), 1.75 (2), 2 (1), 2.25 (1)	OO_{avg} (5), OO_{max} (14)
Tic Tac Toe	1.0625 (2)	OO_{avg} (2)

the representation augmented by the mined features. The number in parentheses behind the training accuracy for enriched data shows on how many folds features were mined at all, "N/A" denotes that no features could be mined. The table with the SVM results in addition lists the average C value used. This parameter trades off training accuracy against model complexity, with higher C denoting a larger penalty for misclassification, leading to more complex models. If our assumptions about the effect of enriching data with additional discriminative features are correct, C should be lower for enriched data.

Data set	Train_{orig}	Test_{orig}	C_{orig}	Train_{enr}	Test_{enr}	C_{enr}
breast-w	97.0752	96.2836	30.4000	98.6172 (10)	**96.5714**	34.5000
iris	97.1852	96.0000	80.0000	N/A	N/A	
segment	93.8384	93.5931	128.0000	99.2352 (10)	**97.0563**	92.8000
diabetes	77.7781	77.2283	86.4000	*81.3810* (10)	75.5263	11.3000
segnoise	99.8815	87.5333	80.0000	99.8519 (10)	**94.7333**	3.6000
ecoli	88.7235	87.5045	128.0000	*88.3601* (10)	83.3244	83.2000
liver-disorders	61.8050	59.7143	121.6000	76.0697 (10)	**63.5462**	64.8000
sonar	88.5701	80.7857	52.8000	*91.0798* (10)	79.3095	68.8000
glass	64.1186	60.3896	96.0000	88.0505 (10)	**66.4502**	100.8000
optdigits	99.5215	98.6299	52.8000	*99.8418* (10)	98.3452	32.0000
spambase	91.8810	91.5889	128.0000	98.0801 (10)	**94.7622**	31.6000
heart-statlog	85.4321	83.7037	34.9000	*88.9301* (10)	83.7037	16.6000
page-blocks	94.1633	93.9703	128.0000	98.7859 (10)	**96.8939**	43.2000
spectrometer	78.4473	53.4731	128.0000	*83.7445* (10)	41.8204	28.8000
ionosphere	95.1881	92.5873	100.8000	*95.3573* (9)	90.8289	73.6000
pendigits	99.2024	98.9811	128.0000	*99.9252* (10)	98.9811	80.0000
vehicle	78.9990	76.2297	128.0000	*92.2906* (10)	74.3375	94.4000
audiology	98.3780	79.6047	35.2000	*99.2618* (10)	79.1304	28.8000
mol. biology (promoters)	99.8947	91.3636	1.3000	100.0000 (1)	**100.0000**	0.4000
breast-cancer	80.3380	72.0443	51.6000	82.4002 (10)	**73.8054**	9.8000
nursery	99.9520	99.9228	128.0000	99.9991 (10)	**99.9846**	12.8000
car	99.2220	98.0901	128.0000	99.7621 (10)	**99.0748**	76.8000
post. patient	71.1111	71.1111	1.0000	71.1111 (10)	71.1111	1.0000
primary-tumor	62.0458	48.3868	36.8000	*62.7631* (10)	46.3458	8.4000
dermatology	99.0892	97.0045	4.0000	98.8768 (10)	**97.8228**	1.9000
soybean	96.2581	93.7042	12.8000	97.2342 (10)	**94.1432**	12.0000
kr-vs-kp	99.3186	98.9361	128.0000	99.6480 (8)	**99.4139**	96.0000
splice	98.9202	96.1755	1.7000	*99.3069* (10)	96.1442	2.0000
lung-cancer	89.4827	33.3333	6.9000	N/A	N/A	
tic-tac-toe	98.3299	98.3333	8.0000	99.3969 (10)	**98.5406**	62.4000
lymph	91.3646	81.8571	7.0000	96.0941 (10)	**82.4286**	50.9000
vote	96.3731	95.6342	29.2000	*96.9090* (10)	95.6343	15.5000

Table 3. Train and test accuracies for original and enriched data representation for SVM. **Bold** values denote better **test** accuracy on the enriched data, *italics* denotes better *train* accuracy on enriched data while test accuracy stays the same or is worse.

It can be seen that all learners profit from the new representation on a number of data sets (denoted in **bold**), sometimes dramatically so, as in the case of *Segnoise* for the SVM, *Molecular Biology (Promoters)* for J48, or *Glass* and *Vehicle* for Naïve Bayes. We can also see that on the majority of data sets, C decreases for the enriched representation, indicating that decision surfaces become easier to model for the SVM. On the other hand, there are a number of data sets where the test accuracy does not change or even becomes worse, while the training accuracy on the enriched representation increases (denoted in *italics*). This strongly implies overfitting effects.

	J48				Naïve Bayes			
Data set	Train_{orig}	Test_{orig}	Train_{enr}	Test_{enr}	Train_{orig}	Test_{orig}	Train_{enr}	Test_{enr}
breast-w	97.8541	94.2836	97.9018 (10)	**96.1429**	96.0420	95.9979	96.7891	**96.7143**
iris	98.0000	94.0000	N/A	N/A	95.8519	96.0000	N/A	N/A
segment	99.1390	96.5368	98.9033 (10)	**96.6667**	80.4858	80.1732	89.5046	**88.7446**
diabetes	83.4050	73.5732	*90.4947* (10)	72.6572	76.2733	76.1842	74.5659	72.1514
letter	96.2039	88.1900	*97.0444* (10)	87.3650	64.5639	64.0900	72.7344	**71.8450**
segnoise	99.0222	94.8667	98.4815 (10)	93.1333	81.8815	80.8667	90.6963	**89.6667**
ecoli	93.0889	81.8360	91.5004 (10)	80.3565	88.3265	85.4278	86.4420	84.5276
liver-disorders	85.5741	64.9328	*89.7601* (10)	64.3025	56.8778	53.3361	67.9570	**57.7059**
sonar	98.1306	71.1667	97.2767 (10)	70.6667	72.2764	67.8334	73.1830	**68.3095**
glass	93.0961	66.8831	92.1602 (10)	**69.2208**	54.7736	47.3593	69.0045	**59.3723**
optdigits	98.0032	90.3915	97.7778 (10)	**90.8897**	91.8189	91.2990	92.1313	**91.9395**
spambase	97.1987	92.4585	97.1093 (10)	**93.1322**	79.7001	79.6783	88.1137	**88.0027**
heart-statlog	92.7161	76.2963	92.0988 (10)	**79.2593**	85.7613	83.7037	*86.7901*	83.7037
page-blocks	98.5850	97.0219	*98.6276* (10)	96.8756	90.3100	90.2795	91.6580	**91.6317**
spectrometer	90.5630	48.9623	88.5123 (10)	43.8854	62.0842	42.7358	*66.1433*	42.3585
ionosphere	98.4173	90.0238	97.8899 (9)	88.6155	83.5709	82.6270	86.7043	**84.4973**
pendigits	99.2581	96.3701	99.0245 (10)	95.9789	85.8645	85.7168	85.8887	**85.7441**
vehicle	91.5293	74.5966	*94.1951* (10)	73.0504	46.9265	45.2675	64.9719	**62.8852**
audiology	90.0679	77.4111	*91.1004* (10)	76.0277	78.5637	71.6601	78.8093	**72.0356**
mol. biology (prom.)	95.5965	78.3636	95.7895 (1)	**90.9091**	98.9507	91.4545	98.9474	**100.0000**
breast-cancer	76.4582	75.9113	*82.1692* (10)	73.4360	75.5239	72.3645	75.9523	**73.0542**
nursery	98.1490	97.2453	99.5122 (10)	**98.2099**	90.3678	90.3087	93.8674	**93.6960**
car	96.1355	92.3615	97.9810 (10)	**94.0392**	86.9856	85.2987	90.0592	**88.5415**
post. patient	71.3580	68.8889	*71.7284* (10)	68.8889	74.3210	68.8889	73.9506	64.4445
primary-tumor	60.6683	39.5544	65.1912 (10)	**40.7130**	56.6375	50.1604	50.8036	41.6132
dermatology	97.8750	94.5345	97.6018 (10)	92.8979	98.9981	98.3709	*99.3017*	98.3709
soybean	96.0144	92.5362	*96.3885* (10)	91.3747	93.5904	92.8261	92.8418	90.3410
kr-vs-kp	99.6454	99.4685	99.5872 (8)	**99.5311**	88.2075	87.6406	79.4882	79.9353
splice	96.2696	94.3573	*97.2379* (10)	94.0439	95.8899	95.3919	94.9878	94.7649
lung-cancer	86.4655	50.0000	N/A	N/A	88.5222	51.6667	N/A	N/A
tic-tac-toe	93.7020	84.9715	96.3001 (10)	**91.4364**	70.6332	69.8278	75.1797	**74.6327**
lymph	90.6913	78.3333	*91.5155* (10)	77.0000	88.4390	83.9047	88.1399	83.0476
vote	97.1904	96.5592	*97.2670* (10)	96.3266	90.3192	89.8731	93.7172	**92.4102**

Table 4. Train and test accuracies for original and enriched data representation for J48 and Naïve Bayes. **Bold** values denote better **test** accuracy on the enriched data, *italics* denotes better *train* accuracy on enriched data while test accuracy stays the same or is worse.

Overfitting control by minimum support As a straightforward way of controlling spurious features, we therefore evaluate the effect of removing spurious features by requiring a minimum support of each pattern that is used as a feature. Tables 5, 6, and 7 show the resulting accuracies when a minimum support of 2, 3, 4, 5, or 6 instances is required. The number in parentheses again denotes the number of folds on which features remain.

Data set	Test$_{orig}$	Test$_{\sigma=2}$	Test$_{\sigma=3}$	Test$_{\sigma=4}$	Test$_{\sigma=5}$	Test$_{\sigma=6}$
diabetes	**77.2283** (10)	75.5263 (10)	75.2615 (10)	74.2174 (10)	75.5281 (10)	75.6545 (10)
ecoli	**87.5045** (10)	83.0303 (10)	85.4011 (10)	84.1157 (9)	84.1355 (9)	83.4819 (9)
sonar	**80.7857** (10)	76.5000 (10)	76.9286 (10)	75.9762 (10)	75.9524 (9)	75.4233 (9)
optdigits	98.6299 (10)	98.5943 (10)	98.5409 (10)	98.5053 (10)	98.5409 (10)	**98.6477** (10)
heart-statlog	83.7037 (10)	84.8148 (10)	84.4445 (10)	**85.1852** (10)	84.4445 (10)	83.3333 (10)
spectrometer	**53.4731** (10)	43.8854 (10)	47.4458 (10)	51.4081 (10)	52.3515 (10)	52.9071 (10)
ionosphere	92.5873 (10)	91.1464 (9)	91.1464 (9)	91.1464 (9)	91.0204 (7)	**92.8572** (6)
pendigits	98.9811 (10)	98.9993 (10)	98.9720 (10)	99.0266 (10)	99.0539 (10)	**99.0630** (10)
vehicle	**76.2297** (10)	74.5630 (10)	76.0994 (10)	74.6849 (10)	75.3963 (10)	74.8039 (10)
audiology	**79.6047** (10)	78.6957 (10)	79.1502 (10)	79.1502 (10)	79.1502 (10)	79.5850 (10)
post. patient	71.1111 (10)	71.6050 (9)	71.6050 (9)	72.2223 (8)	77.7778 (1)	**77.7778** (1)
primary-tumor	48.3868 (10)	48.7077 (10)	48.9840 (10)	48.4046 (10)	48.1105 (10)	**51.7528** (6)
splice	96.1755 (10)	96.0815 (10)	96.0502 (10)	96.0502 (10)	96.0188 (10)	**96.2069** (10)
vote	95.6342 (10)	95.4017 (10)	95.8615 (10)	**95.8668** (10)	**95.8668** (10)	**95.8668** (10)

Table 5. Test accuracies of the SVM for original data representation, and enriched data under different minimum support constraints.

This attempt at overfitting control does not much to improve J48's results. When inspecting J48's models, we find that the newly constructed features are often the ones considered most important by the learner. This, taken together with the fact that J48 profited less from the fully enriched data representation than the SVM and Naïve Bayes did, implies that moving the modeling of atypical instances from the bottom to the top of a decision tree is not an effective strategy.

Data set	Test$_{orig}$	Test$_{\sigma=2}$	Test$_{\sigma=3}$	Test$_{\sigma=4}$	Test$_{\sigma=5}$	Test$_{\sigma=6}$
diabetes	73.5732 (10)	**74.7454** (10)	71.3517 (10)	**74.7454** (10)	73.3100 (10)	72.3958 (10)
letter	**88.1900** (10)	87.1900 (10)	87.1550 (10)	87.1300 (10)	86.9900 (10)	86.9000 (10)
segnoise	**94.8667** (10)	92.7333 (10)	92.7333 (10)	93.4667 (10)	94.0000 (10)	94.2000 (10)
ecoli	**81.8360** (10)	81.5508 (10)	81.5597 (10)	81.1943 (9)	80.8477 (9)	80.5209 (9)
liver-disorders	**64.9328** (10)	62.8992 (10)	64.6639 (10)	62.6135 (10)	61.4790 (10)	61.7479 (10)
sonar	**71.1667** (10)	68.7619 (10)	69.2381 (10)	69.2381 (10)	68.9947 (9)	68.9947 (9)
page-blocks	**97.0219** (10)	96.8755 (10)	96.9304 (10)	96.7113 (10)	96.9305 (10)	96.8026 (10)
spectrometer	48.9623 (10)	48.9762 (10)	**49.3466** (10)	48.5884 (10)	47.6485 (10)	47.0859 (10)
ionosphere	90.0238 (10)	88.6155 (9)	88.6155 (9)	89.2504 (9)	89.7959 (7)	**90.4762** (6)
vehicle	**74.5966** (10)	71.5098 (10)	72.6877 (10)	75.5308 (10)	73.9930 (10)	72.9286 (10)
audiology	77.4111 (10)	76.5020 (10)	76.5020 (10)	77.4111 (10)	**78.2806** (10)	**78.2806** (10)
breast-cancer	**75.9113** (10)	74.4828 (10)	73.8177 (10)	74.5197 (10)	72.7586 (10)	72.7832 (9)
post. patient	68.8889 (10)	69.1358 (9)	69.1358 (9)	72.2223 (8)	77.7778 (1)	**77.7778** (1)
dermatology	**94.5345** (10)	92.6201 (10)	92.0796 (10)	92.3574 (10)	93.1682 (10)	93.1682 (10)
soybean	**92.5362** (10)	90.1982 (10)	90.4881 (10)	91.0742 (10)	91.3640 (10)	91.0699 (10)
splice	94.3573 (10)	94.4201 (10)	94.8276 (10)	94.7022 (10)	**94.7335** (10)	94.2320 (10)
lymph	**78.3333** (10)	77.0000 (10)	77.0000 (10)	77.0000 (10)	74.9524 (10)	75.6191 (10)
vote	96.5592 (10)	**97.0137** (10)	96.7812 (10)	**97.0137** (10)	**97.0137** (10)	**97.0137** (10)

Table 6. Test accuracies of J48 for original data representation, and enriched data under different minimum support constraints.

The situation is quite different for Naïve Bayes: once overfitting control comes into play, there remain only *five* data sets (out of 33) on which no improvement over the original representation can be observed. The newly constructed features combine already existing attributes, as locally indicated by the class labels. This lessens Naïve Bayes' strong bias concerning the conditional independence of attributes by including relationships existing in the data. Unfortunately, there is no clear trend regarding which minimum support constraints are most effective.

The SVM, finally, also profits from overfitting control and in the case of this learner, removing features that cover only a few instances is clearly the right approach. It is noticeable that there are several data sets on which our approach does not work without overfitting control, no matter the learner (diabetes, ecoli, spectrometer, postoperative patient data, splice). There is however no common thread to these data sets, neither in size, dimensionality, nor number of classes.

5 Summary and Conclusions

Based on the observation that hard to classify instances in a classification setting can be considered *atypical*, we proposed using outlier detection techniques for identifying instances that are outliers w.r.t. the class they are labeled with. By constructing discriminative patterns from the k-neighborhoods of such *class outliers*, we derived features that aid in modeling atypical instances and therefore improve classification accuracy.

Data set	Test_{orig}	$\text{Test}_{\sigma=2}$	$\text{Test}_{\sigma=3}$	$\text{Test}_{\sigma=4}$	$\text{Test}_{\sigma=5}$	$\text{Test}_{\sigma=6}$
diabetes	**76.1842** (10)	73.4467 (10)	73.5749 (10)	74.2259 (10)	73.7116 (10)	74.2259 (10)
ecoli	**85.4278** (10)	83.9394 (10)	84.8218 (10)	83.1551 (9)	83.1452 (9)	83.1452 (9)
heart-statlog	83.7037 (10)	84.0741 (10)	**84.8148** (10)	83.7037 (10)	83.7037 (10)	83.7037 (10)
spectrometer	**42.7358** (10)	41.6038 (10)	42.5506 (10)	42.5472 (10)	42.5506 (10)	**42.7358** (10)
post. patient	68.8889 (10)	65.4321 (9)	65.4321 (9)	**69.4445** (8)	66.6667 (1)	66.6667 (1)
primary-tumor	50.1604 (10)	42.4866 (10)	46.3280 (10)	49.8574 (10)	50.4456 (10)	**50.7130** (6)
dermatology	98.3709 (10)	98.6411 (10)	**98.6487** (10)	**98.6487** (10)	**98.6487** (10)	**98.6487** (10)
soybean	**92.8261** (10)	91.6539 (10)	91.3619 (10)	91.6560 (10)	91.5111 (10)	91.9501 (10)
kr-vs-kp	87.6406 (10)	85.6090 (8)	**86.7034** (8)	87.2906 (8)	87.2906 (8)	87.2906 (8)
splice	**95.3919** (10)	94.5454 (10)	94.5454 (10)	94.5768 (10)	94.6081 (10)	94.9216 (10)
lymph	83.9047 (10)	83.0952 (10)	**85.0952** (10)	84.4286 (10)	84.5238 (10)	83.8571 (10)

Table 7. Test accuracies of Naïve Bayes for original data representation, and enriched data under different minimum support constraints.

We investigated the results of this approach on a variety of UCI data sets, using an SVM, Naïve Bayes, and Decision Tree classifier. In evaluating the usefulness of class outlier-based features experimentally, we find that enriching the data representation with these newly derived features does lead to improvements in classification accuracy on a number of data sets, in several cases remarkably so. On the other hand, using this approach without overfitting control can lead to results where the training accuracy improves while testing accuracy decreases or stays the same. By removing features that cover only few instances in the training data, this situation can be improved on a number of data sets but there are some data sets that are resistant to this solution.

Our proposed approach is also not equally beneficial for all three classes of classifiers: the Naïve Bayes classifier profits most from the enriched representation, since the newly derived features overcome Naïve Bayes' strong bias regarding conditional independence of attributes. The Decision Tree classifier, on the other hand, shows no improvement over the original representation on a third of the used data sets.

Generally, though, we have shown the merits of identifying class outliers and using their neighborhoods to derive discriminative features to improve classification accuracy. We have limited us in this work to attribute-value data but there is no reason why this approach cannot be extended, for instance, to graph-structured data, e.g. second-order representations of molecules.

References

1. Blake, C., Merz, C.: UCI repository of machine learning databases (1998), `http://www.ics.uci.edu/~mlearn/MLRepository.html`
2. Breunig, M.M., Kriegel, H.P., Ng, R.T., Sander, J.: Lof: Identifying density-based local outliers. In: Chen, W., Naughton, J.F., Bernstein, P.A. (eds.) SIGMOD Conference. pp. 93–104. ACM (2000)
3. Cleveland, W., Devlin, S., E., G.: Regression by local fitting. Journal of Econometrics 37, 87–114 (1988)
4. Cohen, W.W.: Fast effective rule induction. In: Prieditis, A., Russell, S.J. (eds.) Proceedings of the Twelfth International Conference on Machine Learning. pp. 115–123. Morgan Kaufmann, Tahoe City, California,USA (Jul 1995)
5. Cortes, C., Vapnik, V.: Support-vector networks. Machine Learning 20(3), 273–297 (1995)
6. Cover, T., Hart, P.: Nearest neighbor pattern classification. Information Theory, IEEE Transactions on 13(1), 21 – 27 (Jan 1967)
7. Frank, E., Witten, I.H.: Data Mining: Practical Machine Learning Tools and Techniques with Java Implementations. Morgan Kaufmann (1999)
8. Lindgren, T., Boström, H.: Resolving rule conflicts with double induction. In: 5th International Symposium on Intelligent Data Analysis. pp. 60–67. Springer, Berlin,Germany (Aug 2003)
9. Pérez, E., Rendell, L.A.: Learning despite concept variation by finding structure in attribute-based data. In: ICML. pp. 391–399 (1996)
10. Quinlan, J.R.: C4.5: Programs for Machine Learning. Morgan Kaufmann (1993)
11. Schapire, R.E.: The strength of weak learnability. Machine Learning 5, 197–227 (1990)
12. Vilalta, R., Drissi, Y.: A characterization of difficult problems in classification. In: Wani, M.A., Arabnia, H.R., Cios, K.J., Hafeez, K., Kendall, G. (eds.) ICMLA. pp. 133–138. CSREA Press (2002)
13. Vilalta, R., Rish, I.: A decomposition of classes via clustering to explain and improve naive bayes. In: Lavrac, N., Gamberger, D., Todorovski, L., Blockeel, H. (eds.) ECML. LNCS, vol. 2837, pp. 444–455. Springer (2003)