Relationship between Variants of One-Class Nearest Neighbours and Creating their Accurate Ensembles

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Abstract—In one-class classification problems, only the data for the target class is available, whereas the data for the non-target class may be completely absent. In this paper, we study one-class nearest neighbour (OCNN) classifiers and their different variants. We present a theoretical analysis to show the relationships among different variants of OCNN that may use different neighbours or thresholds to identify unseen examples of the non-target class. We also present a method based on inter-quartile range for optimizing parameters used in OCNN in the absence of non-target data during training. Then, we propose to use two ensemble approaches based on random subspace and random projection methods to create accurate OCNN ensembles that significantly outperforms the baseline OCNN. We tested the proposed methods on 15 benchmark and real world domain-specific datasets to show their superior performance. The results give strong evidence that the random projection ensemble of the proposed OCNN with optimized parameters perform significantly and consistently better than the single OCNN on all the tested datasets.

Index Terms—one-class classification, nearest neighbour, classifier ensemble, random projection, random subspace

1 Introduction

One-Class Classification (OCC) is a special case of classification problem where the data of the positive (target) class is sufficiently available, whereas the negative class (non-target) data is absent during the training phase. Some examples for OCC are machine fault diagnosis, fraud detection, human fall detection, rare disease, etc. In most of these applications, it is easy to collect samples for the positive class, or the data describing the normal behaviour of the domain under consideration. However, the collection of negative samples may be very difficult or result in high cost in dollars or put health and safety of a person in danger. In other cases, the data in the negative class occur rarely. Therefore, even if some samples are collected for the negative class, the training data will be severely skewed and it is difficult to build generalizable classifiers using the traditional supervised classification algorithms.

The research on OCC problems leads to several approaches to build classification models based on only the positive samples. Earlier approaches on OCC focus on determining the shape of the positive class from the sampled points. A lot of these approaches are suggested for two-dimensional datasets. Generally, these approaches are related with the convex hull of finite points; some of these approaches are extended for high dimensional datasets. However, the complexity of these methods is very large for high dimensional datasets. Therefore, these methods are not very practical for dealing with high dimensional OCC problem. Later approaches for OCC are presented using support vector machines, nearest neighbours, decision trees, bayesian networks, neural networks and classifier ensemble approaches. In this paper, we choose a one-class nearest neighbour (OCNN) approach for detecting unseen samples of the negative class, when they were not present during the training phase. An OCNN method finds the high and low density regions based on the local neighbourhood of a test sample. Using a decision threshold, an OCNN accepts or rejects a test sample as a member of the target class. In its simplest form, an OCNN finds the first nearest neighbour of a test sample in the target class and then finds the first nearest neighbour of this neighbour in the target class. If the ratio of these distances is lower than a user-defined threshold, it is accepted as a member of the target class. This method is simple and effective in finding instances of the unseen negative class. The OCNN does not require training the classifier, has few parameters and can easily be used with different similarity measures. These properties make OCNN a useful method for OCC problems. In an OCNN, the number of nearest neighbours and the value of decision threshold can be optimized but the sensitivity of the classifier w.r.t. noise in the positive class may change. There exists several variants of OCNN in the literature (see Section 2); however, these methods do not make relation between the other OCNN methods and do not clearly explain the reasons for a particular variant to work better than others.

Classifier ensemble approaches have been suggested for different OCC methods to improve their performance. Previous research shows that classifier ensembles consisting of accurate and diverse classifiers perform better than a single classifier. The supervised counterpart of OCNN, i.e., K-nearest neighbour (KNN) is robust to variations in the data set; therefore, ensemble techniques based on data sampling (such as Bagging and Boosting) have not been successful to create diverse KNN classifiers. However, KNN classifiers are sensitive to input features sampling; therefore, diverse and accurate KNN based ensembles can be created by using different feature spaces. We propose that the similar ensemble approaches can be useful for OCNN ensembles. In this paper, we present a holistic view on the general problem of OCNN by discussing their different variants and creating their accurate ensembles. The main contributions of the paper are:
• We theoretically show the relationship between various OCNN approaches and discuss the impact of choosing nearest neighbours on the decision threshold.
• We present a cross-validation method and a modified thresholding algorithm that utilize the outliers from the target class to optimize the parameters of the OCNN.
• We present two different types of OCNN ensemble methods by using random subspace and random projection methods to study their performance when the feature space is either changed or transformed. To the best of our knowledge, the suitability of random projection approach is investigated for the first time for OCNN.

Our results on several benchmark and domain-specific real world datasets show superior performance of the OCNN with random projection ensembles in comparison to single OCNN.

The rest of the paper is structured as follows. In Section 2, we present literature review on different variants of OCNN and their ensembles. Section 3 introduces two variants of OCNN that uses different numbers of nearest neighbours and decision threshold, followed by a theoretical analysis about their relationship with other variants of OCNN. In Section 4 we introduce a cross-validation method and a modified thresholding algorithm to optimize parameters for the OCNN classifiers using only the data from the target class. In Section 5 we present a discussion on various ensemble approaches that are used with the OCNN classifiers. Experimental results are shown on various datasets in Section 6. Conclusions and future work are summarized in Section 7.

2 Related Work

The research on OCC leads to the development of various models that mostly differ in either learning with target examples only; learning with target examples and some amount of poorly sampled outlier examples or artificially generated outliers; learning with labelled target and unlabelled data; methodology used and application domains applied. In this paper, we restrict our literature review to OCNN approaches and the methods that involve their ensemble.

Tax [10] presents an OCNN method called nearest neighbour description (NN-d). The general idea is to find the distance of a test object to its nearest neighbour in the target class, and find the nearest neighbour of this neighbour, and average distance of a test object to its nearest neighbour and distance of this neighbour to its nearest neighbour. They order these distances and find the best threshold based on the percentile of the sorted sequence. Angiulli [13] present a prototype based domain description algorithm (PDD) for OCC tasks, which is equivalent to NN-d under the infinity Minkowski metric and generalizes statistical tests for outlier detection. Angiulli introduces the concept of PDD consistent subset prototypes, which is a subset of the original prototype set. The paper presents two algorithms for computing PDD consistent subset: one that guarantees logarithmic approximation factor and the other faster version to manage very large datasets. The faster version does not consider all the pairwise object distances but it is shown to return almost identical subset size at lower computational cost. Krawczyk et al. [14] use prototype reduction techniques using evolutionary approaches that follow either selection or generation of examples from the training data and perform NN-d approach. They report no significant accuracy losses using their prototype reduction technique on several datasets from UCI repository. Cabral et al. [15] propose an OCNN method that uses the concept of structural risk minimization. They remove redundant samples from the training set, thereby obtaining a compact representation aiming at improving generalization performance of the classifier. They achieve considerable reduction in the number of stored prototypes and improved performance than the NN-d classifiers.

Cabral et al. [16] extend their work and present another approach where they not only consider one but K-nearest neighbours of a test object and find a nearest neighbour of each of these K neighbours. A decision is arrived based on majority voting. Their results show that K nearest neighbour version of their classifier outperforms the NN-d. However, it is not shown how the optimal value of K nearest neighbour is arrived at for better classification results. Muñoz and Madden [17] extend the idea of NN-d to tackle the recognition of vehicles using a set of features extracted from their frontal view and presented high accuracy of classification. They compute the average of the K nearest neighbours of the first nearest neighbour to arrive at a decision. However, the computation of best fitting value of K is not illustrated clearly in their work. Halvani et al. [18] use the similar idea for authorship verification task. They generate different types of features for a given document. For every feature type, the distance is calculated for its nearest neighbour and average distance of its K nearest neighbours, and a decision is taken for a given threshold. The decisions from all the feature types are combined using majority voting rule to take a final decision. Huang et al. [19] present an OCNN method for the identification of protein carbamylated as they play important role in a number of biological conditions. They compute threshold from the positive class based on a fixed false negative ratio, compute distance of a test sample with its K neighbours and if it is below a threshold, it is accepted as a member of the positive class. Gesù et al. [20] present an OCNN algorithm and tested it on synthetic data that simulate microarray data for the identification of nucleosomes and linker regions across DNA. They present a decision rule which states that if there are at least K data objects in the positive class that are dissimilar from the test object at most φ, then it is classified as a member of the positive class. They propose to calculate optimal values for K and φ using the ROC curve. Their results show good recognition rate on synthetic data for nucleosome and linker regions across DNA. However, the
paper does not explain the construction of validation set and parameters optimization in detail. Datta [21] modifies the standard KNN algorithm to learn only from the positive class. This algorithm learns a threshold, which is the maximum distance a test example can be from any learned example and still be considered a member of the positive class. Any test example that has a distance greater than the threshold from any training example is not considered a member of the positive class. Datta also present another modification that involves learning a vector of thresholds, where each threshold corresponding to every sample in the positive class and then employing a classification rule based on them to accept or reject a test sample. Khan [22] presents a variant of the $NN-d$ method that finds the distances of $J$ nearest neighbours of the test sample in the target class and compute the $K$ nearest neighbours of each of the $J$ neighbours in the target class. The distance ratio is computed for each of the $J$ neighbours and a majority voting rule is used to take a final decision. They use gaussian and polynomial kernel as a distance metrics and show that this method can perform better than the traditional $NN-d$ on chemical spectral data.

A single one-class classifier might not capture all the characteristics of the data. Therefore, an ensemble of one-class classifiers is a viable solution to improve the performance of base one-class classifiers, which may differ in complexity or in the underlying training algorithm used to construct them [2]. Peckalska et al. [23] use the proximity of target object to its class as a ‘discriminatory representation’ (DR) and show that the discriminative properties of various DRs can be enhanced by combining them properly. They use three types of one-class classifier, namely $NN-d$, Generalized Mean Class and Linear Programming Dissimilarity Data Description. They make two types of ensembles: (i) combine different DR from individual one-class classifiers into one representation after proper scaling using fixed rules, for e.g. average, product and train single one-class classifier based on this information, (ii) combine different DR of training objects over several base classifiers using majority voting rule. Their results show that both methods perform significantly better than the OCC trained with a single representation. Seguí et al. [24] present an ensemble method based on non-parametric weighted bagging strategy for OCC. Their method estimates a probability density based on a forest structure of the data instead of assuming uniform data distribution and constructs bootstrap samples according to the data density ranking, where higher density imply greater likelihood of being selected for a bootstrap of the ensemble. They use three types of one-class classifiers: $NN-d$, OSVM and Minimum Spanning Tree Class Descriptor (MST) [25] and show experimentally that the ensemble bagging and non-parametric weighted bagging obtain better rankings than the base one-class classifier methods and show a statistically significant improvement for MST and $NN-d$. Menahem et al. [26] propose an ensemble meta-learning algorithm which learns a combining function upon aggregates of the ensemble-members prediction. This algorithm depends on the classification properties of the ensemble-members and not on the fix-rule scheme. They use four one-class classifiers; two of them are based on OCNN, the rest are based on density estimation and OSVM. They combine these classifiers by four ensembles rules (majority voting, mean voting, max rule and product rule) and show that their proposed ensemble algorithm outperform traditional ensemble schemes. Gesù and Bosco [27] present an ensemble method for combining fuzzy OCNN classifiers. Their classifier combining method is based on a genetic algorithm optimization procedure by using different similarity measures. They test their method on two categorical datasets and show that whenever the optimal parameters are found, fuzzy combination of one-class classifiers may improve the overall recognition rate. Nanni [28] studies combining several one-class classifiers using the random subspace method for the problem of online signature verification. Nanni uses several one-class classifiers: Gaussian model description, Mixture of Gaussian Descriptions, $NN-d$, PCA Description (PCAD), Linear Programming Description (LPD), SVDD and Parzen Window Classifier. It is shown that fusion of various classifiers can reduce the error and the best fusion method is the combination of LPD and PCAD.

The literature review suggests that some papers use one nearest neighbour in the target class, whereas others use more than one nearest neighbours to decide if a test instance is a member of the negative class or not. However, the intuition behind which method will work better under what conditions is not clear. There is not much work done on the optimization of the decision threshold of an OCNN, which is either set arbitrarily or equal to 1. A major challenge in most of the OCC methods is the unavailability of data from the negative class; therefore, optimization of parameters is very difficult [29]. Hence, optimizing different nearest neighbours and the decision threshold is very difficult in the OCNN approach. We also observed that the ensembles of OCNN (such as random subspace) and fusion with other one-class classifiers can perform better than the base OCNN. Below, we present a detailed analysis of different variants of OCNN and perform a theoretical analysis on their relationship.

3 One-Class Nearest Neighbour Classifiers

Based on the literature review in Section 2, various OCNN methods can be categorized into the following four types based on the number of nearest neighbours they use to compute the decision threshold:

(i) Find the first nearest neighbour of the test sample in the target class, and the first nearest neighbour of the first neighbour ($1NN$) [10], [12], [13], [14], [15].

(ii) Find the first nearest neighbour of the test sample in the target class, and the $K$ nearest neighbours of the first neighbours ($1KNN$) [17], [18], [19].

(iii) Find the $J$ nearest neighbours of the test sample in the target class, and the first nearest neighbours of the first $J$ neighbours ($J1NN$) [16].

(iv) Find the $J$ nearest neighbours of the test sample in the target class, and the $K$ nearest neighbours of the first $J$ neighbours ($JKNN$) [22].

These different methods of OCNN can differ in the number of nearest neighbours, distance metric, method of combining distances and the choice of the value of the decision threshold to arrive at a final decision. Figure 1 shows a graphical representation of these methods using artificial data in 2 dimension. The dark circles (●) show the instances of the target class. The red star (+) shows a test sample. The solid line shows the distance of either 1 or $J$ nearest neighbours of the test sample in the target class and the dotted lines show
the distance between the 1 or K nearest neighbours of those 1 or J neighbours. In a JKNN classifier, if J and/or K is set to 1, then it condenses to 11NN, 1KNN or J1NN.

In this method, we take the average of the distances of different neighbour of the test sample and find their average, \( \bar{D}_j \). For a given decision threshold, \( \theta \), if \( \frac{D_j}{\bar{D}_j} < \theta \), then the test data object is considered as a member of the target class or else rejected as a member of the negative class. Algorithm 2 shows the steps to classify a test data object as a member of target class or not. This algorithm is different from the work of Khan [22] that use a similar JKNN variant in two ways. Firstly, they use kernel (gaussian and polynomial) a distance metric, whereas we use euclidean as a distance metric. Secondly, they combine the decision using majority voting of the distances of different K neighbours of each J neighbours, whereas we take the average of the distances of the J and K nearest neighbours.

3.1 One-Class JK Nearest Neighbour

We now present a general OCNN (JKNN) method for detecting non-target samples. In this method, we

1) Find the J nearest neighbour \( (NN_{j^*}^i(z)) \) of the test sample \( (z) \) in the target class and find their average, \( \bar{D}_j \).
2) Find the K nearest neighbours of these J neighbours \( (NN_{K_j}^i(NN_{j^*}^i(z))) \) and find their average, \( \bar{D}_K \).

For a given decision threshold, \( \theta \), if \( \frac{D_j}{\bar{D}_j} < \theta \), then the test data object is considered as a member of the target class or else rejected as a member of the negative class. Algorithm 2 shows the steps to classify a test data object as a member of target class or not. This algorithm is different from the work of Khan [22] that use a similar JKNN variant in two ways. Firstly, they use kernel (gaussian and polynomial) a distance metric, whereas we use euclidean as a distance metric. Secondly, they combine the decision using majority voting of the distances of different K neighbours of each J neighbours, whereas we take the average of the distances of the J and K nearest neighbours.

3.2 Relationship Among Different OCNN approaches

In an OCNN, either the decision threshold \( (\theta) \) is kept as 1 or chosen arbitrarily. In this section, we will show that varying decision threshold \( (\theta) \) with 11NN is similar to other OCNN methods discussed in Section 3.

In Figure 1a for 11NN with \( \theta \) equal to 1, if \( D_1 \) is more than \( D_2 \) the test sample is classified as an outlier. In this case even if \( D_1 \) is slightly more than \( D_2 \) the test sample will be assigned to negative class. Intuitively, an outlier data point should be at a much greater distance to its nearest neighbour \( (D_1) \) than the distance between this nearest neighbour and its nearest neighbour \( (D_2) \). Mathematically this can be represented as

\[
D_1 > \theta D_2
\]

where \( \theta > 1 \).

In this case, many data points that are outliers in the first case \( (D_1 > D_2) \), will not be rejected. The \( D_1 > \theta D_2 \) rule should reject less outliers than \( D_1 > D_2 \) rule because an outlier’s dissimilarity with its nearest data point in the target class should be more than the dissimilarity between that nearest data point to its nearest neighbour (we know that these two data points belong to the target class). However, finding the optimal value of \( \theta \) is problematic as it depends on the properties of a dataset. The optimal value of \( \theta \) may be different for different datasets and depends on the performance measure used. We will now discuss the relation between other variants of OCNN:

1) 1KNN approach – The 1KNN approach can produce similar results as 11NN \((\theta > 1)\). From Figure 1b for a point of negative class, we can write the distances as

\[
(D_1 + D_2 + ... + D_{2i})/K \geq (D_1 + D_2 + ... + D_{2i-1})/K
\]

where \( D_{2i} (K \geq i \geq 1) \) is the distance between the first nearest neighbour of the test sample and the \( i^{th} \) nearest neighbour of this nearest neighbour. As that distance between the first nearest neighbour and its \( i^{th} \) nearest neighbour is greater than or equal to the distance between it and \((i - 1)^{th} \) nearest neighbour,

\[
\therefore D_{2i} \geq D_{2i-1} \implies D_{2i} \geq D_{2i-1}
\]

Expanding the terms, we get

\[
(D_2 + D_3 + ... + D_{2i})/K \geq (D_2 + D_3 + ... + D_{2i-1})/K
\]

\[
(D_2 + D_3 + ... + D_{2i-1})/K \geq K D_{2i}/K
\]

\[
(D_2 + D_3 + ... + D_{2i-1})/K \geq K D_{21}/K
\]

\[
(D_2 + D_3 + ... + D_{2i-1})/K \geq K D_{21}/K
\]

\[
(D_2 + D_3 + ... + D_{2i})/K = \alpha D_{21}
\]

for \( \alpha \geq 1 \).
Using Equations 2 and 3, we get
\[ D_1 > \alpha D_{21} \] (4)

It is highly unlikely that all the \((K - 1)\) nearest neighbours of the first nearest neighbour of the test sample have the same distances as its first nearest neighbour. Hence, \(\alpha > 1\) for most of the cases. Equations 4 and 5 are the same, this suggests that \(1KNN\) is the same as the intuition based calculation for \(11NN\) with \(\theta > 1\).

2) \(1NN\) approach - The calculation for assigning a class to a data point will be opposite to the \(1KNN\) approach; hence, the condition to assign a negative class to a data point will be
\[ \alpha D_1 > D_{11} \] (5)

Eq. 5 with Eq. 1 suggest that \(1JNN\) approach is similar to \(\theta \leq 1\).

3) \(JKNN\) approach - In \(JKNN\) approach, the average distance of \(J\) nearest neighbours of a test sample is compared with the average distance of the \(K\) nearest neighbours of each of these \(J\) nearest neighbours. For a data point to be a negative class (see Figure 1d),
\[ D_J > D_K \] (6)

Using the same argument as discussed for \(1KNN\), we can write Equation 6 as,
\[ \beta D_{11} > \gamma D_{21} \] (7)

Where \(\beta\) and \(\gamma \geq 1\). For most of the cases, \(\beta\) and \(\gamma\) are more than 1
\[ D_{11} > (\gamma/\beta)D_{21} \] (8)

As both \(\gamma\) and \(\beta\) are more than 1. It is likely, they will cancel out each other for high values of \(J\) and \(K\). Hence, for high values of \(J\) and \(K\), they will generate a condition, \(D_{11} > D_{21}\); that is similar to \(11NN\) approach with \(\theta = 1\). For smaller values of \(J\), the value of \(\beta\) will be near to 1. Therefore, for small \(J\) and large \(K\), \((\gamma/\beta)\) will be greater than 1.

The above arguments imply that \(1KNN\) or \(JKNN\) with small \(J\) and \(\theta = 1\) will be similar to \(11NN\) with \(\theta > 1\). Thus, they are more likely to reject less outliers than \(11NN\) with \(\theta = 1\). Whereas, \(1JNN\) or \(JKNN\) with a large value of \(J\) may accept more non-targets as members of the target class; similar to \(11NN\) with \(\theta < 1\). Finding the optimized values of \(J\) and \(K\) for \(JKNN\) with \(\theta = 1\) or the optimized value of \(\theta\) for \(11NN\) is an important step in designing an efficient OCNN classifier. The parameter optimization techniques are discussed in Section 4.

4 Parameter Optimization for OCNN
Optimizing parameters in one-class classifiers is difficult because only the data from the positive class is available during training. In this section, we will discuss a method by which noisy samples within the positive class can be used to optimize the parameters of OCNN classifiers. We note that the different variants of OCNN discussed in Section 3 (shown in Figure 1) can suffer from either or both of the following problems:

1) False Positives - The real-world target data may contain noisy observations due to non-calibrated data collection devices, human errors in labelling or inadvertent artifacts. The above discussed OCNN approaches ignore this fact and presence of such deviant observations in the target class can make these classifiers sensitive to noise. This case can arise when most of the target data objects are dense toward their center but some data objects are far from it. This behavior can lead to outliers being accepted as members of the target class.

2) False Negatives - If noisy observations are removed from the dataset but the decision threshold is not properly adjusted, an OCNN can reject a target test sample as an outlier.

Yin et al. [31] mention that in the OCC setting, due to the scarcity of negative data, it is a challenging problem to design a detection system that can reduce both the false positives and false negatives. In general, OCC methods are very sensitive to the choice of parameters [32]. In the case of OCNN, choosing a particular value of \(J\) and \(K\) nearest neighbours or moving the decision threshold \(\theta\) can affect both the false positive and false negative rates. However, in a given OCC problem, a classifier’s parameters cannot be optimized directly because there is no training set and validation set available for the negative class. Therefore, choosing the optimal parameters for a given OCC problem in the absence of non-target class is very challenging [33]. One approach to handle such a scenario is to generate artificial data for the unseen negative class [34], [35], [36] by assuming some distribution for the instances of the negative class. However, these approaches are prone to overfitting. Other possibility is to build models for the unseen negative class based on the parameters of the positive class [30], [57]. However, such approaches depend on the estimated parameters of the positive class. A true distribution for positive class is hard to estimate due to limited availability of data and the assumptions on the dataset. We take an alternative view by attempting to find classification boundary from the existing training data for the target class. We now present a method for optimizing the parameters of an OCNN in the absence of training samples for the negative class by:

1) Removing the noisy observations from the target class using a method based on Inter-Quartile Range.

2) Using the rejected noise data as a proxy for the unseen negative class and performing a new cross-validation method to optimize the best \(J\) and \(K\) neighbours or the decision threshold, \(\theta\).

4.1 Removing noise from the target class
As discussed in the previous section, noise in the target data can arise due to various reasons and its presence can adversely affect the performance of \(NN-d\) based classifiers in terms of accepting outliers as members of target class during the testing phase. Khan et al. [35] show that for the human fall detection problem, where the data for falls is difficult to obtain, deviant normal human motion sequences can be removed from the normal human activities using the IQR technique. These deviant sequences can act as a proxy for real falls and help in optimizing the parameters of the probabilistic classifiers. They use Hidden Markov Model based classification technique, and obtain log-likelihoods of the training sequences from the normal activities and apply Inter-Quartile Range (IQR) technique on them to remove the noisy sequences. Although this
technique is specifically developed for probabilistic classifiers, it can be modified to other types of classification techniques. In the nearest neighbour approach, we compute distances instead of probabilities and IQR technique can be adapted to work on this problem. In order to obtain distances, we use a center based distance computation method \[\text{dist}(i) = ||(T_i, T_i)||\], where \(||\cdot||\) is the euclidean distance between two vectors \(T_i\) and \(T_i\).

The instances that are far away from the center of the data are to be removed and are used as proxy for negative class. The algorithmic steps to remove noisy observations from the target class is shown in the Figure [4]. These rejected noisy observation can help in the optimization of the \(J\) and \(K\) neighbours or the decision threshold \((\theta)\) for the OCNN using a cross-validation step, which is described next.

**4.2 Cross Validation**

In OCC problems, estimating the parameters becomes very challenging due to the absence of negative data in the validation set. We now introduce a cross-validation method to optimize the nearest neighbours \(J\) and \(K\) for the JKNN classifier when the decision threshold \((\theta)\) is set to 1. In a given target training data (with no negative samples), we employ the IQR technique (discussed in Section 4.3) to reject some noisy observation from the target class. These rejected noisy observations serves as a proxy for the negative class. Then we employ an inner cross-validation step, with \(G\) folds. We split the target and rejected noisy data such that in one fold we have target data from all the \((G - 1)\) folds and test on target and rejected noisy observations of the \(G^{th}\) fold. We use the one-class JKNN classifier for the inner cross-validation step and test it on different values of \(J\) and \(K\) neighbours and the values that gives the best average value for the performance metric over all \(G\) folds is chosen as the best value of the parameter. The algorithmic steps are shown in Figure [5].

**Input:** \(N\) number of \(T\) target data objects with dimension \(d\), rejection rate \(\omega\)

**Output:** \(O\): rejected noisy observations from the target class

1. Compute the center of the target class, \(T = \sum_{i=1}^{N} \frac{T_i}{N}\)
2. Compute the distance of each target member from \(T_i\), \(\text{dist}(i) = ||(T_i, T_i)||\)
3. Set counter for rejected noisy targets, \(\text{counter} = 0\)
4. for every \(T_i\) do
5. if \(\text{dist}(i) > (Q_3 + \omega \times \text{IQR})||\text{dist}(i) < (Q_1 - \omega \times \text{IQR})\)
6. then \(\text{O[counter]} = T_i\)
7. \(\text{counter} = \text{counter} + 1\)
8. end
9. end
10. if \(\text{counter} == 0\) then
11. Reduce the value of \(\omega\) and repeat from step 4
12. else
13. return \(O\)
14. end

**Fig. 4:** Removing Noisy data from the Target Class

**4.3 Optimizing Decision Threshold**

We discussed the relationship between JKNN with \(\theta = 1\) and 11NN with variable \(\theta\) in Section 3.2. To optimize the decision threshold \(\theta\) for 11NN, we use the same strategy for optimizing \(J\) and \(K\) as discussed above, that uses the rejected noise data from the positive class as a proxy for unseen negative class. Then we use a modified empirical thresholding algorithm to optimize the decision threshold \(\theta\) \[40\]. The general idea of the original thresholding algorithm is to select an empirical threshold from the training instances according to the missclassification cost. This method can convert any cost-insensitive algorithm to cost-sensitive one by searching for the probability that minimizes the misclassification costs.
Input: Target training data (D), Rejected Outliers from Target (N), Remaining Target training data D, Total Number of Target training data, 
\[ N = |D| = |D + N|, J \text{ and } K \text{ nearest neighbours} \]

Output: Optimized Neighbours, \( J_{\text{opt}} \) and \( K_{\text{opt}} \)

1. Apply inner G-fold cross validation. For each fold
   (i) Create internal training set, \( \mathcal{T} \), by combining \( D \) and \( N \) from the \( G-1 \) folds
   (ii) Create validation set, \( V \) by combining \( D \) and \( N \) from the \( G^{th} \) fold
   (iii) foreach \( j \in 1, \ldots, J \) do
      foreach \( k \in 1, \ldots, K \) do
         foreach \( x \in V \) do
            Apply JKNN with \( \theta = 1 \) on \( V \)
            end
            Compute the performance metric, \( gmean[j][k] \) \( \forall x \in V \)
         end
      end
   end

After the above step, a \( gmean \) vector of length \( J, K, N \) is created

2. Find \( gmean_{\text{opt}} = \max_{i,j,n}(gmean[j][k][n]) \)
3. Find the corresponding neighbours, i.e., \( J_{\text{opt}} \) and \( K_{\text{opt}} \)
4. return \( J_{\text{opt}} \) and \( K_{\text{opt}} \)

Fig. 5: Finding Optimized Nearest Neighbours for JKNN with \( \theta = 1 \)

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Input: Target training data (D), Rejected Outliers from Target (N), Remaining Target training data D, Total Number of Target training data, 
\[ N = |D| = |D + N| \]

Output: Empirical Threshold, \( \theta_{\text{emp}} \)

1. Apply inner G-fold cross validation. For each fold
   (i) Create internal training set, \( \mathcal{T} \), by combining \( D \) and \( N \) from the \( G-1 \) folds
   (ii) Create validation set, \( V \) by combining \( D \) and \( N \) from the \( G^{th} \) fold
   (iii) Apply 11NN on \( V \), i.e., \( \forall x \in V \), compute the decision threshold by computing the ratio of their first neighbours and their first neighbours (i.e., \( J = K = 1 \)) in \( \mathcal{T} \)

After the above step, a decision threshold vector \( \{\theta_V\} \) of length \( N \) is created

2. foreach \( i \in 1, \ldots, N \) do
   Choose \( \tau = \theta_{V_i} \) as the threshold
   foreach \( j \in 1, \ldots, N \) do
      Compare \( \tau \) with \( \theta_{V_{ij}} \)
      Compute the class of each data
   end
   Compute the performance metric, \( gmean_i \)
end

10. Find \( \theta_{\text{emp}} = \max_i(gmean_i) \)
11. return \( \theta_{\text{emp}} \)

Fig. 6: Finding Empirical Decision Threshold(\( \theta \)) for 11NN

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4.4 How many noisy observation to reject from the target class?

As discussed earlier, noisy data can be removed from the training data using the IQR technique (Section 4.1.1) to create a validation set for optimizing the parameters OCNN classifier. The amount of observations to be rejected depends upon the rejection rate, \( \omega \). A large value of \( \omega \) results in less rejections and smaller value means more rejections. In the inner cross-validation method described in Section 4.2 the validation set should have at least one observation as a proxy for outliers in each of the inner fold \( G \). As a rule of thumb, the value of \( \omega \) should be chosen such that at least \( G \) data points are rejected from the target class as proxy for outliers. Therefore, the value of \( \omega \) can either be chosen using domain knowledge or hit-and-trial method. In our experiments, we mostly chose \( \omega = 1.5 \), if that did not yield desired number of rejected targets, it is reduced until the desired number of data points from the target class are rejected to generate the validation set.
creating KNN ensembles for multi-class classification [9]. RP has also been used to approximate the convex-hull in high dimensional spaces for one-class problem [47]. However, in this method RP is used to create two or three dimensional low-dimensional spaces. Hence, there may be a large loss of information. The conceptual similarity between KNN and OCNN methods motivate us to employ RP approach for creating ensembles of OCNN methods. The algorithm for OCNN ensembles by RS or RP (with parameter optimization) is illustrated in Figure 8.

Fig. 8: OCNN ensembles with Parameter Optimization

### 5 Ensembles of OCNN

The key to build good ensembles is to create accurate and diverse classifiers [8]. Creating diverse feature spaces to create diverse classifiers is a popular method for supervised KNN based ensembles. We will apply similar approaches for ensembles of OCNN classifiers, i.e. Random Subspace (RS) and Random Projection (RP).

In RS ensembles technique [43], in each run, a classifier is trained on a randomly selected feature subspace of the original feature space. This creates diverse classifiers that in turn creates an accurate ensemble. Random subspace technique has also been used to create ensembles for outlier detection [44]. However, ensembles of various OCNN methods created by RS method have not been extensively studied. RP is a method for dimensionality reduction problem [45]. RP maps a number of points in a high-dimensional space into a low dimensional space with the property that the euclidean distance of any two points is approximately preserved through the projection. Using matrix notation where $D_{d \times n}$ is the original set of $n$, $d$ dimensional observations. The projection of the data onto a lower $p$-dimensional space is defined as

$$D_{p \times n}^{RP} = R_{p \times d}D_{d \times n}, \quad (10)$$

where $R_{p \times d}$ is a random matrix whose rows have unit lengths and $D_{p \times n}^{RP}$ is the new $p \times n$ projected matrix. The elements $r_{ij}$ of a random matrix $R$ can be computed as [46]:

$$r_{ij} = \sqrt{3} \begin{cases} +1, & \text{with probability } \frac{1}{6} \\ 0, & \text{with probability } \frac{2}{3} \\ -1, & \text{with probability } \frac{1}{6} \end{cases} \quad (11)$$

Different random projections of a dataset create different new datasets with different features. RP has been used for creating KNN ensembles for multi-class classification [9]. RP has also been used to approximate the convex-hull in high dimensional spaces for one-class problem [47]. However, in this method RP is used to create two or three dimensional low-dimensional spaces. Hence, there may be a large loss of information. The conceptual similarity between KNN and OCNN methods motivate us to employ RP approach for creating ensembles of OCNN methods. The algorithm for OCNN ensembles by RS or RP (with parameter optimization) is illustrated in Figure 8.

### 6 Results

#### 6.1 Performance Metric

Some of the popular supervised classification performance metrics, such as accuracy, precision, recall, F-measure etc., cannot be used in the OCC scenario. OCC presents a unique scenario when target data is sufficiently present during training and negative data is not. Therefore, during testing the OCC, we would expect to observe a highly skewed distribution of negative data w.r.t. the target data. In that sense, during testing, the problem becomes the evaluation of the performance of a classifier with severely imbalanced test set. Due to this nature of test data, conventional performance metrics (e.g. accuracy) may not be directly employed because the numbers it produce may be misleading. Other measures such as, F-measure depends on precision and recall and if all the test data is classified as target or negative, then it can give NaN values to precision or recall. Kubat and Matwin [48] use the Geometric Mean ($gmean$) of accuracies measured separately on each class i.e., it combines True Positive Rate (TPR) and True Negative Rate (TNR) (where target is the positive class and non-target is the negative class), defined as

$$gmean = \sqrt{\text{TPR} \times \text{TNR}}$$

An important property of $gmean$ is that it is independent of the distribution of positive and negative samples in the test data. It is to be noted that in the extreme case when all the test data is either classified as belonging to only target or non-target, $gmean$ will become zero. This measure is more useful in our application where we expect a skewed distribution of non-target w.r.t. target and we want to evaluate the performance on both the target and non-target.
6.2 Datasets

There are no standard datasets available for testing OCC algorithms; therefore, we test our methods on datasets that have high imbalance ratio of the number of positive and negative labelled data. This is done to highlight the OCC problem where the data of the negative class is rare. In our experiments, only the data from the positive class is used during training and parameter optimization i.e., no data from negative class is used during training. However, the data from negative and positive class is available during testing. We show results on 9 benchmark datasets from KEEL repository and 6 domain specific real-world datasets.

6.2.1 KEEL Benchmark datasets

KEEL dataset repository [49] provides several datasets for testing machine learning algorithms. We choose 9 datasets that have real valued attributes and high imbalance ratio. The details of these datasets are shown in Table 1.

| Dataset                        | #Attributes | #Instances | Imbalance Ratio |
|-------------------------------|-------------|------------|-----------------|
| yeast6                        | 8           | 1484       | 41.4            |
| yeast5                        | 8           | 1484       | 32.73           |
| yeast4                        | 8           | 1484       | 28.1            |
| glass5                        | 9           | 214        | 22.78           |
| glass4                        | 9           | 214        | 15.43           |
| winequality-red-3-vs-5 (Wine1)| 11          | 691        | 68.1            |
| winequality-white-3-9-vs-5 (Wine2)| 11       | 1482       | 58.28           |
| winequality-red-8-vs-6-7 (Wine3)| 11         | 855        | 46.5            |

TABLE 1: KEEL Benchmark Datasets

6.2.2 German Aerospace Center (DLR) [50]

This dataset is collected using an Inertial Measurement Unit (IMU) with integrated 3D magnetometers. The dataset contains samples from 19 people of both genders of different age groups. The data is recorded in indoor and outdoor environments under semi-natural conditions. The sensor is placed on the belt either on the right or the left side of the body or in the right pocket in different orientations. In total the dataset contains labelled data of over 4 hours and 30 minutes of the following 7 activities: Standing, Sitting, Lying, Walking (up/downstairs, horizontal), Running/Jogging, Jumping and Falling. Each sample in the dataset consists of a 9-dimensional vector that has 3 readings each for the accelerometer, gyroscope and magnetometer in the x, y and z directions. We only use the data from accelerometer and gyroscope. One of the subjects did not perform fall activity; therefore, their data is omitted from the analysis.

6.2.3 MobiFall (MF) [51]

This dataset is collected using a Samsung Galaxy S3 mobile device with inertial module integrated with 3D accelerometer and gyroscope. The mobile device was placed in a trouser pocket freely chosen by the subjects in random orientations. For falls, the subjects placed the mobile phone in the pocket on the opposite side of falling direction. All falls were monitored to be done in a specific way. The mean sampling of 87 Hz is reported for the accelerometer and 200Hz for the gyroscope. The dataset is collected from 11 subjects performing various normal and fall activities and 2 subjects only performing falls activity; therefore, they are removed from the analysis. The following 8 normal activities are recorded in this dataset: step-in car, step-out car, jogging, jumping, sitting, standing, stairs (up and down grouped together) and walking. Four different types of falls are recorded – forward lying, front knees lying, sideward lying and back sitting chair. These data from different types of falls are joined together to make one separate class for falls.

6.2.4 Coventry Dataset (COV) [52]

This dataset is collected using two SHIMMER™ sensor nodes strapped to the chest and thighs of subjects that consists of a 3D accelerometer, 3D gyroscope, and a Bluetooth device [53]. The data was gathered at 100 Hz and transmitted to a remote PC and annotated. Two protocols were followed to collect data from subjects. In Protocol 1, data for four types of falls, near falls, falls induced by applying a lateral force and a set of ADL (standing, sitting, walking and lying) is collected. Protocol 2 involved ascending and descending stairs. 42 young healthy individuals simulated various ADL and fall scenarios, with 32 took part in Protocol 1 and 10 in Protocol 2. For Protocol 1, the activities were collected in a real-life circumstances where subject would make phone calls, read books, or talk to others while maintaining various postures. The following normal ADL were collected in Protocol 1 – standing, lying, sitting on a chair or bed, walking, crouching and near falls. Six types of fall scenarios are captured – forward, backward, right, left, real fall-backward and real fall forward. The data for real fall-forward/backward is collected by standing the subject on a wobble board while they are blindfolded and try to balance themselves, then they are pushed from behind/front to fall forward/backward onto a cushion and remain lying down for 10 seconds. These data from different types of falls are joined together to make one separate class for falls. The subjects for Protocol 2 did not record corresponding fall data; therefore, it is not used. In our analysis, we used accelerometer and gyroscope data from the sensor node strapped to the chest.

These DLR, MF and COV datasets are pre-processed and 31 time-domain and frequency-domain features are computed as discussed in Khan [54]. After pre-processing, the DLR dataset has 26576 normal activities and 84 fall segments, the MF dataset has 5430 normal activities and 488 fall segments and the COV dataset has 12392 normal activities and 908 fall segments. The ratio of normal to fall activities in the DLR, MF and COV datasets is 305.67, 11.13 and 13.65.

6.2.5 Aging-related bugs and software complexity metrics

This dataset contains information on the aging-related bugs found in the Linux kernel and MySQL DBMS open source projects [55]. This dataset is meant to investigate defect prediction for aging-related bugs by using software complexity metric and machine learning techniques. The data repository contains several datasets and we choose two of them, namely: Linux Drivers (LD) and MySQL InnoDB (MI). Both the datasets contains 82 attributes (plus one class label) related to program size, aging-related bugs and software complexity metrics. The LI dataset contains 2283 positive instances and 9 negative instances (imbalance ratio of 253.66), whereas the MI dataset contains 370 positive instances and 32 negative
instances (imbalance ratio of 11.56). The reason to use this dataset is to motivate OCC applications, where the examples of the negative class are very less than the number of positive class, in this case defect is rare than normal functioning of the software. In the LI dataset, 31 attributes have zero values and they are removed. In the MI dataset, 30 attributes have zero values that are removed. One attribute has all zero values except at 2 instances; however, during 5-fold cross-validation, all the instances with zero attribute value may appear and will cause problem in the normalization of the data. Therefore, this attribute is also removed and both the datasets are used with 51 attributes.

6.2.6 Breast Cancer Dataset

The original Breast Cancer dataset is available at the UCI repository [56] and modified by the German Research Center of Artificial Intelligence [57] to be used for unsupervised outlier detection. The modified data has 30 attributes with 357 normal instances and 10 negative samples with an imbalanced ratio of 35.7.

6.3 Experimental Setup

To perform the experiment, we set the following values of the parameters

- F-fold cross-validation is used in the experiment to report the average performance metric. We split the dataset such that target data from \((F - 1)\) partitions are joined together and outliers from \((F - 1)\) partitions are ignored s.t. this set is used during training and the remaining targets and outliers of the \(F^{th}\) fold are used during testing. The value of \(F\) is set to 5 in our experiments.
- The value of G-fold inner cross-validation for parameter optimization is set to 2.
- The minimum and maximum number of \(J\) and \(K\) neighbours to optimize in OCNN is set to 1 and 10. For the DLR, MF and COV dataset, this number is set to 5 because we could not obtain results in reasonable time with large number of nearest neighbours due to large data size.
- Size of random subspace is set to 50% and 75% of the total size of attributes that are selected randomly [43].
- Size of the ensemble for random subspace, random projection is set to 25 [58].
- The dimension of new dataset created by RP is kept same as the original dataset.
- Rejection rate, \(\omega\), is set to 1.5. For some datasets, \(\omega\) is manually decreased until all the classifiers are able to reject at least 5 instances from the positive class (corresponding to the number of outer F-cross-validation folds).
- The data is normalized using the min-max method to lie within \([0, 1]\) [29], i.e., \(y_i = \frac{x_i - \min(x)}{\max(x) - \min(x)}\), where \(x = (x_1, x_2, ..., x_n)\), \(n\) is the number of training data and \(y_i\) is the normalized value.

We performed two kinds of experiments with the above mentioned dataset [4].

1) To compare the performance of different types of single OCNN methods i.e., 11NN vs 11NN(\(\theta\)) vs JKNN, where 11NN means at 11NN at \(\theta = 1\), 11NN(\(\theta\)) means 11NN for optimized \(\theta\) and JKNN means JKNN for optimized \(J\) and \(K\) and \(\theta = 1\).

2) To compare the performance of two types of ensembles of OCNN i.e., RP and RS ensemble for each OCNN method.

6.4 Experimental Analysis

6.4.1 KEEL Benchmark Datasets

The results of the first experiment on the KEEL benchmark datasets are presented in Table 2 under the column ‘singe’ for each of the specific OCNN technique i.e., 11NN, 11NN(\(\theta\)) and JKNN. The results show that 11NN performed best \((gmean)\) for 6 out of 9 datasets. We observe that, 11NN gives high values of TNR for all the datasets, whereas 11NN(\(\theta\)) and JKNN produced better TPR in comparison to 11NN. This means that the class boundary set by 11NN(\(\theta\)) and JKNN favours accepting test samples as member of target class resulting in fewer false positives, whereas the boundary for 11NN favours rejecting more samples as negatives resulting in fewer false negatives. Since gmean combines both TPR and TNR with equal weights, it gives a higher value of performance metric to 11NN. Alternatively, we can infer that 11NN(\(\theta\)) and JKNN shift the decision boundary such that the these classifiers are biased for the positive class. We believe that KEEL benchmark datasets are not good representatives for the one class problems. Two classes in the given problems may not be far apart and not necessarily demonstrate the outlier concept. Hence, a large number of negative class data points were predicted as member of the positive class by 11NN(\(\theta\)) and JKNN and a lot of positive samples were predicted as members of the negative class by 11NN. Due to this large misclassification (i.e., more false positives or false negatives), the overall values of gmean are small and none of these methods can be considered for robust classification for both the targets and unseen non-targets. If this misclassification can be reduced, then the gmean values will improve. The improvement in performance can be achieved by applying the ensemble approach on OCNN, which is described next.

The results of the second experiment on the KEEL benchmark datasets are presented in Table 2 under the columns ‘RS(50)’, ‘RS(75)’ and ‘RP’ for each of the specific OCNN technique. The results show that the RP ensembles of 11NN(\(\theta\)), JKNN and 11NN always performed better \((gmean)\) than their single counterparts. The performance advantage is more for 11NN(\(\theta\)) and JKNN. RP ensembles of 11NN(\(\theta\)) performed best for all datasets. Results suggest that RP ensembles show the TNR value equal to 1, which means that these ensembles predicted all the members of the negative class correctly. As discussed above, 11NN(\(\theta\)) and JKNN give large TPR as they are biased for positive class. The combination of high TPR and high TNR for RP ensembles of 11NN(\(\theta\)) and JKNN lead to their high gmean values.

For most of the cases, RS ensemble perform \((gmean)\) worse than single classifier. Though RS ensembles of 11NN(\(\theta\)) and JKNN generally have better TPR than that of single 11NN(\(\theta\)) and single JKNN respectively, lower values of TNR for ensembles of 11NN(\(\theta\)) and JKNN lead to lower values of gmean for these ensembles. The RS method creates diverse classifiers; however, these classifiers may not necessarily be accurate, which affected their overall performance. The ‘single’
version trained on all the features gave poor values for \textit{gmean}. Training these classifiers with smaller amount of features (and creating an ensemble) still suffer from classification boundary bias and the ensemble did not improve the results.

The performance of RP ensembles are best among all the ensemble methods for various OCNN approaches. It has been shown that the performance of supervised KNN classifiers is not affected much in feature space created by RP. The less loss of information can be the reason for it. In our case, we are creating OCNN classifiers that have the same characteristics of supervised KNN classifiers. Hence, these OCNN classifiers trained on feature spaces created by RPs are accurate. Different RPs are creating diverse classifiers. The combination of these accurate and diverse classifiers are helping RP ensembles to correctly predict the negative class points. 11NN(\(\theta\)) may not work appropriately because it depends on the choice of \(\theta\) chosen empirically from training data. Since the training data is limited, we can get sub-optimal choice for it. Therefore, in practice, the results of 11NN(\(\theta\)) may be different than \(JKNN\) with \(\theta=1\).

One of the most important implications of the proposed methodology is finding the optimized values of \(\theta\) for 11NN(\(\theta\)) and, \(J\) and \(K\) for \(JKNN\). We observe that generally the optimized values of the \(\theta\) for 11NN(\(\theta\)) were between 1 and 2. The optimal values of \(J\) were between 1 and 3 whereas the optimized values of \(K\) were always 10 (the maximum set value in the experiment). These values verify our discussion in Section 3.2 that 11NN(\(\theta\)) with \(\theta>1\), 1KNN and \(JKNN\) (for smaller values of \(J\)) have similar decision boundaries.

### 6.4.2 Domain-Specific Real Datasets

The results of the first experiment on the MobiFall, DLR, Coventry, Linux-driver, MySQL-IDB and Breast-Cancer datasets are shown in Table 5 under the column ‘single’ for each of the specific OCNN technique i.e., 11NN(\(\theta\)), JKNN and 11NN. Similar to the results on KEEL benchmark datasets, we observe that JKNN and 11NN(\(\theta\)) are more biased to the positive class than the 11NN, thus resulting in higher TPR at the cost of lower TNR. However, in these datasets, single JKNN always performed better than single 11NN in terms of \textit{gmean}. For three datasets (DLR, Coventry and Breast-Cancer) single 11NN(\(\theta\)) performed better than single 11NN. These datasets better represent OCC problems and the negative class may lie in low-density regions; however, we notice that 11NN(\(\theta\)) is most biased towards the positive class than the other two methods. This means that it gave highest TPR but at the cost of missing to identify negative samples in the test set (low TNR) leading to low \textit{gmean} values. Nonetheless, JKNN and 11NN(\(\theta\)) generally show better performance against 11NN. In 11NN(\(\theta\)) method, since the value of \(\theta\) is calculated from the training data, it may suffer from overfitting problem. Hence, for some datasets 11NN performed better than 11NN(\(\theta\)).

The results of the ensembles are shown in Table 3 under the column ‘RS(50)’, ‘RS(75)’ and ‘RP’ for each of the specific OCNN technique i.e., 11NN(\(\theta\)), JKNN and 11NN. The results about the ensembles suggest that for four datasets (MobiFall, DLR, Coventry, and Breast-Cancer) RP ensembles of 11NN(\(\theta\)) perform the best whereas for other two datasets (Linux-driver and MySQL-IDB) RP ensembles of JKNN perform best in terms of \textit{gmean}. The RP ensembles for

| Data Set | 11NN with optimized \(\theta\) | JKNN | 11NN(\(\theta\)) | Single |
|----------|-----------------------------|------|----------------|-------|
| Glass2   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Glass3   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Glass4   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Glass5   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yolot2   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yolot3   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yolot4   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yolot5   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yolot6   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yeast1   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yeast2   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yeast3   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yeast4   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
| Yeast5   | TPR: 0.951(0.049)           | 0.872(0.067) | TPR: 0.878(0.071) | 0.801(0.075) |
11NN(θ), JKNN and 11NN always gave high TNR and comparable TPR in comparison to RS ensembles. Combining both high TPR and TNR results in high gmean for RP ensembles in comparison to RS ensemble. The member classifiers in RP ensembles of 11NN(θ) and JKNN are created independently. As ensembles in which classifiers are created independently are robust to overfitting problem, this could be one of the reasons for the accurate RP ensembles of 11NN(θ) and JKNN.

### 6.4.3 Statistical Testing

To compare the different OCC methods over several datasets, we perform the Iman-Davenport modification of Friedman’s test [61]. This test suggests that among different classifiers that are run over several datasets, one of them may perform differently than the rest. We then use the post-hoc Nemenyi test that result in a plot, which is quite illustrative to show the rankings of different classifiers. We perform the Iman-Davenport and Nemenyi test on the KEEL Benchmark datasets and domain-specific datasets separately and show the plot of the ranking of different algorithms in figures 9a and 9b. The dark line (−) shows the critical difference (CD). Any two algorithms whose performance difference is greater than the CD are considered as significantly different. The CD plot shows that the RP ensemble method always appear as a highest ranking method among all other OCC methods for both type of datasets. This finding is coherent with the results presented in the previous two sections.

### 7 Conclusions and Future Work

In this paper, we presented a theoretical analysis to demonstrate the generalization and relationship among different variants of OCNN. We further enhance the discriminatory power of OCNN classifier by creating accurate ensembles of different variants of OCNN. We presented a technique to optimize the parameters for the general JK OCNN that only uses data from the target class as the data for the negative data may be absent during the training phase. We tested the proposed methods on 15 benchmark and domain specific datasets and show that RP ensembles of JKNN and 11NN(θ) are highly accurate, specially in identifying the unseen negative samples along with a good balance in identifying the members of the target class. The results also give definitive evidence that single OCNN classifiers are not a good choice for dealing with OCC problems. When OCNN is employed, their ensembles with optimized θ and J, K neighbours perform much better. The success of these ensembles is attributed to two facts: (i) using the proposed optimization method, accurate 11NN(θ) and JKNN models are created and (ii) RP ensemble methods create diverse 11NN(θ) and JKNN models. The combination of these diverse and accurate models created successful RP ensembles of 11NN(θ) and JKNN. Thorough these experiments, we also found that finding the optimal values of J and K is a time consuming task in JKNN approach. However, on the basis of our experiments, we can suggest that only low values of J with high values of K could be used as a good choice for classifying unseen samples, especially when the negative concept is very different from the target class. In future, we would like to use a kernel as a distance measure for OCNN and will study the effects of their ensembles.
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