Kernels for One-Class Nearest Neighbour Classification and Comparison of Chemical Spectral Data

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Dedicated to

my

beloved mother, Zarina Khan

&

sweet daughter, Aliza

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Abstract

The One-class Classification (OCC) problem is different from the conventional binary / multi-class classification problem in the sense that in OCC, the examples in the negative / outlier class are either not present, very few in number, or not statistically representative of the negative concept. Researchers have addressed the task of OCC by using different methodologies in a variety of application domains. This thesis formulates a taxonomy with three main categories based on the way OCC is envisaged, implemented and applied by various researchers in different application domains. Based on the proposed taxonomy, we present a comprehensive research survey of the current state-of-the-art OCC algorithms, their importance, applications and limitations.

The thesis explores the application domain of Raman spectroscopy and studies several similarity metrics to compare chemical spectra. We review some standard, non-standard and spectroscopy-specific spectral similarity measures. We also suggest a modified Euclidean metric to aid in effective spectral library search. These spectral similarity methods are then used to build the kernels for developing one-class nearest neighbour classifiers. Our results suggest that these new similarity measures indeed lead to better precision and recall rates of target spectra in comparison to studied standard methods.

The thesis proposes the use of kernels as distance metric to formulate a one-class nearest neighbour approach for the identification of a chemical target substance in mixtures. The specific application considered is to detect the presence of chlorinated solvents in mixtures, although the approach is equally applicable for any form of spectral analysis. We use several kernels including polynomial (degree 1 and 2), radial basis function and spectral data specific kernels. Our results show that the radial basis function kernel consistently outperforms other kernels in one-class nearest neighbour setting. But the polynomial and spectral kernels perform no better than the linear kernel (which is directly equivalent to the standard Euclidean metric).

Chapter 1

One-Class Classification

In this chapter we introduce the concept of one-class classification (OCC) and formulate the motivation and the problem definition for employing them in the classification of chemical spectral data. In Section 1.1, an introduction to the definition of OCC is presented. Section 1.2 compares OCC with the multi-class classification problem and outlines their characteristics. In Section 1.3 we discuss the methods to measure the performance of OCC algorithms. Section 1.4 discusses the motivation and problem formulation for employing OCC algorithms for the classification of chlorinated solvent data. Section 1.5 summarizes the overall structure of the thesis and Section 1.6 details the research publications that resulted from this research work.

1.1. Introduction to One-class Classification

The traditional multi-class classification paradigm aims to classify an unknown data object into one of several pre-defined categories (two in the simplest case of binary classification). A problem arises when the unknown object does not belong to any of those categories. Let us assume that we have a training data set comprising of instances of fruits and vegetables. Any binary classifier can be applied to this problem, if an unknown test object (within the domain of fruits and vegetables e.g. apple or potato) is given for classification. But if the test pattern is from an entirely different domain (for example a cat from the category animals), the behaviour of the classifier would be 'undefined'. The binary classifier is confined to classifying all test objects into one of the two categories on which it is trained, and will therefore classify the cat as either a fruit or a vegetable. Sometimes the classification task is just not to allocate a test sample into predefined categories but also to decide if it belongs to a particular class or not. In the above example an apple belongs to class fruits and the cat does not.

In one-class classification [1][2], one of the classes (which we will arbitrarily refer to as the positive or target class) is well characterized by instances in the training data, while the

other class (negative or outlier) has either no instances or very few of them, or they do not form a statistically-representative sample of the negative concept.

To motivate the importance of one-class classification, let us consider some scenarios. A situation may occur, for instance, where we want to monitor faults in a machine. A classifier should detect when the machine is showing abnormal / faulty behaviour. Measurements on the normal operation of the machine (positive class training data) are easy to obtain. On the other hand, most faults would not have occurred hence we may have little or no training data for the negative class. Another example is the automatic diagnosis of a disease. It is relatively easy to compile positive data (all patients who are known to have the disease) but negative data may be difficult to obtain since other patients in the database cannot be assumed to be negative cases if they have never been tested, and such tests can be expensive. As another example, a traditional binary classifier for text or web pages requires arduous pre-processing to collect negative training examples. For example, in order to construct a "homepage" classifier [3], sample of homepages (positive training examples) and a sample of non-homepages (negative training examples) need to be gleaned. In these and other situations, collection of negative training examples is challenging because it either represent improper sampling of positive and negative classes or involves manual bias.

1.2. One-class Classification Vs Multi Class Classification

In a conventional multi class classification problem, data from two (or more) classes are available and the decision boundary is supported by the presence of example samples from each class. Most conventional classifiers assume more or less equally balanced data classes and do not work well when any class is severely under-sampled or is completely absent.

Moya et al. [4] originate the term "One-Class Classification" in their research work. Different researchers have used other terms such as "Outlier Detection[1]" [6], "Novelty Detection[2]" [9] or "Concept Learning" [10] to represent similar concept. These terms originate as a result of different applications to which one-class classification has been applied. Juszczak [11] defines One-Class Classifiers as class descriptors that are able to learn restricted domains in a multi-dimensional pattern space using primarily just a positive set of examples.

[1] Readers are advised to refer to detailed literature survey on outlier detection by Chandola et al. [5]

[2] Readers are advised to refer to detailed literature survey on novelty detection by Markou and Singh[7,8]

As mentioned by Tax [2], the problems that are encountered in the conventional classification problems, such as the estimation of the classification error, measuring the complexity of a solution, the curse of dimensionality, the generalization of the classification method also appear in OCC and sometimes become even more prominent. As stated earlier, in OCC tasks either the negative examples is absent or available in limited amount, so only one side of the classification boundary can be determined using only positive data (or some negatives). This makes the problem of one-class classification harder than the problem of conventional two-class classification. The task in OCC is to define a classification boundary around the positive (or target) class, such that it accepts as many objects as possible from the positive class, while it minimizes the chance of accepting the outlier objects. Since only one side of the boundary can be determined, in OCC, it is hard to decide on the basis of just one-class how tightly the boundary should fit in each of the directions around the data. It is also harder to decide which features should be used to find the best separation of the positive and outlier class objects. In OCC a boundary has to be defined in all directions around the data, particularly, when the boundary of the data is long and non-convex, the required number of training objects might be very high.

1.3. Measuring Classification Performance of One-class Classifiers

As mentioned in the work of Tax [2], a confusion matrix (see Table 1) can be constructed to compute the classification performance of one-class classifiers. To estimate the computation of the true error (as in multi class classifiers), the complete probability density of both the classes should be known. In the case of one-class classification, the probability density of only the positive class is known. This means that only the number of positive class objects which are not accepted by the one-class classifier i.e. the false negatives (F^-) can be minimized. In the absence of examples and sample distribution from outlier class objects, it is not possible to estimate the number of outliers objects that will be accepted by the one-class classifier (false positive, F^+). Furthermore, it can be noted that since $T^+ + F^- = 1$ and $F^+ + T^- = 1$, thus the main complication in OCC is that only T^+ and F^- can be estimated and nothing is known about F^+ and T^-. Therefore, limited amount of outlier class data is required to estimates the performance and generalize the classification accuracy of a one-class classifier.

	Object from target class	Object from outlier class
Classified as a target object	True positive, T^+	False positive, F^+
Classified as an outlier object	False negative, F^-	True negative, T^-

Table 1: Confusion Matrix for OCC. (Source: Tax [2])

1.4. Motivation and Problem Formulation

As discussed above in Sections 1.1, 1.2 and 1.3, OCC presents a classification scheme in which the samples from negative / outlier class are not present, very rare or statistically do not represent the negative concept. It also imposes a restriction on estimating the errors of the one-class classifier model when the negative samples are not abundant. If there is a severe lack of negative examples, the performance one-class classifier can be estimated using artificially generated outliers [1]. Improper or biased choice of outliers may not be able to generalize the one-class classifier's performance. Tax and Duin [1] propose to generate artificial outliers uniformly in a hypershpere such that it fits the target class as tight as possible to estimate errors (see detailed discussion of this method in Section 2.4.2).

Raman Spectroscopy [12] is spectroscopic method based on inelastic scattering of monochromatic light when a chemical substance is illuminated using a laser. A Raman spectrum is produced due to the vibration and rotational motions of the molecules of the substance which shows the intensities at different wavelengths. A Raman spectrum of every pure substance is unique and it can be regarded as its 'molecular fingerprint'. This property can be used as a signature for unambiguous identification of chemical substances.

In practice, chemical substances may not occur in their pure form but as mixtures of two or more chemical substances in various proportions. This makes the task of identification of target substance more challenging as the peaks in the resulting Raman spectrum get convolved because of the influence of other chemical substances in the mixture. An example would be the spectral library search, where the presence of a substance in a mixture is being

searched in a spectral database. There exist standard library search methods; however they may not be able to capture the intricacies outlined above. Therefore, there is a room for the development of new spectral search methods that can work efficiently in conditions where standard search methods fail.

It is exigent to build classifiers for the detection of target substance in mixtures, when the outliers are absent or not properly sampled. For our research, we undertake the task of identifying the presence or absence of chlorinated solvents in a mixture of various chlorinated and non-chlorinated solvents. Chlorinated solvents are environmentally hazardous and there needs to be proper disposal scheme for such substances, if present in their raw form or as a constituent of mixture. It is easy to collect samples for training a one-class classifier that contains chlorinated solvents in pure or mixture form. However to build a set of samples that are representative of negative concept is very difficult. Because any mixture that does not contain chlorine can be considered an outlier sample, therefore the choices are unlimited and the training samples thus gleaned will not statistically represent the negative concept. In such a case, it is very difficult to build a multi-class classifier (binary classifier here) for detecting the presence or absence of chlorine in a mixture that can generalize the results. This limitation paves the way for the deployment of OCC scheme that uses the target samples only (or with few outliers) during training phase.

There are various methods quoted in literature to tackle the problem of OCC (see Section 2.3, 2.4 and 2.5 for detailed discussion). Recently there is a growing interest in the study of kernels in machine learning tasks [13,14]. In our research work, we have used the kernels as distance metric to implement one-class nearest neighbour approach to detect the presence or absence of chlorinated solvents in a mixture.

1.5. Overview of Thesis

The thesis is divided into five chapters. In Chapter 2, we propose a taxonomy for the study of OCC methods based on the availability of data, algorithms used and the application domains applied. Such a taxonomy is useful for researchers who plan to work in the vast field of OCC, to limit their research effort and focus more on the problem to be tackled. Based on the proposed taxonomy, we provide a comprehensive literature review on the recent advances in the field of OCC, followed by guidelines for the study of OCC and open research areas in this field.

In Chapter 3, we briefly introduce the concept of Raman Spectroscopy. We also present various similarity and dissimilarity measures used to compare spectra. These (dis)similarity methods includes the standard, non-standard and more recent measures that are used in spectral library search for the identification of substances in mixtures. We also introduce two domain-specific spectral kernels and propose a modified Euclidean metric specific for chemical spectral data. The chlorinated solvent data used in our research work is explained in this chapter. We introduce the concept of spectral library search and conduct spectral search experiments on the chlorinated solvent data and present the results.

Chapter 4 captures the importance of kernels in the machine learning tasks. We present a short research review on incorporating kernels as distance metrics for multi class classification using the nearest neighbour approach. We later present the already existing one-class nearest neighbour approach and propose the use of kernels as distance metric instead of the conventional methods like Euclidean metric for implementing the one-class nearest neighbour approach.

Chapter 5 presents the results of our experimentation on the chlorinated solvent dataset using the proposed approach of kernel-based one-class nearest neighbours. We discuss several aspects of our experiments including parameter setting, choice of kernels, varying the number of neighbours etc. Then we summarize our conclusions and present the future work.

1.6. Publications Resulting from the Thesis

The work in the present thesis resulted in the following publications:

- A Survey of Recent Trends in One-class Classification, Shehroz Khan and Michael G. Madden, Proceedings of the 20th Irish Conference on Artificial Intelligence and Cognitive Science, Dublin, 2009, in the LNAI volume 6206, pp181-190, Springer-Verlag
- Kernel-Based One-Class Nearest Neighbor Approach for Identification of Chlorinated Solvents, Shehroz S. Khan and Michael G. Madden, Pittsburgh Conference (PITTCON-2010), Orlando, USA.

Chapter 2

Review: One-class Classification and its Applications

The OCC problem has been studied by various researchers using different methodologies in a wide range of application domains. In this chapter we briefly present the related research review work in the field of OCC in Section 2. In Section 2.2, we propose a new taxonomy to be used for the study of OCC problems. This differentiating factor of this taxonomy from the previous survey work in OCC is that the previous surveys have been more focussed on either specific application domains or centred on specific algorithms or methods. Since the area of OCC is quite large, our proposed taxonomy gives a researcher the opportunity to focus on specific area as per their research requirements. Based on the taxonomy we present a comprehensive literature review of the state-of-the-art OCC algorithms, their importance, applications and limitations in Sections 2.3, 2.4 and 2.5. In Section 2.6 we discuss certain open questions in the field of OCC.

2.1. Related Review Work in OCC

In recent years, there has been a considerable amount of research work carried out in the field of OCC. Researchers have proposed several OCC algorithms to deal various classification problems. Mazhelis [15] presents a review of OCC algorithms and analyzed its suitability in the context of mobile-masquerader detection. In the paper, the author proposes a taxonomy of one-class classifiers classification techniques based on:

- The internal model used by classifier (density, reconstruction or boundary based)
- The type of data (numeric or symbolic), and
- The ability of classifiers to take into account temporal relations among feature (yes or no).

This survey on OCC describes a lot of algorithms and techniques; however it does not cover the entire spectrum studied under the field called one-class classification. As we describe in subsequent sections, one-class classification has been termed and used by various

researchers by different names in different contexts. The survey presented by Mazhelis [15] proposes a taxonomy suitable to evaluate the applicability of OCC to the specific application domain of mobile-masquerader detection. In our review work, we neither restrict ourselves to a particular application domain, nor to any specific algorithms that are dependent on type of the data or model. Our aim is to cover as many algorithms, designs, contexts and applications where OCC has been applied in multiple ways (as briefed by way of examples in Section 1.1). Little of the research work presented in our review may be found in the survey work of Mazhelis, however our review on OCC encompasses a broader definition of OCC and does not intend to duplicate or re-state their work.

2.2. Proposed Taxonomy

Based on the research work carried out in the field of OCC using different algorithms, methodologies and application domains, we propose a taxonomy for the study of OCC problems. The taxonomy can be categorized into three categories on the basis of (see Figure 1):

(i) Availability of Training Data: Learning with positive data only or learning with positive and unlabeled data and / or some amount of outlier samples.

(ii) Methodology Used: Algorithms based on One-class Support Vector Machines (OSVMs) or methodologies based on algorithms other than OSVMs.

(iii) Application Domain Applied: OCC applied in the field of text / document classification or in the other application domains.

The proposed categories are not mutually exclusive, so there may be some overlapping among the research carried out in each of these categories. However, they cover almost all of the major research conducted by using the concept of OCC in various contexts and application domains. The key contributions in most OCC research fall into one of the above-mentioned categories. In the subsequent subsections, we will consider each of these categories in detail.

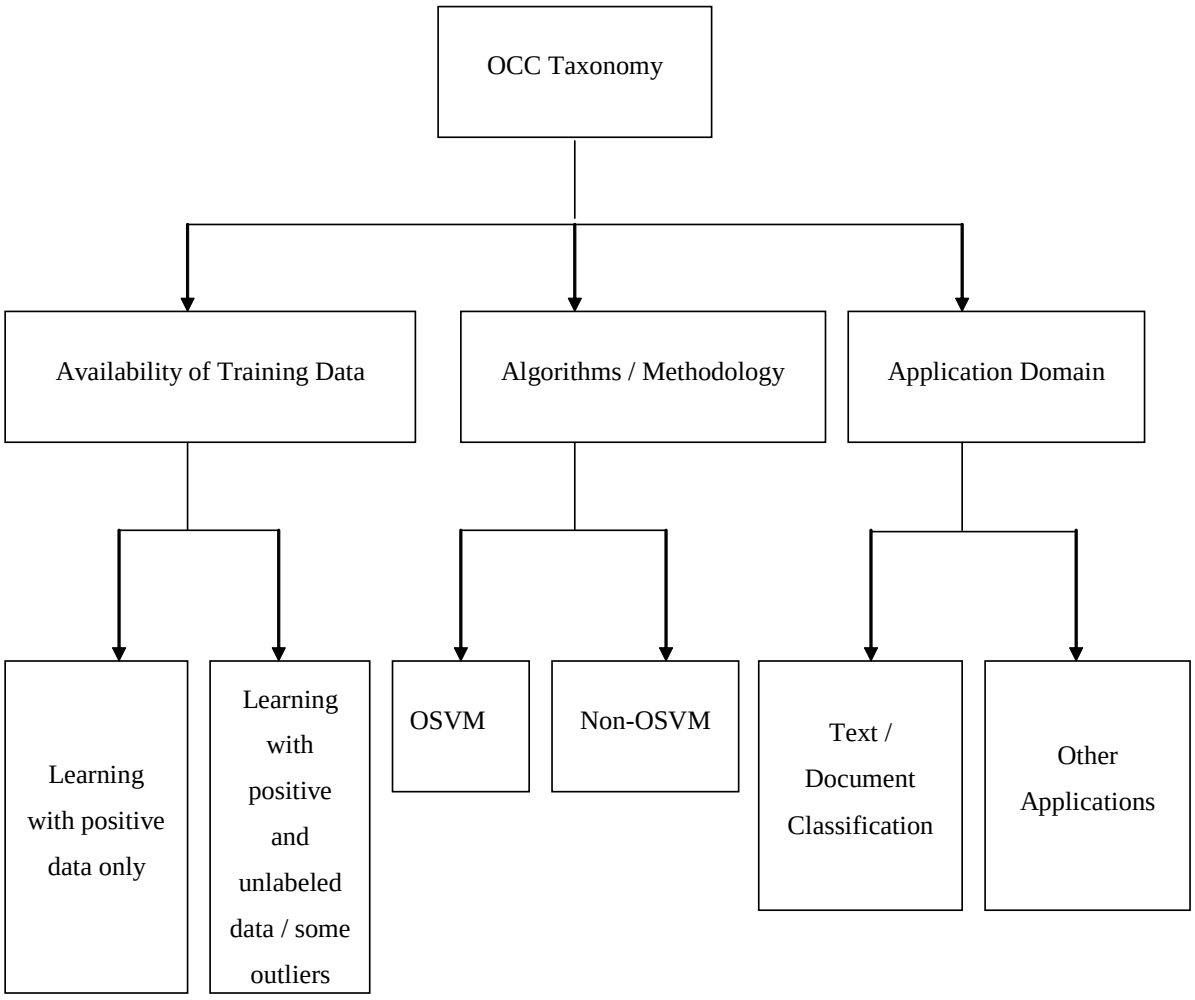


Figure 1: The Proposed Taxonomy for the Study of OCC Techniques

2.3. Category 1: Availability of Training Data

Availability of training data plays a pivotal role in any OCC algorithm. Researchers have studied OCC extensively under three broad categories:

a) Learning with positive examples only.
b) Learning with positive examples and some amount of poorly sampled negative examples.
c) Learning with positive and unlabeled data.

Category c) has been a matter of much research interest among the text / document classification community [16-18] that has been discussed in detail in Section 2.5.1.

Tax and Duin [19,20] and Schölkopf et al. [21] develop various algorithms based on support vector machines to tackle the problem of OCC using positive examples only; for a detailed discussion on them, refer to Section 2.4.2. The main idea behind these strategies is to construct a decision boundary around the positive data so as to differentiate them from the outlier / negative data.

For many learning tasks, labelled examples are rare while numerous unlabeled examples are easily available. The problem of learning with the help of unlabeled data given a small set of labelled examples was studied by Blum and Mitchell [22] by using the concept of co-training. The co-training settings can be applied when a data set has natural separation of their features. Co-training algorithms incrementally build classifiers over each of these feature sets. Blum and Mitchell show the use co-training methods to train the classifiers in the application of text classification. They show that under the assumptions that each set of features is sufficient for classification, and the feature sets of each instance are conditionally independent given the class, PAC (Probably Approximately Correct) learning [23] guarantees on learning from labelled and unlabeled data. Assuming two views of examples that are redundant but not correlated, they prove that unlabeled examples can boost accuracy. Denis [24] was the first to conduct a theoretical study of PAC learning from positive and unlabeled data. Denis proves that many concepts classes, specifically those that are learnable from statistical queries, can be efficiently learned in a PAC framework using positive and unlabeled data. However, the trade-off is a considerable increase in the number of examples needed to achieve learning, although it remains polynomial in size. DeComite et al. [25] give evidence with both theoretical and empirical arguments that positive examples and unlabeled examples can boost accuracy of many machine learning algorithms. They noted that the learning with positive and unlabeled data is possible as soon as the weight of the target concept (i.e. the ratio of positive examples) is known by the learner. An estimate of the weight can be obtained from a small set of labelled examples. Muggleton [26] presents a theoretical study in the Bayesian framework where the distribution of functions and examples are assumed to be known. Liu et al. [27] extend their result to the noisy case. Sample complexity results for learning by maximizing the number of unlabeled examples labelled as negative while constraining the classifier to label all the positive examples correctly were presented in their research work. Further details on the research carried out on training classifiers with labelled positive and unlabeled data is presented in Section 2.5.1.

2.4. Category 2: Algorithms Used

Most of the major OCC algorithms development can be classified under two broad categories, as has been done either using:

- One-class Support Vector Machines (OSVMs), or
- Non-OSVMs methods (including various flavours of neural networks, decision trees, nearest neighbours and others).

Before we move on to discuss OSVM we briefly introduce the support vector machines for standard two class classification problem in the next section.

2.4.1. Support Vector Machines

The support vector machine (SVM) [13][28] is a training algorithm for learning classification and regression rules from the data. The support vector machines are based on the concept of projecting a data set in high dimension feature space and determining optimal hyper-planes for separating the data from different classes [13]. Two key elements in the implementation of SVM are the techniques of mathematical programming and kernel functions [28]. The parameters are found by solving a quadratic programming problem with linear equality and inequality constraints; rather than by solving a non-convex, unconstrained optimization problem.

For training data that is linearly separable, a hyper-plane is constructed that separates the positive from the negative examples with maximum margin. The points x which lie on the hyper-plane satisfy $w.x+b=0$, where w is normal to the hyper-plane, $|b|/\|w\|$ is the perpendicular distance from the hyper-plane to the origin, and $\|w\|$ is the Euclidean norm of w **(**as shown in Figure 2**)**. Let d_+ (and d_-) be the shortest distance from the separating hyper-plane to the closest positive (negative) example, and define the "margin" of a separating hyper-plane to be $d_+ + d_-$. For the linearly separable case, the support vector algorithm simply looks for the separating hyper-plane with largest margin.

This can be formulated as follows: suppose that all the training data satisfy the following constraints:

$$w.x_i + b \geq +1, \qquad y_i = +1 \qquad \text{Equation 1}$$

$$w.x_i + b \leq -1, \qquad y_i = -1 \qquad \text{Equation 2}$$

with the decision rule given by

$$f_{w,b}(x) = \text{sign}\,(w.\,x + b) \qquad \text{Equation 3}$$

The SVM can be used to learn non-linear decision functions by first mapping the data X to some higher dimensional feature space H and constructing a separating hyper-plane in this space. Denoting the mapping to feature space by

$$X \rightarrow H \qquad \text{Equation 4}$$

$$x \mapsto \phi(x) \qquad \text{Equation 5}$$

where $\phi(x)$ is the projection of x in the feature space H.

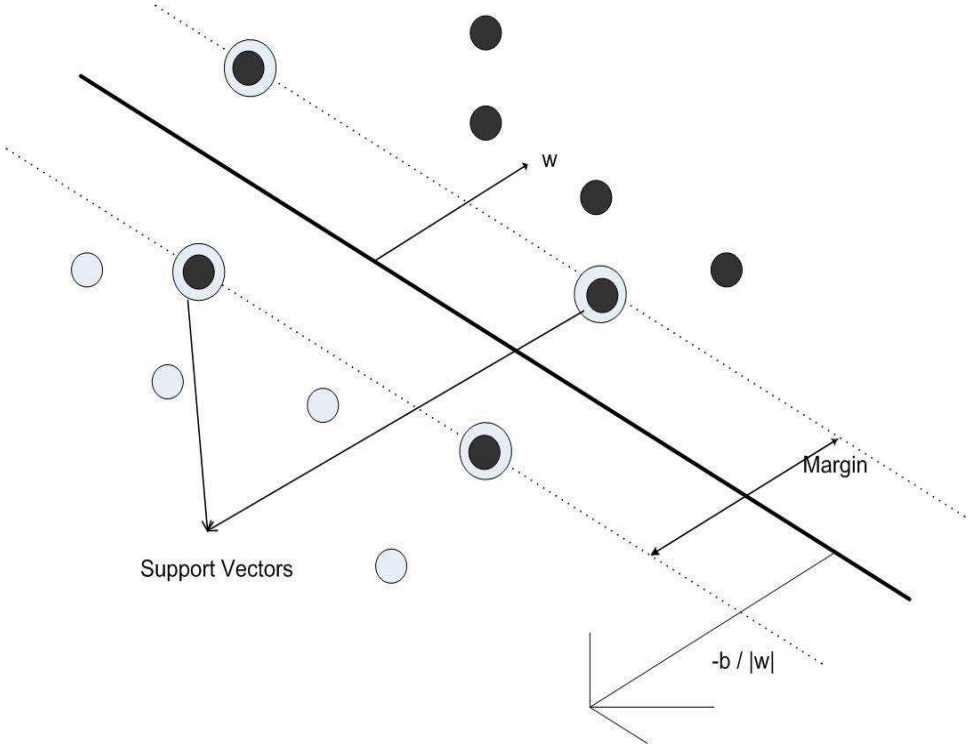


Figure 2: Separating hyper-plane for the separable case. The support vectors are shown with double circles (Source [28].

Omitting mathematical calculations, the decision function as mentioned in

Equation 3, comes in the form of inner products $\phi(x).\phi(z)$. Mapping the data to H is time consuming and storing it may be impossible, e.g. if H is infinite dimensional. However, the data only appear in inner products, a computable function is required that gives the value of the inner product in H without performing the mapping. Hence a kernel function can be introduced [28]:

$$K(x, z) = (\phi(x).\ \phi(z)) \qquad \text{Equation 6}$$

The kernel function allows constructing an optimal separating hyper-plane in the space H without explicitly performing calculations in this space. Commonly used kernels include [29]:

Polynomial kernel → $K(x, y) = (1 + (x, y))^d$

Radial Basis Function (RBF) → $K(x, y) = \exp\left(-\|x - y\|^2 / (2\sigma^2)\right)$

where σ is width of the kernel

Sigmoidal → $K(x, y) = \tanh(\kappa(x.y) + \Theta)$, with gain κ and offset Θ

This is called 'kernel trick' or 'kernel approach' and gives the SVM great flexibility. With a suitable choice of parameters, SVM can separate any consistent data set. For noisy data, slack variables can be introduced to allow training errors.

In the following subsection we explain the main algorithms that have been used in the OSVM framework and then in Section 2.4.3 we discuss other main Non-OSVM algorithms to handle OCC problem.

2.4.2. One-class Support Vector Machine (OSVM)

The one-class classification problem is often solved by estimating the target density [4], or by fitting a model to the data support vector classifier [13]. Tax and Duin [19,20] seek to solve the problem of OCC by distinguishing the positive class from all other possible patterns in the pattern space. They constructed a hyper-sphere around the positive class data that encompasses almost all points in the data set with the minimum radius. This method is called the Support Vector Data Description (SVDD).

Assume a data set containing N data objects, $\{x_i, i = 1,2,\ldots, N\}$ and the hyper-sphere is described by centre **a** and radius R (See Figure 3). To fit the hyper-sphere to the data, an error function L is minimized that contains the volume of the hyper-sphere and the distance from the boundary of the outlier objects. The solution is constrained with the requirement that (almost) all data is within the hyper-sphere. In operation, an SVDD classifier rejects a given test point as outlier if it falls outside the hyper- sphere. To allow the possibility of outliers in the training set, the distance from x_i to the centre **a** should not be strictly smaller than R, but larger distances should be penalized. Therefore, slack variables $\boldsymbol{\xi}$ is introduced which measure the distance to the boundary, if an object is outside the description. An extra

parameter C has to be introduced for the trade-off between the volume of the hyper-sphere and the number of target objects accepted. This results in the following error and constraints:

$$L(R, a, \xi) = R^2 + C\sum_i \xi_i \qquad \text{Equation 7}$$

$$\|x_i - a\|^2 \le R^2 + \xi_i \ , \forall_i \qquad \text{Equation 8}$$

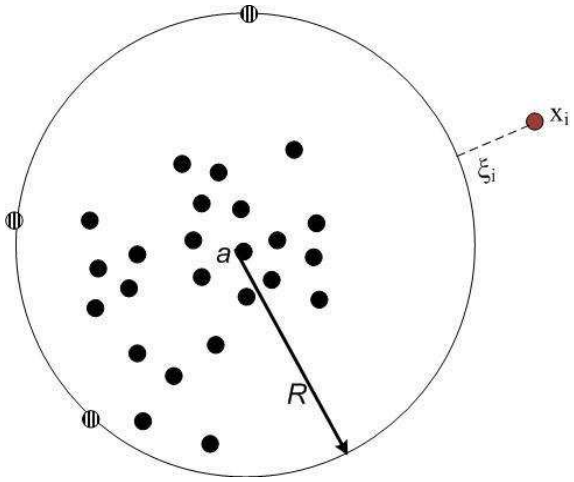


Figure 3 : The hyper-sphere containing the target data, with centre a and radius R. Three objects are on the boundary are the support vectors. One object x_i is outlier and has $\xi_i > 0$ (Source: Tax [2]).

In order to train this model, there is a possibility of rejecting some fraction of the positively-labelled training objects, when volume of the hyper-sphere decreases. Furthermore, the hyper-sphere model of the SVDD can be made more flexible by introducing kernel functions. Tax [2] considers Polynomial and a Gaussian kernel and found that the Gaussian kernel works better for most data sets (Figure 4). Tax uses different values for the width of the kernel, s. The larger the width of the kernel, the fewer support vectors are selected and the description becomes more spherical. In Figure 4 it can be seen that except for the limiting case where s becomes very large, the description is tighter than the original spherically shaped description or the description with the Polynomial kernels. Increasing s decreases the number of support vectors. Also, using the Gaussian kernel instead of the Polynomial kernel results in tighter descriptions, but it requires more data to support more flexible boundary. Their method becomes inefficient when the data set has high dimension. This method also doesn't work well when large density variation exist among the objects of data set, in such case it starts rejecting the low-density target points as outliers. Tax shows the usefulness of the approach on machine fault diagnostic data and handwritten digit data.

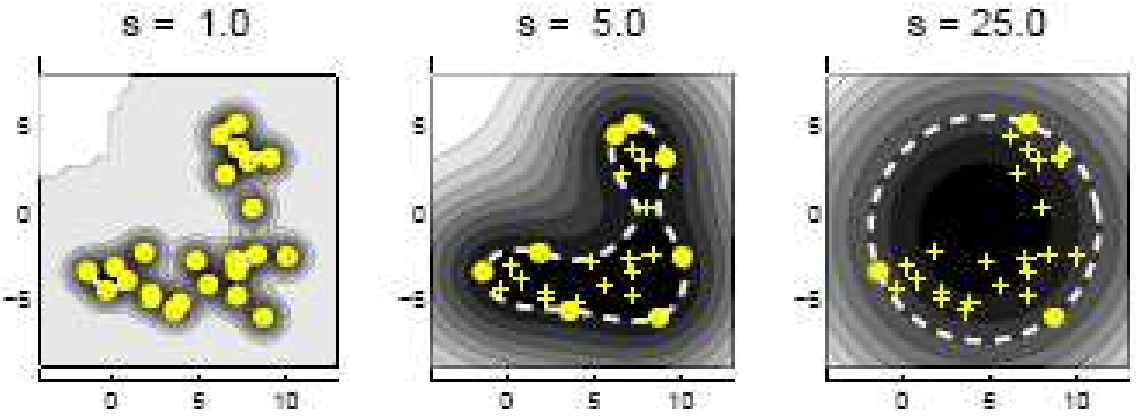


Figure 4 : Data description trained on a banana-shaped data set. The kernel is a Gaussian kernel with different width sizes s. Support vectors are indicated by the solid circles; the dashed line is the description boundary (Source: Tax [2]).

Tax and Duin [1] suggest a sophisticated method which uses artificially generated outliers, uniformly distributed in the hyper-sphere, to optimize the OSVM parameters in order to balance between over-fitting and under-fitting. The fraction of the accepted outliers by the classifier is an estimate of the volume of the feature space covered by the classifier. To compute the error without the use of outlier examples, they uniformly generate artificial outliers in and around the target class. If a hyper-cube is used then in high dimensional feature space it becomes infeasible. In that case, the outlier objects generated from a hyper-cube will have very low probability to be accepted by the classifier. The volume in which the artificial outliers are generated has to fit as tight as possible around the target class. To make this procedure applicable in high dimensional feature spaces, they propose to generate outliers uniformly in a hyper-sphere. This is done by transforming objects generated from a Gaussian distribution. Their experiments suggest that the procedure to artificially generate outliers in a hyper-sphere is feasible for up to 30 dimensions.

Schölkopf et al. [30,31] present an alternative approach to the above-mentioned work of Tax and Duin on OCC, using a separating hyper-plane. In their method they construct a hyper-plane instead of a hyper-sphere around the data, such that this hyper-plane is maximally distant from the origin and can separate the regions that contain no data. They propose to use a binary function that returns +1 in 'small' region containing the data and -1 elsewhere. For a hyper-plane w which separates the data x_i from the origin with maximal margin ρ, the following holds

$$w.x_i \geq \rho - \xi_i \ , \ \xi_i \geq 0 \ , \ \forall_i \qquad \text{Equation 9}$$

And the function to evaluate a new test object **z** becomes

$$f_\nu(z, w, \rho) = I(w.z \le \rho)$$ Equation 10

Schölkopf et al. [31] then minimizes the structural error of the hyper-plane measured by $\|w\|$ and some errors, encoded by the slack variable ξ_i are allowed. To separate the dataset from the origin, a quadratic program needs to be solved. This results in the following minimization problem

$$\min\left(\frac{1}{2}\|w\|^2 - \rho + \frac{1}{\nu N}\sum_i \xi_i\right)$$ Equation 11

with the constraints given by equation $w.x_i \ge \rho - \xi_i$, $\xi_i \ge 0$, $\forall_i$.

A variable ν is introduced that takes values between 0 and 1 that controls the effect of outliers i.e. the hardness or softness of the boundary around the data. This variable ν can be compared with the parameter C presented in the Tax's SVDD. Schölkopf et al. [31] suggest the use of different kernels, corresponding to a variety of non-linear estimators. In practical implementations, this method and the SVDD method of Tax [2] operate comparably and both perform best when the Gaussian kernel is used. As mentioned by Campbell and Bennett [32], the origin plays a crucial role in this method, which is a drawback since the origin effectively acts as a prior for where the class abnormal instances are assumed to lie (termed as the problem of origin). The method has been tested on both synthetic and real-world data. Schölkopf et al. [31] present the efficacy of their method on the US Postal Services dataset of handwritten digits. The database contains 9298 digit images of size 16×16=256; the last 2007 constitute the test set. They trained the algorithm using a Gaussian kernel of width s=0.25, on the test set and used it to identify outliers. In their experiments, they augmented the input patterns with ten extra dimensions corresponding to the class labels of the digits, to help to identify mislabelled data as outliers. Their experiments show that the algorithm indeed extracts patterns which are very hard to assign to their respective classes and a number of outliers were in fact identified.

Manevitz and Yousef [33] investigate the usage of one-class SVM for information retrieval. Their paper proposes a different version of the one-class SVM as proposed by Schölkopf et al. [21], which is based on identifying outlier data as representative of the second class. The idea of this methodology is to work first in the feature space, and assume that not only the origin is member of the outlier class, but also all the data points close enough to the origin

are considered as noise or outliers (see Figure 5). Geometrically speaking, the vectors lying on standard sub-spaces of small dimension i.e. axes, faces, etc., are to be treated as outliers. Hence, if a vector has few non-zero entries, then this indicates that the pattern shares very few items with the chosen feature subset of the database. Therefore, this item will not serve as a representative of the class and will be treated as an outlier. Outliers can be identified by counting features with non-zero values and if they are less than a predefined threshold. The threshold can either be set globally or determined individually for different categories. Linear, sigmoid, polynomial and radial basis kernels were used in this work. They evaluate their results on the Reuters Data set [34] using the 10 most frequent categories. Their results were generally somewhat worse than the OSVM algorithm presented by Schölkopf et al. [21]. However they observe when the number of categories was increased, their version of SVM obtains better results.

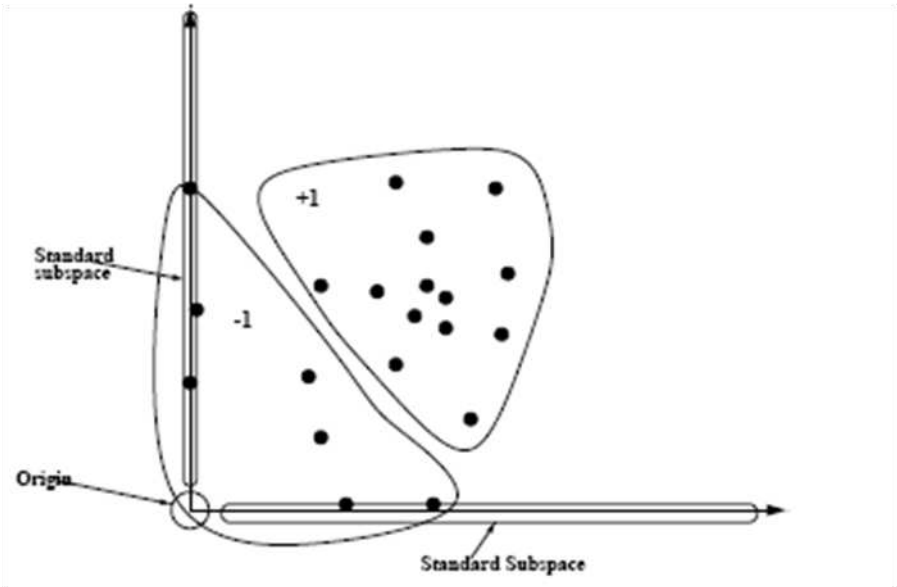


Figure 5 : Outlier SVM Classifier. The origin and small subspaces are the original members of the second class. The diagram is conceptual only (Source: Manevitz and Yousef [33]).

Li et al. [35] present an improved version of the OCC presented by Schölkopf et al. [21] for detecting anomaly in an intrusion detection system, with higher accuracy than other standard machine learning algorithms. Zhao et al. [36] used this method for customer churn prediction for the wireless industry data. They investigate the performance of different kernel functions for this version of one-class SVM, and show that the Gaussian kernel function can detect more churners than the Polynomial and Linear kernel.

An extension to the work of Tax and Duin [19,20] and Schölkopf [30] is proposed by Campbell and Bennett [32]. They present a kernel OCC algorithm that uses linear programming techniques instead of quadratic programming. They construct a surface in the input space that envelopes the data, such that the data points within this surface are considered targets and outside it are regarded as outlier. In the feature space, this problem condenses to finding a hyper-plane which is pulled onto the data points and the margin remains either positive or zero. To fit the hyper-plane as tight as possible, the mean value of the output of the function is minimized. To accommodate outliers, a soft margin can be introduced around the hyper-plane. Their algorithm avoids the problem of origin (as is apparent in the OCC algorithm presented by Schölkopf et al.[31]) by attracting hyper-plane towards the centre of data distribution rather than by repelling it away from a point outside the data distribution. Different kernels can be used to create hyper-planes; however they showed that RBF kernel can produce closed boundaries in input space while other kernels may not. A drawback of their method is that it is highly dependent on the choice of kernel width parameter, σ. However, if the data size is large and contains some outliers then σ, can be estimated. They showed their results on artificial data set, Biomed Data [37] and Condition Monitoring data for machine fault diagnosis.

Yu [38] proposes a one-class classification algorithm with SVMs using positive and unlabeled data and without labelled negative data and discuss some of the limitations of other OCC algorithms [1][[33]. On the performance of OSVMs under such scenario of learning with unlabeled data with no negative examples, Yu comments that to induce accurate class boundary around the positive data set, OSVM requires larger number of training data. The support vectors in such a case come only from positive examples and cannot create proper class boundary, which also leads to overfitting and underfitting of the data. Figure 6 (a) and (b) show the boundaries of SVM trained from positives and negatives and OSVM trained from only positives on a synthetic data set in a two-dimensional space. In this low-dimensional space, the ostensibly “smooth” boundary of OSVM is the result of incomplete SVs due to not using the negative SVs, and not as a result of the good generalization. This becomes much worse in high-dimensional spaces where more SVs around the boundary are needed to cover major directions. When the numbers of SVs in OSVM were increased, it overfits the data rather than being more accurate as shown in Figure 6 (c) and (d). However, such OSVM boundary might be the best achievable one when only positive data are available. Yu [39] presents an OCC algorithm called Mapping

Convergence (MC) to induce accurate class boundary around the positive data set in the presence of unlabeled data and without negative examples. The algorithm has two phases: mapping and convergence. In the first phase, a weak classifier (e.g. Rocchio [40][41]) is used to extract strong negatives from the unlabeled data. The strong negatives are those examples that are far from the class boundary of the positive data. In the second phase, a base classifier (e.g. SVM) is used iteratively to maximize the margin between positive and strong negatives for better approximation of the class boundary. Yu [39] also presents another algorithm called Support Vector Mapping Convergence (SVMC) that works faster than the MC algorithm. At every iteration, SVMC only uses minimal data such that the accuracy of class boundary is not degraded and the training time of SVM is also saved. However, the final class boundary is slightly less accurate than the one obtained by employing MC. They show that MC and SVMC perform better than other OCC algorithms and can generate accurate boundaries comparable to standard SVM with fully labelled data.

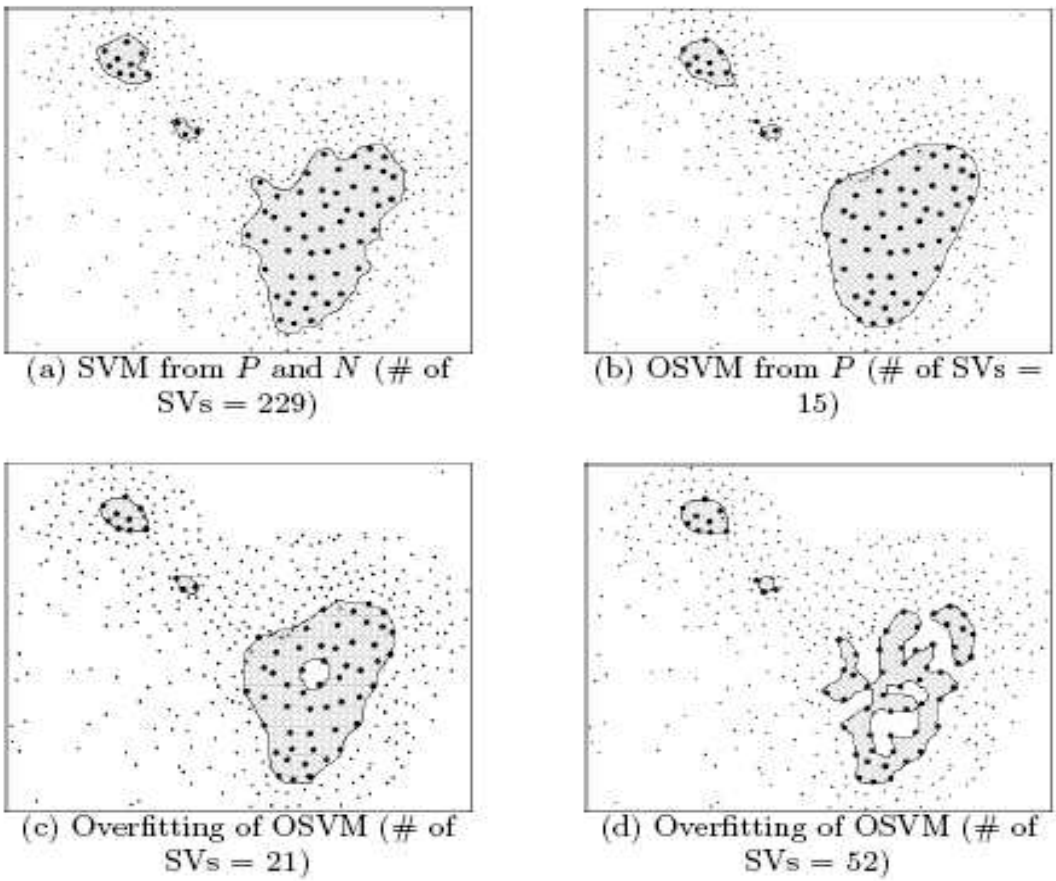


Figure 6 : Boundaries of SVM and OSVM on a synthetic data set: big dots: positive data, small dots: negative data (Source Yu, H. [38])

2.4.3. One-Class Classifiers other than OSVMs

2.4.3.1. One-Class Classifier Ensembles

As in the normal classification problems, one classifier hardly ever captures all characteristics of the data. However, using just the best classifier and discarding the classifiers with poorer performance might waste valuable information [42]. To improve the performance of different classifiers which may differ in complexity or training algorithm, an ensemble of classifiers is a viable solution. This may not only increase the performance, but can also increase the robustness of the classification [43]. Classifiers are commonly ensembled to provide a combined decision by averaging the estimated posterior probabilities. This simple algorithm already gives very good results for multi-class problems [44]. When Bayes' theorem is used for the combination of different classifiers, under the assumption of independence, a product combination rule can be used to create a classifier ensemble. The outputs of the individual classifiers are multiplied and then normalized (this is also called the logarithmic opinion pool [45]). In the combination of one-class classifiers, the situation is different. One-class classifiers cannot directly provide posterior probabilities for target (positive class) objects, because accurate information on the distribution of the outlier data is not available. In most cases, however, assuming that the outliers are uniformly distributed, the posterior probability can be estimated. Tax [2] mentions that in some OCC methods distance is estimated instead of probability. If there exists a combination of distance and probability outputs, the outputs should be standardized before they can be combined. To use the same type of combining rules as in conventional classification ensembles, the distance measures must be transformed into a probability measure. As a result, combining in OCC improves performance, especially when the product rule is used to combine the probability estimates. Classifiers can be combined in many ways. One of the ways is to use different feature sets and to combine classifiers trained on each of them. Another way is to train several classifiers on one feature set. Since the different feature sets contain much independent information, combining classifiers trained in different feature spaces provide better accuracy.

Tax and Duin [46] investigate the influence of the feature sets, their inter-dependence and the type of one-class classifiers for the best choice of the combination rule. They use a normal density and a mixture of Gaussian and the Parzen density estimation [9] as two types of one-class classifiers. They use four models, the SVDD [20], K-means clustering [9], K-

center method [47] and an auto-encoder neural network [10]. The Parzen density estimator emerged as the best individual one-class classifier on the handwritten digit pixel dataset [48]. They showed that combining classifiers trained in different feature spaces is useful. In their experiments, the product combination rule gave the best results. The mean combination rule suffers from the fact that the area covered by the target set tends to be overestimated. As a result of that more outlier objects may be accepted than it is necessary.

Juszczak and Duin [49] extend combining one-class classifier for classifying missing data. Their idea is to form an ensemble of one-class classifiers trained on each feature, pre-selected group of features or to compute a dissimilarity representation from features. The ensemble should be able to predict missing feature values based on the remaining classifiers. As compared to standard methods, their method is more flexible, since it requires much fewer classifiers and do not require re-training of the system whenever missing feature values occur. They also show that their method is robust to small sample size problems due to splitting the classification problem to several smaller ones. They compare the performance of their proposed ensemble method with standard methods used with missing features values problem on several UCI datasets [50]. Lai et al. [51] study combining one-class classifier for image database retrieval and showed that combining SVDD-based classifiers improves the retrieval precision. Ban and Abe [52] address the problem of building multi class classifier based on one-class classifiers ensemble. They studied two kinds of once class classifiers, namely, SVDD [20] and Kernel Principal Component Analysis [53]. They constructed a minimum distance based classifiers from an ensemble of one-class classifiers that is trained from each class and assigns a test sample to a given class based on its prototype distance. Their method gave comparable performance as SVMs on some benchmark data sets; however it is heavily dependent on the algorithm parameters. They also commented that their process could lead to faster training and better generalization performance provided appropriate parameters are chosen.

Boosting methods have been successfully applied to classification problems [54]. Their high accuracy, ease of implementation and wide applicability make them as a suitable choice among machine learning practitioners. Rätsch et al. [55] propose a boosting-like one-class classification algorithm based on a technique called barrier optimization [56]. They also show an equivalence of mathematical programs that a support vector algorithm can be translated into an equivalent boosting-like algorithm and vice versa. It has been pointed out by Schapire et al. [57] that boosting and SVMs are ‘essentially the same’ except for the way

they measure the margin or the way they optimize their weight vector: SVMs use the l_2-norm and boosting employs the l_1-norm. SVMs use the l_2-norm to implicitly compute scalar products in feature space with the help of kernel trick, where as boosting perform computation explicitly in feature space. They comment that SVMs can be thought of as a 'boosting' approach in high dimensional feature space spanned by the base hypotheses. Rätsch et al. [55] exemplify this translation procedure for a new algorithm called the one-class leveraging. Building on barrier methods, a function is returned which is a convex combination of the base hypotheses that leads to the detection of outliers. They commented that that the prior knowledge that is used by boosting algorithms for the choice of weak learners can be used in one-class classification. They show the usefulness of their results on artificially generated toy data and the US Postal Service database of handwritten characters.

2.4.3.2. Neural Networks

Ridder et al. [58] conduct an experimental comparison of various OCC algorithms. They compare a number of unsupervised methods from classical pattern recognition to several variations on a standard shared weight supervised neural network [59] proposed by Viennet [60]. The following unsupervised methods were included in their study:

a) Global Gaussian approximation
b) Parzen density estimation
c) 1-Nearest Neighbour method
d) Local Gaussian approximation (combines aspects of a) and c)).

They use samples from scanned newspaper images (at 600 dpi) as experimental datasets. The binary images were then reduced six-fold to approximately 1000×750 pixel grey value images. They show that Gaussian methods give the worst results, while the Parzen method suffers less from the problems of the Gaussian method. The 1- Nearest Neighbor method very clearly distinguishes the images from text better than any other method. The Local Gaussian performs much worse than the Parzen and the 1-nearest neighbor method, but it outperforms the simple Gaussian method. It is also the only method which does not suffer from the fact that background is classified as text. They also show that adding a layer with radial basis function improves performance.

Manevitz and Yousef [61] show how a simple neural network can be trained to filter documents when only positive information is available. In their design of the filter, they used a basic feed-forward neural network. To incorporate the restriction of availability of

only positive examples, they used the design of a feed forward network with a "bottleneck". They chose three level network with m input neurons, m output neurons and k hidden neurons, where k < m. The network is trained using standard back-propagation algorithm [62] to learn the identity function on the positive examples. The idea is that while the bottleneck prevents learning the full identity function on m-space; the identity on the small set of examples is in fact learnable. The set of vectors for which the network acts as the identity function is a sort of sub-space which is similar to the trained set. For testing a given vector, it is shown to the network, if the result is the identity; the vector is deemed interesting i.e. positive or else an outlier. Manevitz and Yousef [63] apply the auto-associator neural network to document classification problem. To determine acceptance threshold, they used a method based on a combination of variance and calculating the optimal performance. During training, they check the performance values of the test set at different levels of error. The training process is stopped at the point where the performance starts a steep decline. Then they perform a secondary analysis to determine an optimal real multiple of the standard deviation of the average error that serves as a threshold. The method was tested and compared with a number of competing approaches, i.e. Neural Network, Naïve Bayes, Nearest Neighbour, Prototype algorithm, and shown to outperform them.

Skabar [64] describes to learn a classifier based on feed-forward neural network using positive examples and corpus of unlabeled data containing both positive and negative examples. In conventional feed forward binary neural network classifier, positive examples are labelled as 1 and negative examples as 0. The output of the network represents the probability that an unknown example belongs to the target class, with threshold of 0.5 is set to decide whether an unknown sample belongs to either of the case. However, in this case, since unlabeled data contain some unlabeled positive examples, the output of the trained neural network may be less than or equal to the actual probability that an example belongs to the positive class. If it is assumed that the labelled positive examples adequately represent the positive concept, it can be hypothesized that the neural network will be able to draw a class boundary between negative and positive examples. Skabar shows [64] the application of the technique to the prediction of mineral deposit location.

2.4.3.3. Decision Trees

Various researchers have used decision tress to classify positive samples from a corpus of unlabeled examples. Decomite et al. [25] present experimental results showing that positive examples and unlabeled data can efficiently boost accuracy of the statistical query learning algorithms for monotone conjunctions in the presence of classification noise and experimental results for decision tree induction. They modify standard C4.5 [65] to get an algorithm that uses unlabeled and positive data and show the relevance of their method on UCI data sets [[50]]. Letouzey et al. [66] design an algorithm which is based on positive statistical queries (estimates for probabilities over the set of positive instances) and instance statistical queries (estimates for probabilities over the instance space). The algorithm guesses the weight of the target concept (the ratio of positive instances in the instance space) and then uses a hypothesis testing algorithm. They show that their algorithm can be estimated in polynomial time and is learnable from positive statistical queries and instance statistical queries only. Then, they design a decision tree induction algorithm, called POSC4.5, using only positive and unlabeled data. They present experimental results on UCI data sets [50] that are comparable to C4.5 algorithm [65]. Yu [38] comments that such rule learning methods are simple and efficient for learning nominal features but are tricky to use for problems of continuous features, high dimensions, or sparse instance spaces.

2.4.3.4. Other Methods

Wang et al. [67] investigate several one-class classification methods in the context of Human-Robot interaction for face and non-face classification. Some of the important methods used in their study are:

- Support Vector Data Description (SVDD) [2]
- Gaussian data description (GAUSS-DD) - that models the target class as a simple Gaussian distribution. Mahalanobis distance is used to avoid the density estimate that leads to numerical instabilities, which is defined as:

$$f(x) = (x - \mu)^T \sum^{-1} (x - \mu) \qquad \text{Equation 12}$$

- KMEANS-DD - where a class is described by k clusters, placed such that the average distance to a cluster centre is minimized. The cluster centres c_i are placed using the standard K-means clustering procedure. The target class is then characterized by

$$f(x) = \min_i (x - c_i)^2 \qquad \text{Equation 13}$$

The above two classifiers are defined as:

$$\text{Class}(x) = \begin{cases} \text{target}, & \text{if} \quad \text{Measurement}(x) \le \text{threshold}; \\ \text{non-target}, & \text{if} \quad \text{otherwise} \end{cases}$$

- The PCA-DD method, based on Principal Component Analysis, describes the target data by a linear subspace defined by the eigenvectors of the data covariance matrix Σ. Only k eigenvectors are used, which are stored in a d×k matrix W (where d is the dimensionality of the original feature space). To check if a test object is outlier, the reconstruction error is computed, which is the difference between the original object and its projection onto the subspace. This projection is computed by:

$$\chi_{proj} = W(W^T W)^{-1} W_X \qquad \text{Equation 14}$$

The reconstruction error is then given by $f(x) = \left\| x - \chi_{proj} \right\|^2$

- LP-DD is a linear programming method [68]. This data descriptor is constructed to describe target classes that can be represented in terms of distances to a set of support objects. This classifier uses the Euclidean distance by default. This classifier has the following form $f(x) = \sum w_i d(x, x_i)$. The weights w_i are optimized such that just a few weights stay non-zero, and the boundary is as tight as possible around the data,

Wang et al. [67] study the performance of these one-class classification methods on the object recognition dataset described in Wang and Lopes [69]. This dataset contains two parts. There are 400 pictures from AT&T/ORL face database [70] and 402 non-face pictures from their previous work [71]. They resize all patterns to 32×32 and all the experiments were carried out based on the PRTOOLS [72] and DDTOOLS [2]. For their analysis, they set face as the target class. In their experimentation they observe that SVDD attains better performance in comparison to other studied OCC methods. They comment that the good performance of SVDD in comparison to other methods can be attributed to its flexibility. The other methods use very strict models, such as planar shapes. They also investigate the effect of varying the number of features. They remark that more features do not always guarantee better results, because with an increase in the number of features, more training data are needed to reliably estimate the class models.

Ercil and Buke [73] report a different technique to tackle the OCC problem, based on fitting an implicit polynomial surface to the point cloud of features, to model the target class to

separate it from the outliers. They show the utility of their method for the problem of defect classification, where there are often lot of samples for the non-defective class but only a few samples for various defective classes. They use an implicit polynomial fitting technique and show a considerable improvement in the classification rate, in addition to having the advantage of requiring data only from non-defective motors in the learning stage.

Tax [2] presents a one-class nearest neighbour method, called nearest neighbour description (NN-d). In NN-d, a test object z is accepted when its local density is larger or equal to the local density of its nearest neighbour in the training set $NN^{tr}(z) = NN_1^{tr}(z)$. The first nearest neighbour is used for the local density estimation. The following acceptance function is used:

$$f_{NN^{tr}}(z) = I\left(\frac{\left\| z - NN^{tr}(z) \right\|}{\left\| NN^{tr}(z) - NN^{tr}\left(NN^{tr}(z)\right) \right\|} \leq 1 \right) \qquad \text{Equation 15}$$

This means that the distance from object z to its nearest neighbour in the training set $NN^{tr}(z)$ is compared to the distance from this nearest neighbour $NN^{tr}(z)$ to its nearest neighbour (see Figure 7).

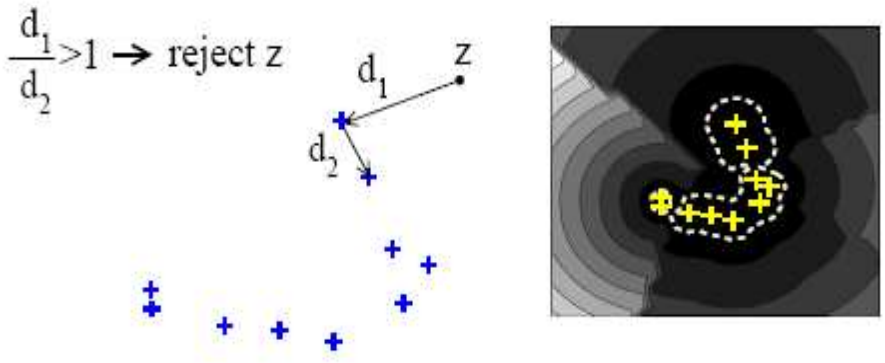


Figure 7 : The Nearest Neighbour Data Description (Source: Tax [2]).

This NN-d has several predefined choices to tune various parameters. First of all, different numbers of neighbours can be considered. One can use the distance to the k^{th} nearest neighbour, or the average of the k distances to the first k neighbours. Then this model can be termed as KNN-d. The value of threshold (default 1.0) can be changed to either higher or lower values. Increasing the number of neighbours will decrease the local sensitivity of the method, but it will make the method less noise sensitive. The other variations of one-class nearest neighbours are described in Section 4.3.

Tax and Duin [74] proposes a nearest neighbour method capable of finding data boundaries when the sample size is very low. The boundary thus constructed can be used to detect the targets and outliers. The method compares the distance from a test object to the training set to the nearest neighbour distance within the training set. This method has the disadvantage that it relies on the individual positions of the objects in the target set. Their method seems to be useful in situations where the data is distributed in subspaces. They tested the technique on both real and artificial data and found to be very useful when very little amount of training data exist (less than 5samples per feature).

Datta [75] modify the standard nearest neighbour algorithm [76] appropriate to learn a single class, called the positive class. The modified algorithm, NN-PC (nearest neighbour positive class), takes examples from only one-class as input. NN-PC learns a constant δ 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 δ from any training example will not be considered a member of the positive class. δ is calculated by

$$\delta = \text{Max}\{\forall x \ \text{Min}\{\forall y \neq x \ \text{dist}(x, y)\}\} \qquad \text{Equation 16}$$

where x and y are two examples of the positive class, and Euclidean distance (dist(…)) is used as the distance function.

While classifying test examples, if it varies too much from the positive examples, then it is classified as an outlier. Mathematically, if $\exists x : \text{dist}(x, \text{test}) < \delta$ then the test example is classified as member of the positive class, otherwise it is not. Datta also experimented with another similar modification called NN-PCN, that involves learning a vector $< \delta_1, \ldots \delta_n >$,where δ_i is the threshold for the i^{th} example. This modification records the distance to the closest example for each example. δ_i is calculated by

$$\delta_i = \text{Min}\{\forall y \neq x_i \ \text{dist}(x_i, y)\} \qquad \text{Equation 17}$$

where x_i is the i^{th} training example. To classify a test example same classification rule as above is used, that is, if $\exists x_i : \text{dist}(x_i, \text{test}) < \delta_i$ then the test example is classified as a member of the positive class.

Datta [75] also suggests a method to learn a Naive Bayes classifier from samples of positive class data only. Traditional Naive Bayes [76] attempts to find $p(C_i \mid A_1 = v_1 \ \& \ldots \& \ A_n = v_n)$,

that is, the probability of a class given an unlabeled example. By assuming that the attributes are independent and applying Bayes' theorem the previous calculation is proportional to:

$$\left[\prod_{j}^{attributes} p\left(A_j = v \mid C_i\right)\right] p\left(C_i\right) \qquad \text{Equation 18}$$

where A_j is an attribute, v is a value of the attribute, C_i is a class, and the probabilities are estimated using the training examples.

When only the positive class is available, the calculation of $p\left(C_i\right)$ (from Equation 18) cannot be done correctly. Datta [75] modify Naive Bayes to learn in a single class situation and call their modification as NB-PC (Naive Bayes Positive Class) that uses the probabilities of the attribute-values. NB-PC computes a threshold t as

$$t = Min\left[\forall x \prod_{j}^{attributes} p\left(A_j = v_i\right)\right] \qquad \text{Equation 19}$$

where $A_j = v_i$ is the attribute value for the example x and $p\left(A_j = v_i\right)$ is the probability of the attribute's i^{th} value. The probabilities for the different values of attribute A_j is normalized by the probability of the most frequently occurring v. During classification, if for the test example $\prod_{j}^{attributes}\left(A_j = v_i\right) \geq t$, then the test example is predicted as a member of the positive class. Datta tested the above positive class algorithms on various data sets taken from UCI repository [50] and conclude that NN-PCN seems to perform the worst, since it typically has precision and recall values lower than other discussed algorithms. Learning a different δ for each example does not intuitively seem like a reliable or stable way of predicting class membership, since δs can easily change depending on the training examples. They also observed that NN-PC and NB-PC have classification accuracy (both precision and recall values) close to C4.5's [65] value, although C4.5 was learning from all classes and they were learned using only one-class.

2.5. Category 3: Application Domain Applied

2.5.1. Text / Document Classification

Traditional text classification techniques require an appropriate distribution of positive and negative examples to build a classifier; thus they are not suitable for this problem of OCC. It is of course possible to manually label some negative examples, though depending on the

application domain, this may be a labour-intensive and a time consuming task. However, the core problem remains, that it is difficult or impossible to compile a set of negative samples that provides a comprehensive characterization of everything that is `not' the target concept, as is assumed by a conventional binary classifier. It is a common practice to build text classifiers using positive and unlabeled examples[3] as collecting unlabeled samples is relatively easy and fast in many text or Web page domains [27], [78]. In this subsection, we will discuss some of the algorithms that exploit this methodology with application to text classification.

The ability to build classifiers without negative training data is useful in a scenario if one needs to extract positive documents from many text collections or sources. Liu et al. [27] propose a method (called Spy EM) to solve this problem in the text domain. It is based on Naïve Bayesian classification (NB) and the Expectation Maximization (EM) algorithm [79]. The main idea of the method is to first use a technique to identify some reliable / strong negative documents from the unlabeled set. It then runs EM to build the final classifier. Yu et al. [3,80] propose a SVM based technique called PEBL (Positive Example Based Learning) to classify Web pages with positive and unlabeled pages. Once a set of strong negative documents is identified, SVM is applied iteratively to build a classifier. PEBL is sensitive to the number of positive examples. When the positive data is small, the results are often very poor. Li and Liu [17] propose an alternative method to learn to classify texts using positive and unlabeled data. Their method differs from PEBL in that they perform negative data extraction from the unlabeled set using the Rocchio method [40][4]. Although the second step also runs SVM iteratively to build a classifier, there is a key difference in selection of final classifier. Their technique selects a ‘good’ classifier from a set of classifiers built by SVM, while PEBL does not. Liu et al. [16] study the same problem and suggest that many algorithms that build text classifier with positive and unlabeled data are based on two strategies:

[3] For further reading on this topic , readers are advised to refer to survey paper by Zhang and Zuo [77]

[4] The basic idea of the algorithm is to represent each document, **e**, as a vector in a vector space so that documents with similar content have similar vectors. The value e_i of the i^{th} key-word is represented as the tf-idf weight [81]

- Identifying a set of reliable / strong negative documents from the unlabeled set. In this step, Spy-EM [27] uses a Spy technique, PEBL uses a technique called 1-DNF [3], and Roc-SVM [16] uses the Rocchio algorithm [40].
- Building a set of classifiers by iteratively applying a classification algorithm and then selecting a good classifier from the set. In this step, Spy-EM uses the Expectation Maximization (EM) algorithm with a NB classifier, while PEBL and Roc-SVM use SVM. Both Spy-EM and Roc-SVM have some methods for selecting the final classifier. PEBL simply uses the last classifier at convergence, which can be a poor choice.

These two steps together work in an iterative manner to increase the number of unlabeled examples that are classified as negative, while at the same time maintain the correct classification positive examples. It was shown theoretically by Liu et al. [27] that if the sample size is large enough, maximizing the number of unlabeled examples classified as negative while constraining the positive examples to be correctly classified will give a good classifier. Liu et al. [16] introduce two new methods, one for Step 1 (i.e. the Naïve Bayes method) and Step 2 (i.e. SVM alone) and perform an evaluation of all 16 possible combinations of methods for Step 1 and Step 2 (discussed above). They develop a benchmarking system called LPU (Learning from Positive and Unlabeled data) [82]. They also propose an approach based on a biased formulation of SVM that allows noise (or error) in positive examples. This soft margin version of biased-SVM uses two parameters, C_+ and C_- respectively, to weight both positive and negative errors differently. It can be expressed mathematically as:

$$\text{Maximizing} \quad \frac{1}{2}w^T w + C_+ \sum_{i=1}^{k-1} \xi_i + C_- \sum_{i=1}^{k-1} \xi_i \qquad \text{Equation 20}$$

$$\text{Subject to:} \quad y_i\left(w^T x_i + b\right) \geq 1 - \xi_i, \qquad i = 1,2,\ldots n$$

$$\xi_i \geq 0, \qquad i = 1,2,\ldots n$$

They experiment on two data sets, namely Reuters [34] and Usenet articles as compiled by Lang [83], and conclude that the biased-SVM approach outperforms all existing two-step techniques.

Yu et al. [84] explore SVMC [38,39] (for detail on this technique refers to Section 2.4.2) for performing text classification without labelled negative data. They use two commonly used corpora for text classification – Reuters [34] and WebKb [85] and compare their method

against six other methods: (1) Simple Mapping Convergence (MC); (2) OSVM; (3) Standard SVM trained with positive examples and unlabeled documents substituted for negative documents; (4) Spy-EM; (5) Naïve Bayes with Negative noise; (6) Ideal SVM trained from completely labelled documents. In their results they show that with a reasonable amount of positive documents, the MC algorithm gives the best results among all the methods considered. Their analysis shows that when the positive training data is not under-sampled, SVMC significantly outperforms other methods because SVMC tries to exploit the natural gap between positive and negative documents in the feature space, which eventually helps to improve the generalization performance.

Peng et al. [86] present a text classifier from positive and unlabeled documents based on Genetic Algorithms (GA) by adopting a two stage strategy (as discussed above). Firstly, reliable negative documents were identified by improved 1-DNF algorithm. Secondly, a set of classifiers were built by iteratively applying SVM algorithm on training example sets. Thirdly, they discuss an approach to evaluate the weighted vote of all classifiers generated in the iteration steps to construct the final classifier based on a GA. They comment that the GA evolving process can discover the best combination of the weights. Their problem statement is shown in Figure 8. They perform experiments on the Reuter data set [34] and compare their results against PEBL [80] and OSVM and showed that their GA based classification performs better.

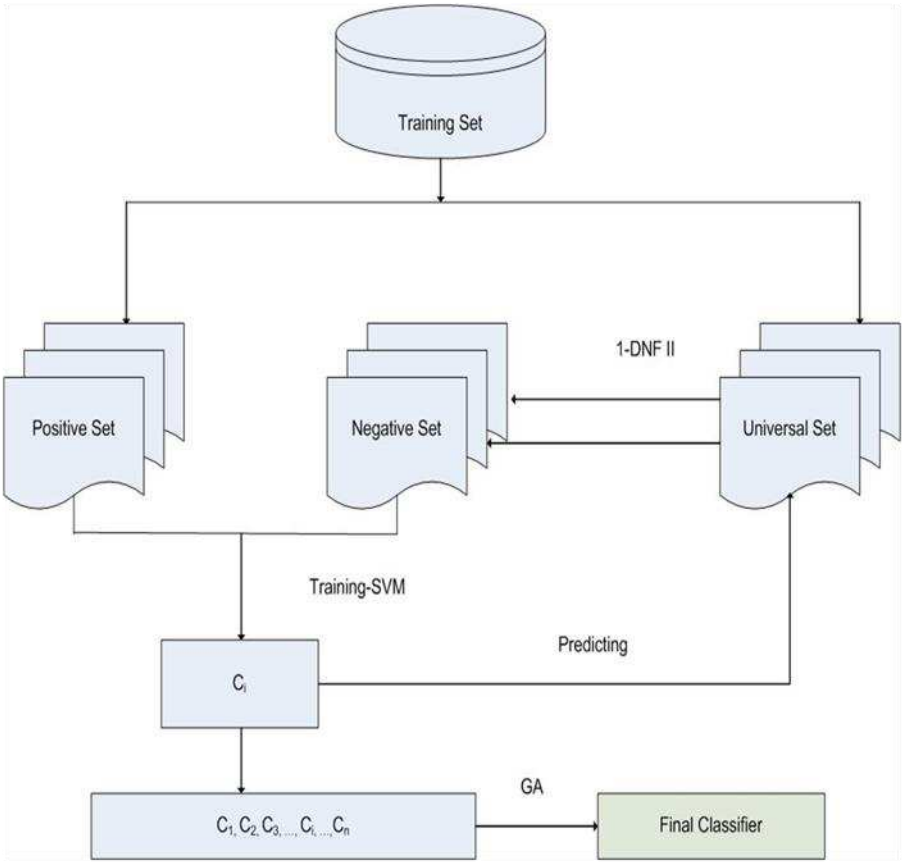


Figure 8 : Illustration of the procedure to build text classifiers from labeled and unlabeled examples based on GA. Ci represents the individual classifier produced by the ith iteration of the SVM algorithm. (Source: Peng et al. [86]).

Pan et al. [87] extend the concept of classifying positive examples with unlabeled samples in the Collaborative Filtering (CF) application. In CF, the positive data is gathered based on user interaction with the web like news items recommendation or bookmarking pages etc. However, due to ambiguous interpretations, limited knowledge or lack of interest of users, the collection of valid negative data gets hampered. Sometime negative and unlabeled positive data are severely mixed up and difficult to discern. Manually labelling negative data is not only intractable considering the size of the web but also will be poorly sampled. Traditional CF algorithms either label negatives data, or assume missing data as negative. Both of these approaches have their inherent problem of being expensive and biasing the recommendation results. Pan et al. [87] propose two approaches to one-class CF to handle the negative sparse data to balance the extent to which to treat missing values as negative examples. The first approach is based on weighted low rank approximation [88] that works on the idea of providing different weights to error terms of both positive and negative examples in the objective function. The second is based on sampling some missing values as negative examples based on some sampling strategies. They perform their experimentation

on real life data from social bookmarking site del.icio.us and Yahoo News data set and show that their method outperforms other state of the art CF algorithms.

Onoda et al. [89] report a document retrieval method using non-relevant documents. Users rarely provide a precise query vector to retrieve desired documents in the first iteration. In subsequent iterations, the user evaluates whether the retrieved documents are relevant or not, and correspondingly the query vector is modified in order to reduce the difference between the query vector and documents evaluated as relevant by the user. This method is called relevance feedback. The relevance feedback needs a set of relevant and non-relevant documents to work usefully. However, sometimes the initial retrieved documents that are presented to a user do not include relevant documents. In such a scenario, traditional approaches for relevance feedback document retrieval systems do not work well, because the systems need relevant and non relevant documents to construct a binary classification problem. To solve this problem, Onoda et al. propose a feedback method using information of non-relevant documents only, called non-relevance feedback document retrieval. A diagrammatic representation of the problem of non relevance feedback is shown in Figure 9. Their design of non-relevance feedback document retrieval is based on OSVM [21]. Their proposed method selects documents which are discriminated as not non-relevant and near the discriminant hyper-plane between non-relevant document and not non-relevant documents. In their experiments they compare their approach with conventional relevance feedback methods and vector space model without feedback. Their method gives consistently better performance than other compared methods. They comment that this method is very useful to retrieve relevant documents using information of non-relevant documents only.

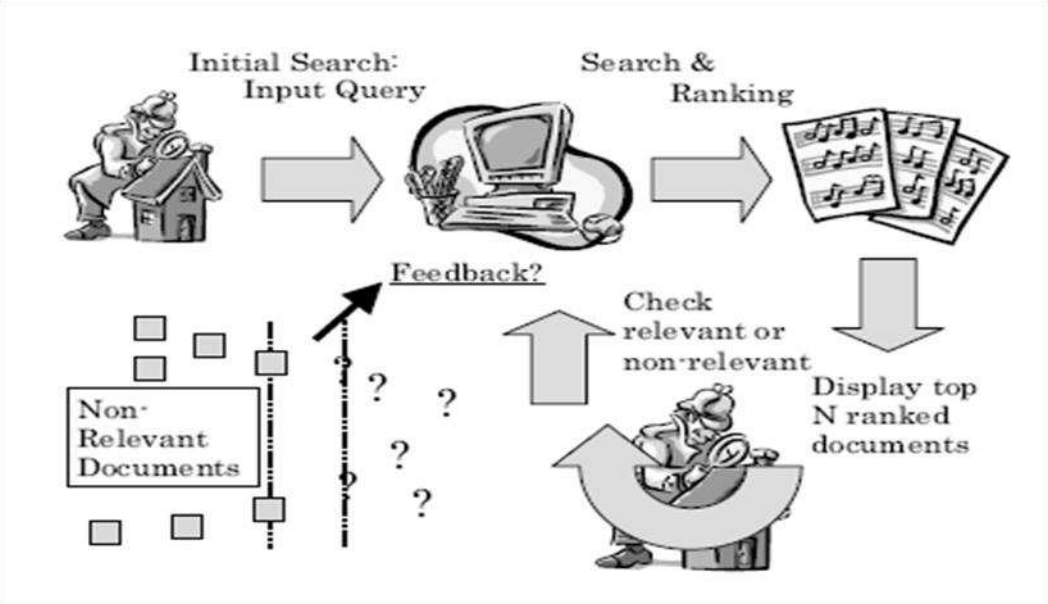


Figure 9 : Outline of a problem in the relevance feedback documents retrieval (Source: Onoda et al. [89]).

Koppel et al. [90] study the 'Authorship Verification' problem where only examples of writings of a single author is given and the task is to determine if given piece of text is or is not written by this author. They begin their study by choosing a feature set that might be used consistently by a single author over a variety of writings. These features could be frequency of words, syntactic structures, parts of speech n-grams [91], complexity and richness measures [92] or syntactic and orthographic idiosyncrasies [93]. The traditional approaches of text classification doesn't work in this kind of classification problem, hence they presented a new technique called 'unmasking'. The basic idea of unmasking is to iteratively remove those features that are most useful for distinguishing between books A and B and to gauge the speed with which cross-validation accuracy degrades as more features are removed. Their main hypothesis is that if books A and B are written by the same author, then whatever differences be there between them (of genres, themes etc), the overall essence or regularity in writing style can be captured by only a relatively small number of features. For testing their algorithm, they consider a collection of twenty-one 19^{th} century English books written by 10 different authors and spanning a variety of genres. They obtain overall accuracy of 95.7% with errors almost equally distributed between false positives and false negatives.

Denis et al. [94] introduce a Naïve Bayes algorithm and shows its feasibility for learning from positive and unlabeled documents. The key step in their method is in estimating word

probabilities for the negative class because negative examples were not available. This limitation can be overcome by assuming an estimate of the positive class probability (the ratio of positive documents in the set of all documents). In practical situations, the positive class probability can be empirically estimated or provided by domain knowledge. Their results on WebKB data set [85] show that error rates of Naïve Bayes classifiers obtained from p positive examples, PNB (Positive Naïve Bayes), trained with enough unlabeled examples are lower than error rates of Naïve Bayes classifiers obtained from p labeled documents. Denis et al. [95] consider situations where only a small set of positive data is available together with unlabeled data. Constructing an accurate classifier in these situations may fail because of the shortage of properly sampled data. However, learning in this scenario may still be possible using the co-training framework (introduced by Blum and Mitchell [22], and described earlier in Section 2.3), that looks for two views over the data. For example, in the case of retrieval of bibliographic references, the positive examples are stored in the user database. A first view of the bibliographic fields consists of - title, author, abstract, editor. A second view is the full content of the paper. Unlabeled examples are easily available in the bibliographic databases accessible via the World Wide Web. Co-training algorithms incrementally build basic classifiers over each of the two feature sets. They define a Positive Naïve Co-Training algorithm, PNCT that takes a small pool of positive documents as it seed. PNCT first incrementally builds Naive Bayes classifiers from positive and unlabeled documents over each of the two views by using PNB. Along the co-training steps, self-labelled positive examples and self-labelled negative examples are added to the training sets. They also propose a base algorithm which is a variant of PNB, able to use these self-labelled examples. They perform experiments on the WebKB dataset [85] and show that co-training algorithms lead to significant improvement of classifiers, even when the initial seed is only composed of positive documents.

2.5.2. Other Application Domain

In this subsection we will highlight some of the other applications domains where methodologies based on one-class classification have been utilized.

OSVMs have been successfully applied in a wide variety of application domains such as Handwritten Digit Recognition [1,2,30], Information Retrieval [33], Classifying Missing Data [49], Image Database Retrieval [1,96-98], Face Recognition Applications [67,99,100], Chemometrics [101], Spectroscopy [102][103] Classification of Bio-Acoustic Time Series

[104], Nosocomial Infection Detection [105], Medical Analysis [106-108], Bioinformatics [109-113], Steganalysis [114], Spam Detection [115,116], Detecting Anomalous Windows Registry Access [117], Audio Surveillance [118], Ship Detection [119], Collision Detection [120], Anomaly Detection [35,121-126], Yeast Regulation Prediction [127], Customer Churn Detection [36], Relevant Sentence Extraction [128], Machine Vibration Analysis [129], Machine Fault Detection [73,129-132] and Recommendation Tasks [133]. Compression neural networks for one-sided classification have been used in many areas, these include detecting Mineral Deposits [64], fMRI Analysis [134] etc. One-class Fuzzy ART networks have been explored by Murshed et al. [135] to classify Cancerous Cells. Wang and Stolfo have used one-class Naïve Bayes to detect Masquerade Detection [136] in a network and showed that less effort in data collection is required with comparable performance as that of a multi-class classifier. Munroe and Madden [137] have presented a one-class k-nearest neighbour approach for vehicle recognition from images and showed that the results are comparable to that of standard multi-class classifiers.

2.6. Open Research Questions in OCC

The goal of One-Class Classification is to induce classifiers when only one class (the positive class) is well characterized by the training data. In this chapter, we have presented a survey of current state-of-the-art research work using OCC. We observe that the research carried out in OCC can be broadly presented by three different categories or areas of study, which depends upon the availability of training data, classification algorithms used and the application domain investigated. Under each of these categories, we further provide details of commonly used OCC algorithms. Although the OCC field is becoming mature, still there are several fundamental problems that are open for research, not only in describing and training classifiers, but also in scaling, controlling errors, handling outliers, using non-representative sets of negative examples, combining classifiers and reducing dimensionality.

Classifier ensembles have not been exploited very much for OCC problems, and techniques such as boosting and bagging deserve further attention. Another point to note here is that in OSVMs, the kernels that have been used mostly are Linear, Polynomial, Gaussian or Sigmoidal. We suggest it would be fruitful to investigate some more innovative forms of kernels, for example Genetic Kernels [138] or domain specific kernels (for spectroscopic data), for example, Weighted Linear Spectral Kernel [139], that have shown greater potential in standard SVM classification. The kernels have been used as distance metric in

multi-class classification problems; however, the same is not exploited for the OCC. This particular problem is investigated in the Chapter 4 of this thesis. In the case where abundant unlabeled examples and some positive examples are available, researchers have used many two-step algorithms (as have been discussed in Section 2.5.1). We believe that a Bayesian Network approach to such OCC problems would be an interesting exercise.

This survey provides a broad insight into the study of the field of OCC. Depending upon the data availability, algorithm use and application, appropriate OCC techniques can be applied and improved upon. We hope that this survey will provide researchers with a direction to formulate future novel work in this field and reduce their research time and effort considerably.

Chapter 3

Spectral Data, Similarity Metrics and Library Search

This chapter presents a brief description of the Raman Spectroscopy and the spectral data thus obtained, followed by short review of the common spectral search and comparison algorithms. This chapter highlights some standard spectral search and comparison methods, and some recent / non-standard methods for finding similarity between spectra. A few similarity measures that are specific for comparing the spectra are also introduced in this chapter. The spectrum-specific comparison methods will be used to develop kernels to be used in Chapter 4.

In our present research work we are interested in vibrational spectroscopy and related techniques; therefore we have restricted our review, study and analysis of similarity and search methods that have been applied in those fields, especially the sub-field of Raman Spectroscopy.

3.1. Raman Spectroscopy

Raman Spectroscopy is a spectroscopy technique which is based on scattering of monochromatic light in the visible, near infrared, or near ultraviolet range [12]. When a chemical substance is illuminated by a laser, most of the light is elastically scattered due Rayleigh scattering. A small portion of the light (1 in 10^6), however, is inelastically scattered at a different wavelength to the incident light. This inelastic scattering of incident light is known as Raman scattering. This scattering is due to the interaction of light with the vibrational and rotational motions of molecules and other low-frequency modes within the material. A Raman spectrum is thus obtained which shows the change in frequency of the scattering light as well as its intensity. This Raman scattering can be treated as a 'molecular fingerprint' of a given chemical substance providing information on the vibrational and rotational motions of the chemical bonds between the molecules (see Figure 10). Every

substance has a unique Raman spectrum and for machine learning tasks, this 'molecular fingerprint' can be exploited for unambiguous identification of substances.

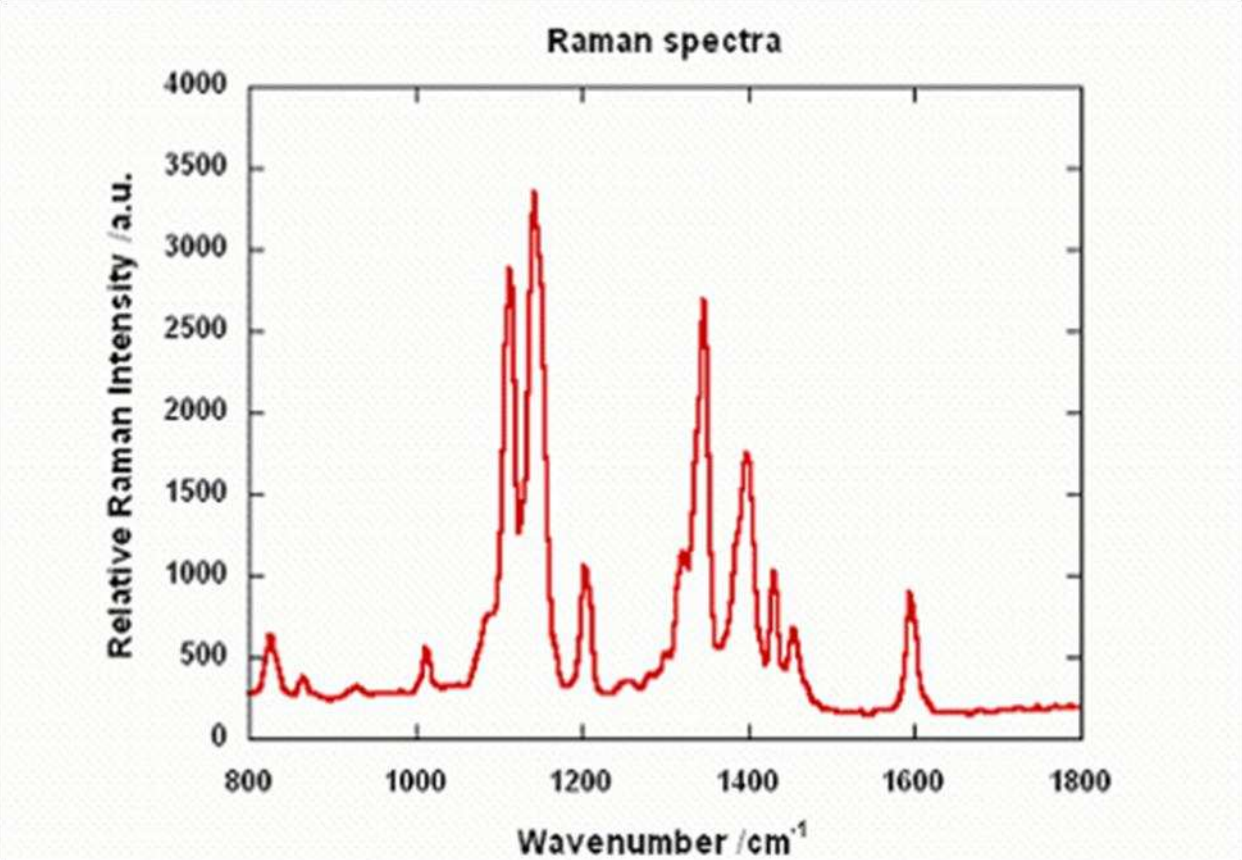


Figure 10: Raman Spectrum of Azobenzene polymer (Source Horiba Scientific [140]

Each point in a Raman spectrum (see Figure 10) represents the value of intensity corresponding to particular frequency. The Raman shift is either represented as wavelengths or wavenumbers. The wavenumber is defined as number of waves per unit length [141], which is directly proportional to the frequency of the scattered light (wavelength is inversely proportional to the frequency). The wavenumber unit, cm^{-1}, is commonly used.

Raman Spectroscopy has been used in wide variety of applications, such as gemstone identification [142], identification and quantification of narcotics [143] and illicit substances [144], chemical identification [145], and explosive detection [146].

Raman spectra can also be used to determine the quantity of a particular chemical substance or estimate its presence within a mixture of various substances [139]. Figure 11 shows Raman spectra of three different compounds, namely, Caffeine, Glucose and Cocaine. It can be seen that all the three pure compounds have distinctive Raman spectra.

3.2. Some Definitions

In this section, we provide some basic definitions of the terms and concepts we will be using in this and subsequent chapters.

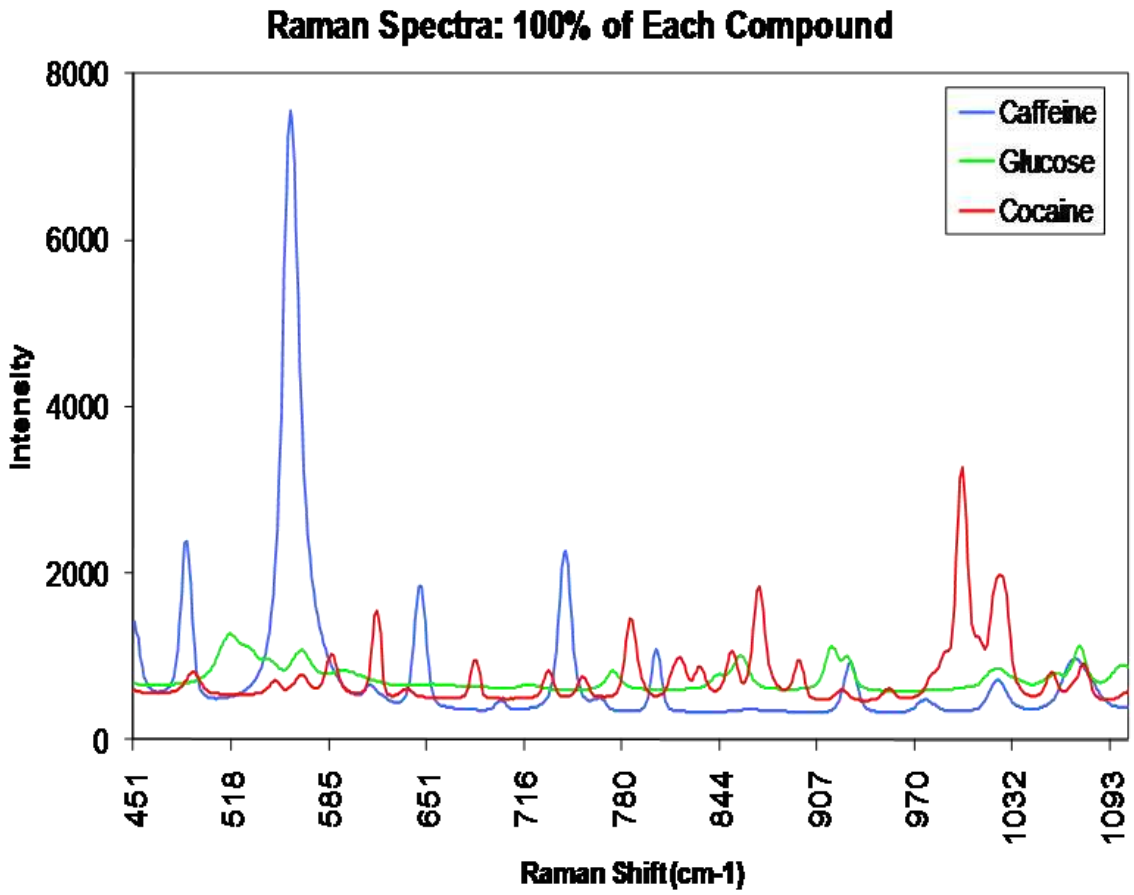


Figure 11: Raman Spectra of three different compounds (Source: [139])

3.2.1. Similarity

Similarity can be defined as a degree of symmetry (quantitative or qualitative) between two or more objects. In text recognition, it can be defined as number of matching characters between two text strings. In Bioinformatics, it can be defined as the number of matching DNA sequences. In geometrical application, it can be expressed as a score that represents some kind of resemblance between two vectors. For spectroscopic data, similarity means matching of peaks and overall shape of the spectrum. Common similarity measures are Cosine and Correlation Coefficient. Each of these measures computes similarity between spectra in its own way (for details refer to Section 3.4).

3.2.2. Dissimilarity

Dissimilarity can be defined as a degree of being distinct or unlike. In geometry, it can be represented as a distance score (Manhattan, Euclidean, Mahalanobis, Chebychev etc) between two or more vectors. The more dissimilar two vectors are the higher the value of score. If two vectors are less dissimilar or bear more resemblance to each other than the dissimilarity score will be low or close to zero.

Note: Similarity and Dissimilarity can be treated as reciprocal concepts in terms of interpreting the value of score.

3.2.3. Comparison

Comparison means comparing two spectra based on some similarity or dissimilarity measure and computes a score. This score can be used to access the degree of resemblance between two spectra and can be employed in a library search (defined below).

3.2.4. Search

In spectroscopy, usually an unknown spectrum is searched against a known library of pure substance to find a match (or nearest matches), called hits, for further analysis [147]. The unknown spectrum is searched for using a search algorithm (see Section 3.4 to 3.6) which computes a score based on similarity or dissimilarity measure it employs and provides a score and a list of nearest matches.

3.2.5. Spectral Library

A spectral library is a database of spectra of known substances [147]. The spectral library is usually used for spectrum search and comparison purposes and as an aid to identify unknown spectrum. The companies that sell digitized spectral libraries for use by researchers and other practitioners include Thermo Scientific, Sigma Aldrich, Bio-Rad Laboratories - Sadtler Division, National Institute of Standards and Technology and many others. Spectral libraries can also be developed within organisations to reflect their own requirements and applications [148].

3.3. Spectral Data Pre-processing

The spectral data in its raw form is usually not used for comparison and spectral search purposes. There are two basic steps that are usually employed to pre-process the raw spectral

data before it can be deemed useful for further use. These methods are discussed in the following subsections.

3.3.1. Normalization

Spectral measurements suffer from variation in intensities in their spectrum. These variations in intensity may arise due to changes in laser-intensity output, a sample's refractive index, opacity, position, absorptivity and density and instrument design [149]. To counter this problem, normalization is employed to the entire spectrum to fix intensities to a known or constant value.

One common way of normalizing a spectrum is to normalize it to a constant Euclidean norm [150]

$$x_{i,norm} = \frac{x_i}{\|x\|} \qquad \text{Equation 21}$$

where x_i is the intensity of the spectrum at the i^{th} wavenumber, $x_{i,norm}$ is the corresponding normalized value at i^{th} wavenumber, $\|x\|$ is the Euclidean norm of the spectral vector x. For a spectral vector X defined as $[x_1, x_2 \ldots x_N]$, where N is the total number of spectral points, then Euclidean norm is defined as $\|x\| = \sqrt{x_1^2 + x_2^2 + \ldots x_N^2}$. This normalization transforms the input spectra on a unit hypersphere, such that all data are approximately in the same scaling.

Another normalization method, called mean normalization [150], where every point of the spectrum is divided by its mean value,

$$x_{i,norm} = \frac{x_i}{\left(\frac{1}{N}\sum_{j=1}^{N} x_j\right)} \qquad \text{Equation 22}$$

where x_i is the intensity of the spectrum at the i^{th} wavenumber, $x_{i,norm}$ is the corresponding normalized value at i^{th} wavenumber, N is the total number of spectral points. After mean normalization all the spectra have the same area.

In the min-max normalization method, all the points in a spectrum are mapped in a desired range (or between 0 and 1) using this formula

$$x_{i,norm} = \frac{x_i - \min}{\max - \min} \qquad \text{Equation 23}$$

where $x_{i,norm}$ is the corresponding normalized value for the spectral point x_i, min and max are the minimum and maximum values of the spectral vector X.

3.3.2. Baseline Correction

Sometime the spectrum obtained for a substance does not have a flat baseline and may come up with curved or sloping baseline. This can happen due to sample scattering, inappropriate choice of background or instrumentation drift [147]. If the baseline is not flat it leads to improper identification of peaks and introduce errors for estimating quantitative measurements [151]. Such spectra with poor baseline are detrimental for the spectral library search methods. Therefore, baseline correction methods are employed so that the resulting spectrum has a flat baseline that makes spectral library search more successful.

There are various ways for correcting the baseline. The general idea is to construct and fit a polynomial function (linear, quadratic or n^{th} degree polynomial) that resembles the shape of baseline in sample spectrum. Once the function is obtained, it is subtracted from the sample spectrum, resulting in spectrum that should have no slope or curved baseline [147][149].

Note: It is a common practice to pre-process the spectral data using normalization and baseline correction before employing searching and comparing with the spectral library to obtain meaningful and interpretable results [147].

Before we introduce next sections on standard and more recent search and comparison methods, we define some notations that we shall use later on.

An unknown spectrum is defined as a vector $\mathrm{X} = [\mathrm{x}_1, \mathrm{x}_2 \ldots \mathrm{x}_\mathrm{N}]$, where x_i denotes the responses at i^{th} wave number.

Similarly, a known spectrum from the database is defined as a vector $\mathrm{Y} = [\mathrm{y}_1, \mathrm{y}_2 \ldots \mathrm{y}_\mathrm{N}]$, where y_i denotes the responses at i^{th} wave number and N is the total number of data points in a spectrum.

3.4. Standard Spectral Search and Comparison Methods

The similarity, search and comparison methods described in this section are well established and standard. These methods are used by several spectroscopy/chemometric companies in their products (e.g. Thermo Fisher Scientific [152]).

3.4.1. Euclidean Distance

The Euclidean Distance method is the most commonly used spectral search algorithm [153]. It can be defined as:

$$\mathrm{Dist}(X,Y) = \sqrt{\sum_{i=1}^{N}(x_i - y_i)^2} \qquad \text{Equation 24}$$

Euclidean distance computes squared difference of responses at every wave number and gives a squared sum over all data points. This method is very fast in computation.

3.4.2. Pearson Correlation Coefficient

The Pearson product-moment correlation coefficient (r) [154] computes linear dependence between two spectra using the following formula:

$$r_{X,Y} = \frac{1}{n-1}\sum\left(\frac{x_i - \bar{X}}{S_X}\right)\left(\frac{y_i - \bar{Y}}{S_Y}\right) \qquad \text{Equation 25}$$

where $\bar{X}$ and $\bar{Y}$ are sample mean and S_X and S_Y are sample standard deviation.

The correlation coefficient ranges from −1 to 1. A value of 1 implies that there exists a linear relationship between spectra X and Y such that when X increases then Y also increases (high positive interdependence). A value of −1 implies that there exists a linear relationship between spectra X and Y such that when X increases then Y decreases (high negative interdependence). A value of 0 means that there exists no linear relationship between spectra X and Y.

In cases where the baseline in the spectrum is not well established (see Section 3.3.2), First Derivative Correlation method instead should be considered; this is described next.

3.4.3. First Derivative Correlation

The First Derivative Correlation method [155] is an extended version of the Correlation search algorithm. The Correlation algorithm can cater for noise and negative spikes present in the spectrum. However, the correlation algorithm cannot correct a bad baseline [155], which can be rectified by using the First Derivative Correlation search algorithm. These algorithms enhances differences in the peak positions and small peak shifts between unknown spectrum and known spectra, and tend to give more importance to position of peaks rather than their intensities [156].

3.4.4. Absolute Value Search

The Absolute Value algorithm [157] calculates the similarity value by taking the average absolute difference between unknown spectrum and the spectra in the database and can be expressed as

$$\text{Score} = \frac{\sum_{i=1}^{N} |x_i - y_i|}{N} \qquad \text{Equation 26}$$

The Absolute Value search algorithm gives more emphasis to the small differences between the unknown spectrum and library spectra. This algorithm, sometimes, works well in scenarios where there exist spurious peaks in the unknown spectrum [157].This method is very similar to the Least Squares method (see Section 3.4.6). In cases where the baseline in unknown spectrum is not well established, First Derivative Absolute Value may be considered to remove baseline effects [158].

3.4.5. Citiblock

The Citiblock or the Manhattan distance metric [159] computes the sum of absolute differences between the absorbance values of two spectrums at every wave number. It can be defined as:

$$\text{Score} = \sum_{i=1}^{N} |x_i - y_i| \qquad \text{Equation 27}$$

This metric is very similar in concept to absolute value search defined in Section 3.4.4

3.4.6. Least Square Search

The Least Squares method [160] is similar to the Absolute Value method in that it computes point-to-point differences between the unknown spectrum and the spectra in the database. However, the similarity value is calculated by averaging the square of the differences between the two spectra, which can be expressed as

$$\text{Score} = \frac{\sum_{i=1}^{N} (x_i - y_i)^2}{N} \qquad \text{Equation 28}$$

This method gives more emphasis on the larger peaks in the unknown spectrum and compensates for noise present in the spectra [160]. First Derivative Least Square [161] method may be used to remove some baseline effects, if the unknown spectrum's baseline cannot be corrected using the method described in Section 3.3.2.

3.4.7. Peak Matching Method

The peak matching algorithm takes each peak occurring in the unknown spectrum and attempt to find its corresponding matching peak in the spectra present in the library and compute a score to assess their similarity [162]. There are two types of peak matching methods: Forward search and Reverse search. In the Forward peak search method, the difference between peak values between the unknown spectrum and the spectra in library is computed and minimum absolute distance is saved. A score is then computed based on this distance. This algorithm penalize spectra in library if they do not have peaks at matching positions to the unknown spectrum, but imposes no penalty if the spectra in the library has more peaks present than the unknown spectrum.

In a Reverse peak search [162], the method of searching reverses in the sense that each peak present in the spectra in library is compared against the corresponding peaks in the unknown spectrum and a score is computed. This algorithm does not penalize the unknown spectrum if it has more peaks than the spectra present in the library.

3.4.8. Dot Product Metric

Dot product [154] computes similarity point to point between unknown and library spectra. It can be expressed as:

$$\text{Score} = X \bullet Y = \sum_{i=1}^{N} x_i y_i \qquad \text{Equation 29}$$

where $\bullet$ is the dot product between spectral vectors X and Y, x_i and y_i are response values at i^{th} wave number . In principle, dot product and least square search method (see Section 3.4.6) provides comparative information, however the former requires less number of computational steps [154].

3.5. More Recent / Non-Standard Spectral Search and Comparison Methods

This section presents a brief description of some recent and non-conventional similarity metrics that are being developed for spectral search and similarity. As will be described below, these methods have been reported to perform equal or better than standard methods described in Section 3.4.

3.5.1. Match Probability

Match probability is a similarity measure developed by Ellison and Gregory [163] for identifying spectra within a spectral library by matching the common peaks between unknown spectrum and spectra from the database. Suppose an unknown spectrum has m peaks and library spectrum has q peaks, and at any p possible position they share n peaks. Then the probability for finding the n peaks common to both m and q, taken from same population of size p, is calculated using hypergeometric distribution and expressed as:

$$P(n, m, q, p) = \frac{{}^{m}C_{n} \cdot {}^{p-m}C_{q-n}}{{}^{p}C_{q}} \qquad \text{Equation 30}$$

Figure 12 [163] shows diagrammatic representation of two spectra with m and q peaks and they share n peaks. Figure 13 [163] shows the Venn diagrammatic representation, which shows the region N as the common region for the two peak sets M and Q taken at random from P positions.

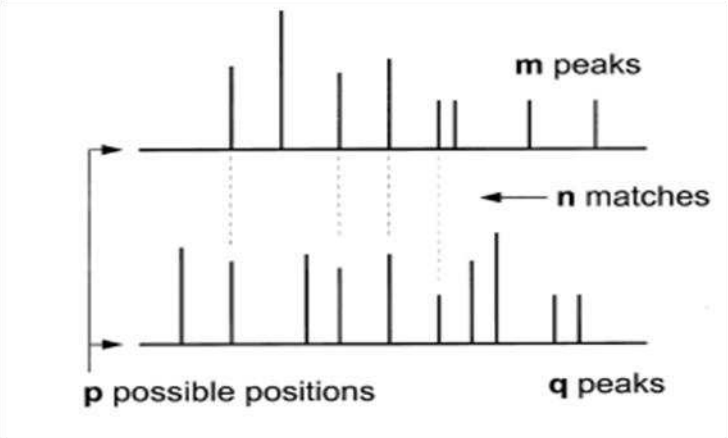


Figure 12: Peak Matching: n matches are common to two spectra with m and q peaks, each from p possible line positions. (Source: Ellison and Gregory[163])

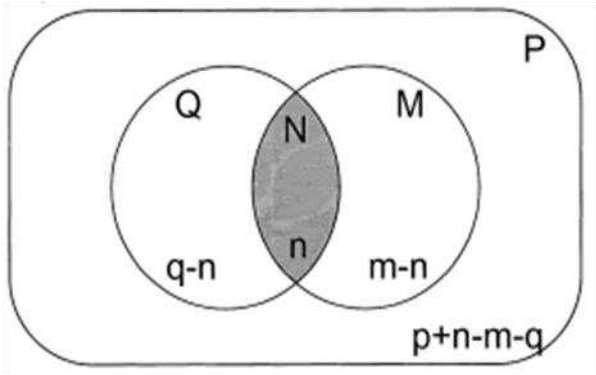


Figure 13: Venn diagram for underlying hypergeometric distribution. (Source Ellison and Gregory [163])

They observe that this method yields better search results when an unknown spectrum is searched against the spectral library than using the simple binomial distribution predictions.

3.5.2. Nonlinear Spectral Similarity Measure

This is a non-linear method for measuring spectral similarity measure between two spectra [164]. The method not only considers the shape similarity of spectra but also the function of various absorption features. The adjacent bands in spectrum are usually highly correlated, which is removed by first projecting the spectral vectors in feature space and applying Kernel Principal Component Analysis (KPCA). In this method, the kernel function of polar coordinates is used. Finally, a linear similarity measure is used to find similarity between the two non-linearly transformed spectra. The method is reported to be effective in spectral similarity measure [164].

3.5.3. A Spectral Similarity Measure using Bayesian Statistics

This spectral similarity method [165] is based on differentiating subtle differences between two spectra. These subtle differences mean that the two spectra may overlap quite well in general except for some local regions. In these local regions, the differences among the spectra may look insignificant, which may not be the case. Such subtle differences will cause problems for many spectral search methods. For example, correlation coefficient will give a similarity index value of approximately 1.0 (or 100%) for these kinds of spectral pairs. This method transforms the spectral similarity measure into a hypothesis test of the similarities and differences between the unknown spectra and the spectra from the library. A difference vectors is defined that denotes the difference between the two spectra and its scalar mean is used as the statistical variable for the hypothesis test. A threshold is also proposed for the

hypothesis that the spectra are different. The Bayesian prior odds ratio is estimated from several spectra of the same sample. The posterior odds ratio is used to quantity the spectral similarity measure of the two spectra. They demonstrated the effectiveness of their method on diffuse reflectance near-infrared spectra of tobacco samples of two formulations and show that their method can detect subtle differences between the spectra.

3.6. Spectral Similarity Methods Specific for Spectral Data

3.6.1. Spectral Linear Kernel

Spectral Linear Kernel [139] (SLK) is a special similarity metric designed specifically for computing the spectral similarity between two Raman spectra. The kernel function is sometimes described as a similarity metric which can be then applied in spectroscopy. This measure compares two sample spectra and returns a score: the higher this score, the more similar the two spectra are to each other. This method utilizes information about the spectra profile such as the presence of peaks or troughs in a particular region. This method not only takes into consideration the original intensity values at each wavenumber, but also includes the difference between the intensity at a point and number of its neighbouring points on the spectrum (called a window). The use of neighbouring points within a window places greater importance on differences between points sharing the same spectral region than on difference between points that are far apart on the spectrum. The similarity metric can be expressed as:

$$\mathrm{Sim}(x_i, y_i) = x_i . y_i + \sum_{j=i-W}^{j=i+W} (x_i - x_j)(y_i - y_j) \qquad \text{Equation 31}$$

where $\mathrm{Sim}(x_i, y_i)$is the similarity value as computed by the SLK, W is the window size that consists of neighbouring points in a spectra at value i. Figure 14 illustrates the working of spectral linear kernel.

3.6.2. Weighted Spectral Linear Kernel

The Weighted Spectral Linear Kernel [166] (WSLK) is similar to SLK with a small modification that it also incorporates the pure spectrum, meaning thereby, it gives more weights to similarities between spectra in those regions where the corresponding pure substance has peaks of high magnitude. The similarity metric can be expressed as:

$$Sim(x_i, y_i) = w_i \cdot x_i \cdot y_i + w_i \sum_{j=i-W}^{j=i+W} (x_i - x_j)(y_i - y_j)\,(w_i - w_j) \qquad \text{Equation 32}$$

where w_i is the intensity of pure substance at wave number i. The value of w is normalized between 0 and 1. Figure 15 shows the comparison of two spectra using WSLK. The kernel gives more importance to similarities between two sample spectra that occur in spectral regions in which strong peaks exist in the pure target spectrum. Similarities in spectral region that do not overlap with target spectrum peaks are given lower weighting.

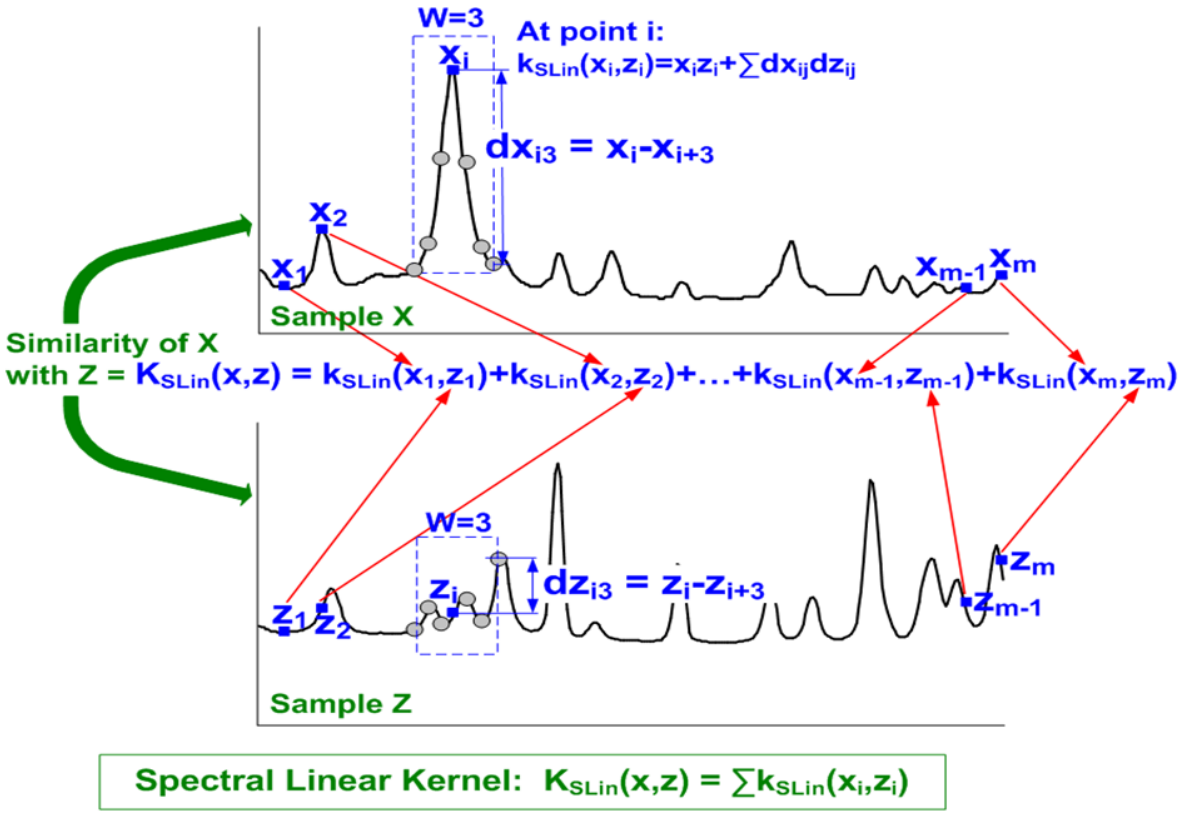


Figure 14: Spectral Linear Kernel (Source [139])

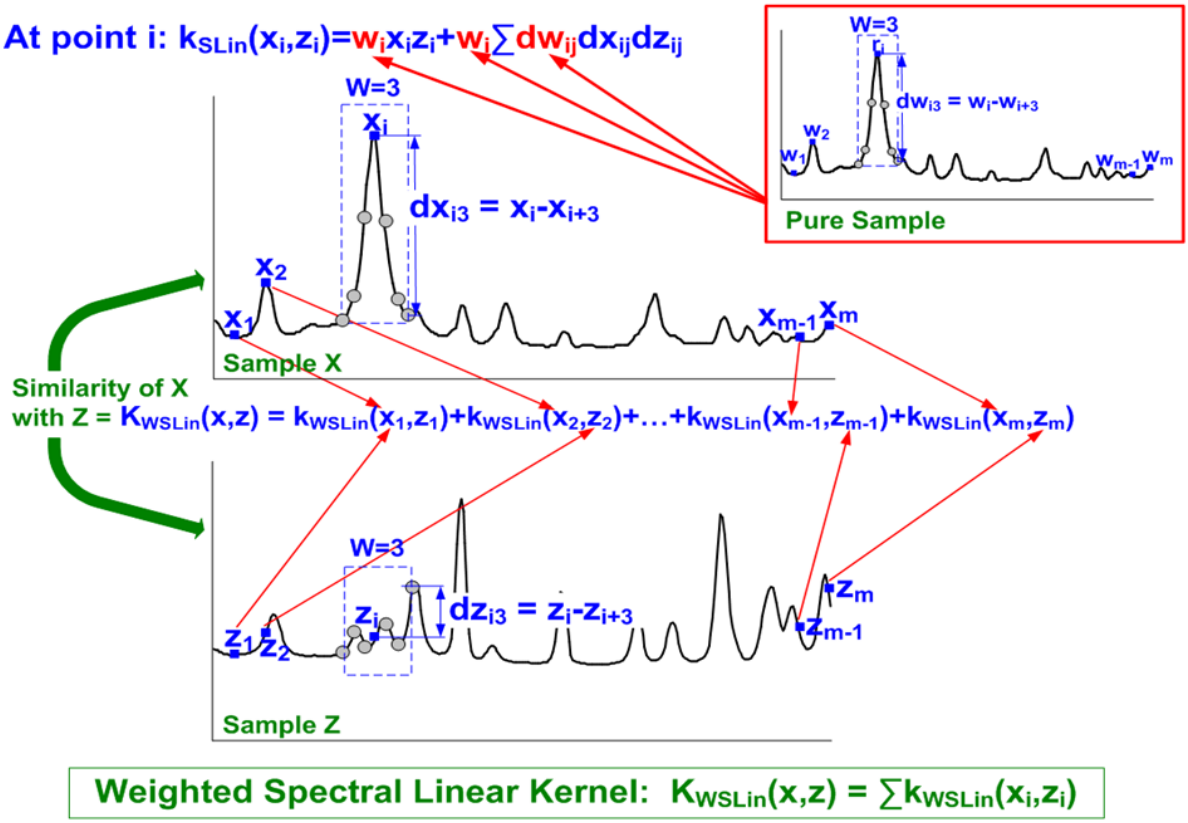


Figure 15: Comparing two spectra using Weighted Spectral Linear Kernel (Source [139])

3.7. A New Modified Euclidean Spectral Similarity Metric

As mentioned in Section 3.2.4, in spectral library search an unknown spectrum is matched against a database of pure materials and based on a match score, a list of nearest matches is produced. The unknown spectrum can be a pure material or a mixture of several pure materials. If the unknown spectrum is a mixture of several pure materials then the task to find a nearest match from the database of pure materials becomes very difficult. A mixture may contain Raman spectra of several pure materials in various proportions which may lead to either summation of the peaks of individual pure materials or appearance of new peaks at certain wavelengths in the resulting spectrum of mixture. The convolution of peaks in the resulting mixture spectrum makes the task of spectral searching more challenging.

The standard Euclidean metric (defined in Section 3.4.1) gives equal importance to peaks of query spectrum and the spectra in spectral library. However, for computing the similarity of a mixture against pure materials, this might be undesirable. In this section, we present a new Modified Euclidean Spectral Similarity Metric that gives weights to the peaks in terms of penalty or reward according to their absence or presence or the difference in intensities in the

unknown spectrum (mixture) and the pure spectra in the spectral library. The performance of this new similarity method is evaluated relative to other similarity methods in Section 3.8.

Before we explain the new similarity metric, we define some notations to be used in this section:

Let X be the query spectrum (mixture),

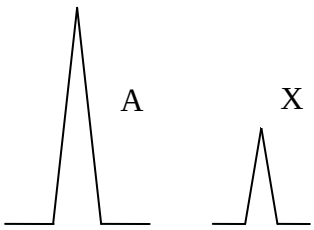
x be the value of intensity of the unknown spectrum at a given wavelength,

A be the pure spectrum from the spectral library, and

a be the value of intensity of the pure spectrum at a given wavelength.

While computing the similarity between an unknown spectrum of mixture against a spectrum of pure material from the spectral library, at any given wavelength, the following four scenarios might occur:

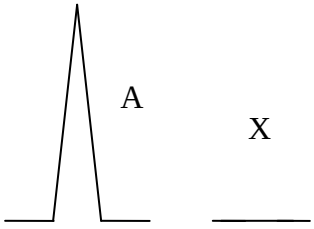
1. When the mixture has a peak smaller than the pure substance



If $A = a, X = x$ and $a > x$

This means that A is (most probably) present in X in some percentage, which means A bears similarity with X. Therefore this condition should be **rewarded** i.e. giving importance to the fact that pure substance is indeed present in the mixture.

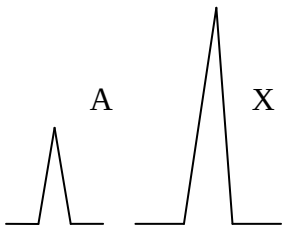
2. When the mixture doesn't have a peak corresponding to the pure substance



If $A = a, X = 0$

This means that A is not present in the mixture. Therefore, its occurrence should be **penalized**, to accommodate scenarios where the mixture has presence of its constituents.

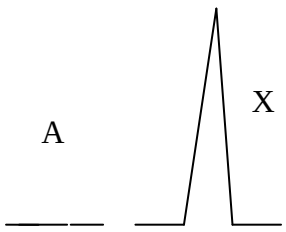
3. When the mixture has a peak larger than the pure substance



If $A = a, X = x$ and $a < x$

This condition means that A is present in X in some proportion. So this is a desirable match. Therefore, no need to penalize it (no reward either).

4. When the mixture has a peak and the corresponding peak in pure substance is absent



If $A = 0, X = x$

Here, if the mixture X has a peak, and A has no peak in the same place, then the peak must come from one of the other constituents in the mixture forming X. However, this is not a proof that A is definitely not a constituent of the mixture X. In this scenario the best we can say is that this situation provides no evidence against A being part of the mixture, and only weak evidence for it. Therefore, it should neither be penalised nor rewarded.

The idea of 'penalty' means that it is a bad match and the metric should be pushed by a constant. The 'reward' means that the match is good and the metric should be reduced. We penalize by multiplying and reward by dividing with the same constant (the variance of the mixture).

The Modified Euclidean Spectral Similarity algorithm can be illustrated by following steps:

i. Compute variance of the mixture, σ

ii. For i=*1, 2 ... N*, where N is the number of points in the spectra, Set SqDist=0, Repeat Step iii.a to iv

iii. Compute distance at every point, as given under:

a. if $A_i > X_i$ AND $X_i \neq 0$, $Distance_i(X_i, A_i) = \sum_{i=1}^{N} \sqrt{(x_i - a_i)^2 / \sigma}$

b. if $A_i > X_i$ AND $X_i = 0$, $Distance_i(X_i, A_i) = \sum_{i=1}^{N} \sqrt{\sigma (x_i - a_i)^2}$

c. Else $Distance_i(X_i, A_i) = \sum_{i=1}^{N} \sqrt{(x_i - a_i)^2}$

iv. $SqDist = SqDist + Distance_i(X_i, A_i)$

v. $Modified\_Euclidean = \sqrt{SqDist}$

The Modified Euclidean metric thus capture certain subtleties that need to be considered while doing a spectral search.

3.8. Comparative Analysis of Spectral Search Methods

In this section we present the measures taken to perform a comparative analysis of various spectral search algorithms defined in Section 3.4, 3.6 and 3.7. This section details the data pre-processing steps taken, methodology adopted to compute search performance and the test strategy formulated for fair comparison of search results. As a representative Raman spectroscopy dataset, we use a set of spectra from chlorinated and non-chlorinated solvents, taken from the work of Conroy et al. [167], which is described next.

3.8.1. Description of the Dataset

The chlorinated data set used in our research work is taken from the work of Conroy et al. [167]. The Raman spectra were recorded on a Labram Infinity (J-Y Horiba) spectrometer. 25 chlorinated and non-chlorinated solvents of different grades were used (see Table 2). These solvents were then mixed in various concentrations to create 225sample mixture of both chlorinated and non-chlorinated solvents (see Table 3). This exercise was done to try and replicate possible industrial scenarios.

Solvents	Grade	Solvents	Grade
Acetone	HPLC	Acetophenol*	Analytical
Toluene	Spectroscopic	n-Pentane	Analytical
Cyclohexane	Analytical & Spectroscopic	Xylene	Analytical
Acetonitrile	Spectroscopic	Nitromethane	Analytical
2-Propanol	Spectroscopic	Dimethylformamide	Analytical
1,4-Dioxane	Analytical & Spectroscopic	Nitrobenzene*	Analytical
Hexane	Analytical	Tetrahydrofuran	Analytical
1-Butanol	Analytical & Spectroscopic	Diethyl Ether	Analytical
Methyl Alcohol	Analytical	Petroleum Acetate	Analytical
Benzene	Analytical	Chloroform	Analytical & Spectroscopic
Ethyl Acetate	Analytical	Dichloromethane	Analytical & Spectroscopic
Ethanol	Analytical	1,1,1-Trichloroethane	Analytical & Spectroscopic
Cyclopentane	Analytical	-	-

Table 2: List of chlorinated and non-chlorinated solvents and the various grades used. *Solvents containing fluorescent impurities (Source Conroy et al. [167])

	Pure Solvents	Binary Mixture	Ternary Mixtures	Quaternary Mixtures	Quintary Mixtures	Total
Chlorinated	3	96	40	12	0	151
Non-Chlorinated	22	23	12	10	7	74
Total Number	25	119	52	22	7	225

Table 3: Summary of various chlorinated and non-chlorinated solvent mixtures (Source Conroy et al. [167])

3.8.2. Data Pre-processing

We implemented quadratic polynomial curve fitting for baseline correction. Here a quadratic polynomial is approximated for each spectrum and then subtracted from the given spectrum to get corrected baseline. The normalization of baseline corrected spectrum is done using min-max normalization method described in Section 3.3.1

3.8.3. Methodology for Measuring Search Performance

The performance of search and comparison algorithms is evaluated using the spectral library search method. In this method an unknown test spectrum (X) is provided by the user as the input. This spectrum, X, is from a material of known composition but its composition is hidden for the purposes of testing. This spectrum can either be a pure material or mixture of two or more materials. The spectrum X will be searched against all the spectra present in the spectral database. The spectral database consists of spectra of pure substances. The searching of unknown spectrum against the spectral library is done using a variety of spectral search algorithms mentioned in Section 3.8.5.

A diagrammatic representation of the Spectral Search method is provided in Figure 16. In the figure, top ten search results are shown in two different colours. Green colour signifies a correct search result or the presence of target chemical in the search results, and red colour signifies an incorrect search result or absence of target chemical in the search results.

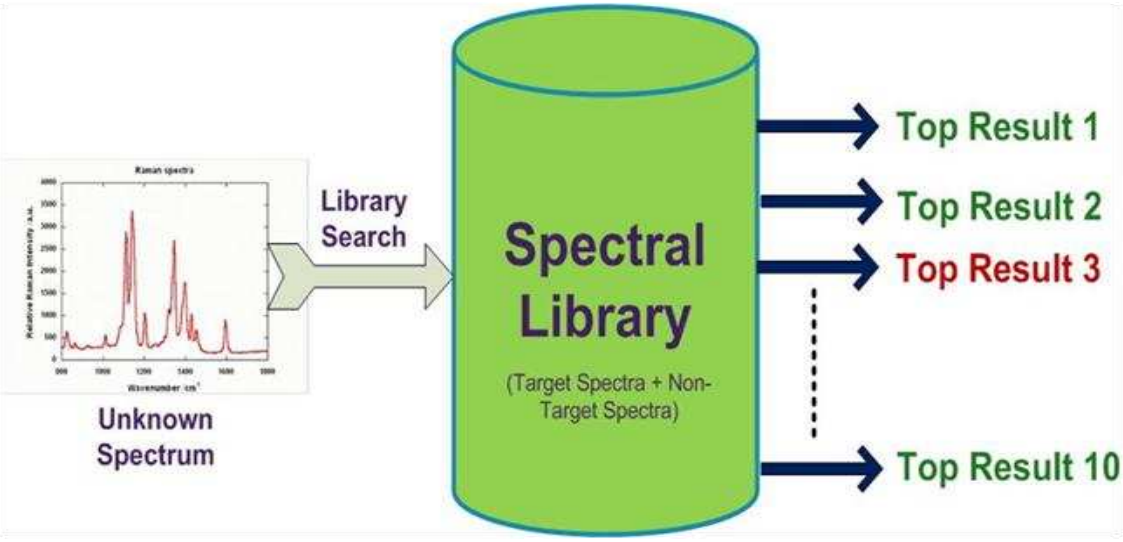


Figure 16: Spectral Search System

The performance of spectral library search result is estimated using the precision and recall values returned by the search algorithm, which are defined as:

- Precision - The ratio between the correct search results and the total number of returned search results.
- Recall - The ratio between the correct search results and the number of results that should have been returned.

For the purpose of experiments, the value of Recall is fixed to 0.5 (i.e. when 50% of the relevant results are retrieved by the query). At this value of recall, value of Precision will be calculated to estimate which search algorithm is performing best.

3.8.4. Testing Strategy

The spectra of three different chlorinated solvents, in pure form or mixtures that are investigated are listed next:

- Dichloromethane (60 targets, 170 non-target)
- Trichloroethane (79 targets, 151 non-targets)
- Chloroform (79 targets, 151 non-targets)

Here the ‘target’ means that the mixture contains the spectra of the given material, and non-target means that the mixture does not contain the spectra of the given material. It is to be noted that the above three datasets are formed from the same dataset described in Section 3.8.1 by relabeling according to the specific ‘target’.

To test search accuracy of spectral search algorithms, three separate sets of experiments have to be executed (for each of the above defined chemical materials). All these experiments have these common steps:

- Randomly Split the target chemical spectra into two parts: 25% for testing the efficiency of the search algorithm (test set), and 75% to be part of spectral library.
- Creating the spectral library by adding to it all the non-target spectra plus 75% of target spectra.
- For every test spectrum i in the test set, do the following,
- For every spectral search algorithm j, fix the value of Recall= 0.5 (approx.)
  - Compute the value of $\text{Precision}_{i,j}$ at this recall value
  - Compute the average value of $\text{Precision}_{i,j}$ across all test set (for a particular spectral search algorithm), to show overall precision of the occurrence of target chemical when (around) 50% of the target chemical spectra in search results have been retrieved successfully.

  Mathematically, it can be expressed as

$$Average\ Precision_j = \frac{\sum_{i=1}^{i=Number\ of\ Test\ Spectra} Precision_{i,j}}{Number\ of\ Test\ Spectra} \qquad \text{Equation 33}$$

- Compare $Average\ Precision$ values of different search algorithms. An algorithm with higher value of $Average\ Precision$ shall be deemed as better than others at a fixed value of recall.

3.8.5. Spectral Search Algorithms

The various spectral search algorithms that will be evaluated are as follows:

1. Euclidean metric
2. Modified Euclidean Metric
3. Citiblock Metric
4. Cosine
5. Spectral Linear Kernel (SLK)
6. Weighted Spectral Linear Kernel (WSLK)

3.9. Evaluation Relative to Standard Algorithms

The data set to be used for evaluation of spectral search algorithms is presented in Section 3.8.1 and 3.8.4. The search algorithms (see Section 3.8.5) are tested on this dataset and the value of $Average\ Precision$ (at fixed recall) is used as a metric to measure the performance of these algorithms.

Note: Although the value of recall is set to 0.5, but in computation it is slightly higher. The reason is that the number of retrieved spectra is always a natural number and cannot be expressed as a decimal. For example, for the dataset described in Section 3.9.1, the total number of target spectra to be retrieved by a given query is 45. The threshold here is to retrieve 50% of the 45 spectra that equals to 22.5 spectra, which is rounded of to 23 spectra and therefore the recall becomes $23/45 = 0.511$. The recall values of datasets in Section 3.9.2 and 3.9.3 can be explained in the same way.

The paired t-test [168] is used as statistic to evaluate significant different between average precision values obtained from search algorithms. The null hypothesis was set so that "the values of average precision from two search algorithms are same". The confidence interval is set to 95% and two-tailed test is employed. If the calculated p-value is lower than this threshold then we reject the null hypothesis and interpret that the mean values of average precision from two search algorithms are not same. MS-Excel 2007's TTEST function [169] is used to compute the p-value and determine whether the two average precision have same mean or not.

3.9.1. Dichloromethane

The details of the Dichloromethane data used for testing the spectral library are as follows:

Total number of Spectra = 230
Number of Targets Spectra = 60
Number of Non-Target Spectra = 170
Number of Test Spectra = 15
Size of Spectral Library = 45 target + 170 Non Target = 215

The results for dichloromethane data set are presented in Table 4.

(Dis)similarity Metrics	Average Precision (Recall = 0.511)	Standard Deviation
Euclidean	0.2194	0.0393
Modified Euclidean	0.2664	0.0480
Citiblock	0.2402	0.0417
Cosine	0.1896	0.0427
SLK	0.1802	0.0152
WSLK	**0.2888**	0.0305

Table 4: Average Precision Results for Dichloromethane Data

These results of Table 4 are presented graphically in Figure 17.

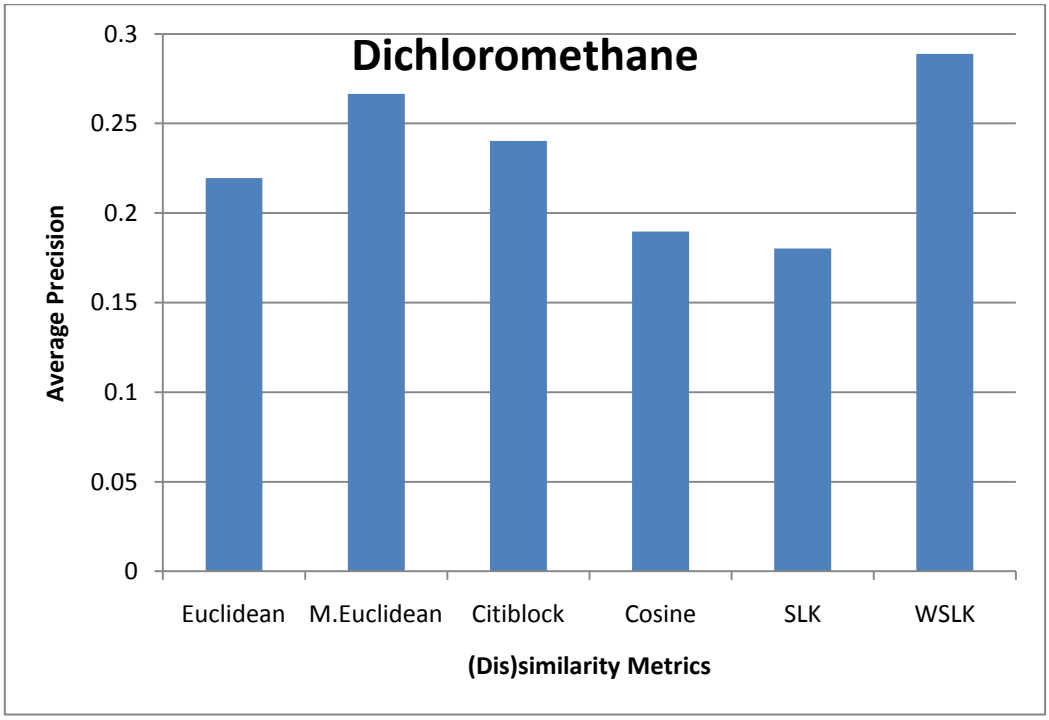


Figure 17: Average Precision search results for Dichloromethane

It can be observed from Table 4 and Figure 17 that for a recall value of 0.511, WSLK performed the best with highest average precision rate. The paired t-test shows that WSLK's average precision value is statistically different from rest of the other search algorithms except Modified Euclidean. Modified Euclidean comes a close second but it is not statistically

much different from WSLK and Citiblock, which comes a close third. The other three search algorithms perform worse in comparison to these algorithms.

3.9.2. Trichloroethane

The details of Trichloroethane data used for testing the spectral library are as follows:

Total number of Spectra = 230

Number of targets Spectra = 79

Number of Non-target Spectra = 151

Number of Test Spectra = 20

Size of Spectral Library = 59 target + 151 Non Target = 210

The results for trichloroethane data set are presented in Table 5

(Dis)similarity Metrics	Average Precision (Recall = 0.508)	Standard Deviation
Euclidean	0.2689	0.0208
Modified Euclidean	0.2909	0.0403
Citiblock	0.2920	0.0331
Cosine	0.2643	0.0405
SLK	0.2860	0.0559
WSLK	**0.3725**	0.0574

Table 5: Average Precision results for Trichloroethane Data

The above tabular results can be visualized graphically in Figure 18.

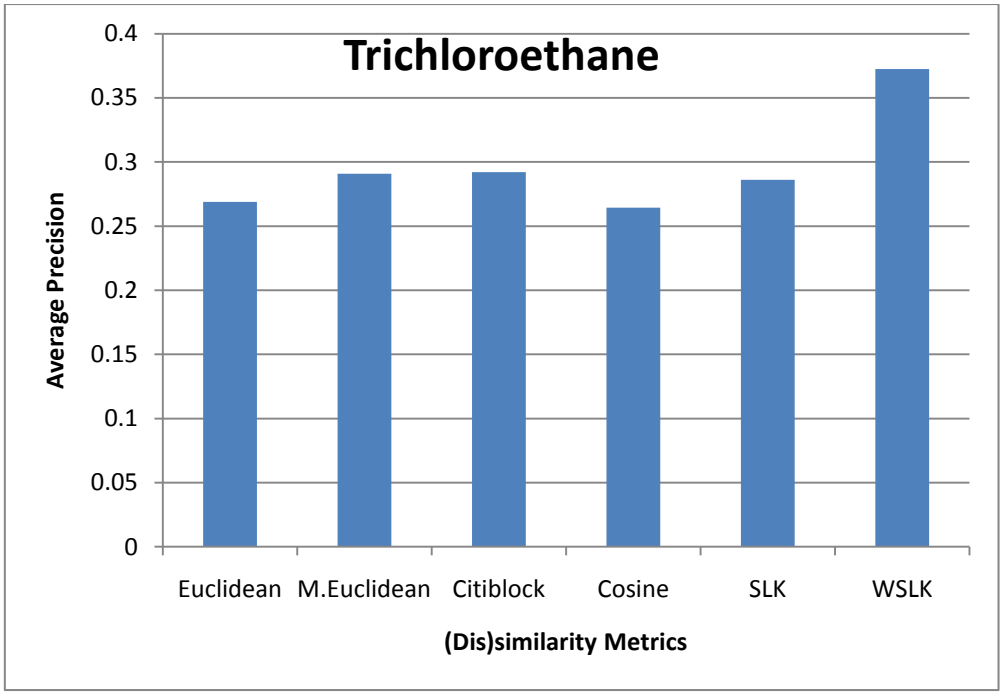


Figure 18: Average Precision search results for Trichloroethane

Table 5 and Figure 18 shows that, for a fixed recall value of 0.508, WSLK metrics performs the best for the Trichloroethane data with highest average precision. The paired t-test shows that it is statistically different from the average precision values obtained from other algorithms. Modified Euclidean and Citiblock comes close second and third with no statistical difference among them. Both of them are not statistically significantly different from SLK either. Therefore it is difficult to say that SLK performs worse than them. Cosine and Euclidean metric performs worst with no statistical difference among them.

3.9.3. Chloroform

The details of Chloroform dataset used for testing the spectral library are as follows:

The data description for testing the spectral library is as under:

Total number of Spectra = 230

Number of targets Spectra = 79

Number of Non-target Spectra = 151

Number of Test Spectra = 20

Size of Spectral Library = 59 target + 151 Non Target = 210

The results for chloroform data set are presented in Table 6

(Dis)similarity Metrics	Average Precision (Recall = 0.508)	Standard Deviation
Euclidean	0.2513	0.0174
Modified Euclidean	0.2718	0.0142
Citiblock	0.2661	0.0177
Cosine	0.2468	0.0166
SLK	0.2710	0.0196
WSLK	**0.9586**	0.0851

Table 6. Average Precision results for Chloroform Data

These tabular results are shown graphically in Figure 19.

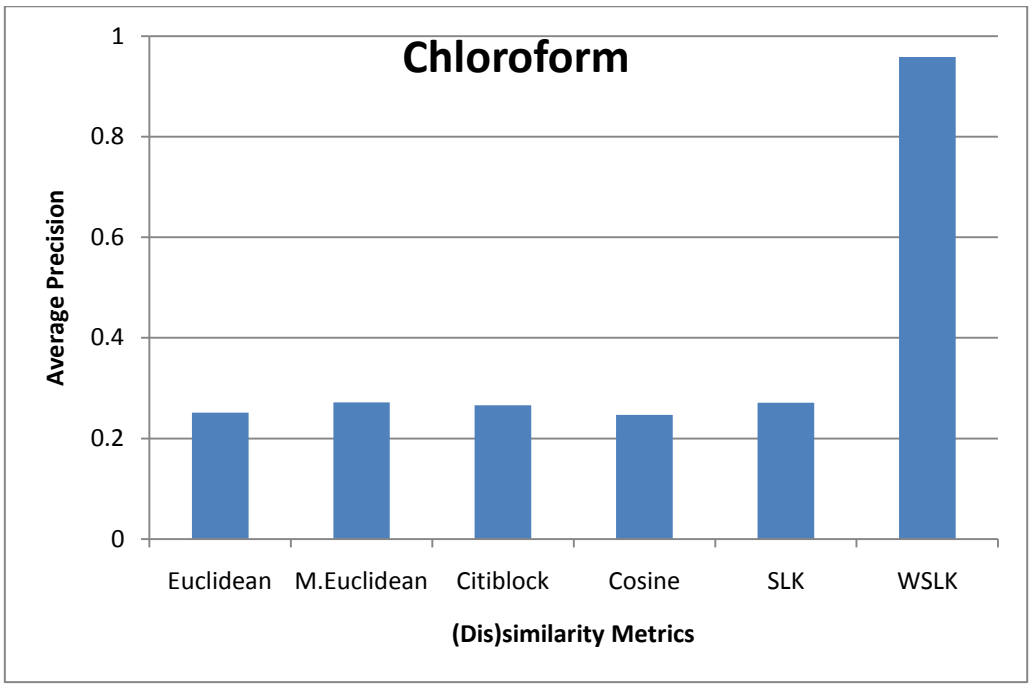


Figure 19: Average Precision search results for Chloroform

From Table 6 and Figure 19, it can be seen that WSLK performed with much superior average precision rate (0.9586) for fixed recall of 0.58. The paired t-test also suggests that it is statistically different from other search algorithms. Modified Euclidean and SLK come second and very close to each other with no statistical difference in the means. Both of them also do not have statistical difference in their means when compared with Citiblock, therefore, it

cannot be interpreted to perform worse than them. Euclidean and Cosine performs the worst and their means are statistically same using paired t-test.

3.9.4. Evaluation of Spectral Search Algorithms

The evaluation is based on the best three search algorithms for the chlorinated solvent test data set. The results are presented in Figure 20.

Data Sets	Best Search Algorithms		
	First	Second	Third
Dicholormethane	WSLK	Modified Euclidean	Citiblock
Trichloroethane	WSLK	Modified Euclidean / Citiblock	SLK
Chloroform	WSLK	Modified Euclidean / SLK	Citiblock

Figure 20: Overall Evaluation of Best 3 Spectral Search Algorithms on Chlorinated Solvent data

It can be seen that WSLK similarity measure gives consistently the best average precision rate for all the three chlorinated solvent data considered. Modified Euclidean dissimilarity measure emerged as the second best spectral search algorithm consistently for the three chlorinated solvent data set. The next best choice for the choice of spectral search algorithm is SLK and Citiblock. The paired t-test shows that some of the spectral algorithms's average precision values may not be significantly different than others, however Euclidean metric perform worst in almost all the cases.

It can be concluded that for the chlorinated solvent data, WSLK is the overall best of the similarity metrics that have been evaluated. The reason for the superior performance of WSLK lies in the fact that it gives importance to those regions in a spectrum where the pure substance has peaks and also the points in the neighbourhood at any point in a spectrum. Modified Euclidean came the modest second among spectral search algorithms we evaluated. The reason for its good and consistent performance is that it does not give equal importance to peaks of an unknown material to be searched in spectral library (unlike Euclidean metric), rather it rewards or penalizes the occurrence or absence of peaks in conjunction with calculating Euclidean distance as well. SLK and Citiblock are the next close choices. SLK's strength lies in the fact that it considers not only a portion of spectrum to be searched against

spectral library but also its nearby points to capture a general similarity spread across a localized region. The better performance of Citiblock in comparison to other standard spectral search methods might be due to the presence of sharp peaks in the unknown spectrum. Standard Euclidean search method never gave good results in comparison to other spectral search algorithms. Cosine metric gave the worse results in all the three chlorinated solvents data.

This study shows that in spectroscopic applications, standard spectral search algorithms are a good starting point to develop an understanding about the spectral search mechanism. However, it does not guarantee the best spectral library search results. The reason is that they do not embody any domain specific insight into the data. Therefore, from our experiments we deduce that spectral search accuracy can be improved by devising customized non-standard spectral search algorithms that are more specific to spectroscopic data and capture more information that traditional spectral search algorithms might not.

Chapter 4

One-class K-Nearest Neighbour Approach based on Kernels

The K-nearest neighbour (KNN) [76] is a standard approach for solving multi class classification problems. It has been modified to tackle the problem of one-class classification by Tax in his thesis [2]. Various other researchers have also presented variants of one-class nearest neighbour approach (see Section 4.3). In this chapter we present modification on the standard one-class KNN based algorithms presented by Tax. We incorporate the use of kernel functions as distance metric instead of the conventional Euclidean based distance metrics. In a traditional KNN classifier, the k nearest neighbours' class labels are used to decide the class allotment of a test case. We extend that approach by not only considering j nearest neighbours, but their k nearest neighbours also and an averaged decision is taken to allocate a class to a test sample.

4.1. Kernel as Distance Metric

The conventional nearest neighbour (NN) classifier uses Euclidean measure as a distance metric to compute similarity between two vectors. This distance metric can be redefined by incorporating the 'kernel approach' and applied to conventional NN classifier [170]. The idea of applying a kernel is to transform the data into high dimensional feature space by performing a nonlinear mapping and then try to define a classification boundary around it in that space. For further details on 'kernel approach', refer to Section 2.4.1.

As described by Yu et al. [170], suppose an n dimensional vector is transformed to m dimensional feature space using some non-linear mapping:

$$\langle x\rangle = (x_1, x_2, \cdots x_n) \xrightarrow{feature\ mapping} \psi(x) = \big(\varphi_1(x), \varphi_2(x), \cdots \varphi_m(x)\big), \qquad x \epsilon S_1, \psi(x) \epsilon S_2$$

Here $S_1$is the original n dimensional space and S_2 is the transformed m dimensional feature space. **x** is a vector in space S_1 and $\psi(x)$ is the corresponding vector is space S_2. ψ is a non

linear mapping that transforms the vector in original space S_1 to a high dimensional space S_2. And $\varphi_i = 1,2,\cdots m$ are the mapping functions.

A kernel function, K(...), can be expressed as inner dot product of the vector in new transformed space without actually carrying out the mapping ψ. Mathematically it can be written as:

$$K(x,y) = \langle \psi(x), \psi(y) \rangle, \qquad \forall\, x, y \,\epsilon S_1 \qquad \text{Equation 34}$$

where $\langle \psi(x), \psi(y) \rangle$ denotes the dot product of $\psi(x)$ and $\psi(y)$. The popular kernel functions that are used commonly are [29] (also see Section 2.4.1):

- Polynomial kernel $\rightarrow$ $\mathrm{K}(\mathrm{x}, \mathrm{y}) = (1 + (\mathrm{x}, \mathrm{y}))^{\mathrm{d}}$, where d is the degree of the polynomial
- Radial Basis Function (RBF) $\rightarrow$ $\mathrm{K}(\mathrm{x}, \mathrm{y}) = \exp\left(-\|\mathrm{x} - \mathrm{y}\|^2 / (2\sigma^2)\right)$, where σ is width of the kernel
- Sigmoidal $\rightarrow$ $\mathrm{K}(\mathrm{x}, \mathrm{y}) = \tanh(\kappa(\mathrm{x}.\mathrm{y}) + \Theta)$, with gain κ and offset Θ

The parameters p,σ, κ and Θ are all adjustable to tune the suitability of a kernel function.

As described by Yu et al. [170], the norm distance between two vectors can be expressed as:

$$d(x,y) = \|x - y\| \qquad \text{Equation 35}$$

By decomposing of $d^2(\psi(x), \psi(y))$ into inner products and substitution of $K(x,y) = \langle \psi(x), \psi(y) \rangle$, $\forall\, x, y \,\epsilon S_1$ Equation 34 for the inner products we get

$$d^2(\psi(x), \psi(y)) = K(x,x) - 2K(x,y) + K(y,y) \qquad \text{Equation 36}$$

Or it can be simplified further as:

$$d_K(x,y) = \sqrt{K(x,x) - 2K(x,y) + K(y,y)} \qquad \text{Equation 37}$$

where $d_K(x,y)$ is the distance metric between vectors x and y in the kernel space.

4.2. Kernel-based KNN Classifiers

The 'kernel approach' has been used by various researchers to implement different flavours of NN-based classifier. Yu et al. [170] applied the 'kernel approach' to modify the norm distance metric and present the Kernel KNN classifier. They proved that the conventional NN

classifier is a special case of the Kernel NN when radial basis kernel or polynomial kernel with degree 1 is chosen. They therefore argue that the Kernel KNN will not perform worse than conventional NN. Also, since the distance metric calculation process is only altered, the computation time of the Kernel NN and the conventional NN shall remain comparable. They show their results on BUPA Liver Disorder data set [50] and US Postal Service data. Their experimental results on Kernel KNN are better than conventional KNN classifiers and can compete with SVM.

Peng et al. [171] present a quasiconformal kernel method for nearest neighbour classification. In traditional NN methods, when the data becomes sparse in high dimensional space, to find nearest neighbourhood one need to look far away from the test sample that may induce severe bias. Their method produces neighbourhoods where the class conditional probabilities tend to be homogenous. This is done by employing quasiconformal kernels as distance metric which tend to move the samples closer to the test example if the class posterior probabilities are similar. Similarly, if the class posterior probabilities of samples are different from the test example, they are moved farther away from it. The resulting effect is to create neighbourhood with homogenous class conditional probabilities. Their experimental results on UCI datasets [50] demonstrate that the algorithm can potentially improve the performance of KNN in some classification and data mining problems.

Daqi and Jie [172] propose a Kernel Fisher Discriminant used with KNN algorithm to solve large scale learning problems. Their main idea is to first, to decompose a large scale multi-class classification problem into multiple two class problems. Secondly, the samples in each class of the two class problems are covered by hyper-dimensional spheres with different sizes, and repeat the process until all of them are included within hyper-spheres of different sizes. Such spheres can be considered as new prototypes and they are relatively less than the original number of samples. Finally, if the Euclidean distance between a test sample and the surface of the sphere of a class is smallest, the sample is assigned the class of the sphere. This kind of kernel KNN classifier only needs to store a small proportion of samples in the form of prototypes. Their results on USPS and letter recognition data show that their method has higher classification accuracy than the standard classification methods they compared with.

4.3. One-class KNN Classifiers

Tax [2] presents a one-class nearest neighbour method, called nearest neighbour description (NN-d). In NN-d, a test object z is accepted when its local density is larger or equal to the

local density of its nearest neighbour in the training set (for detail refer to Section 2.4.3.4). Munroe and Madden [137] extends the idea of one-class KNN to tackle the recognition of vehicles using a set of features extracted from their frontal view and presented high accuracy of classification. They also implemented multi class classifiers to compare their method. They comment that it is not reasonable to draw direct comparisons between the results of the multi-class and single-class classifiers, because the experimental methodology and underlying assumptions are quite different. They also make a note that the performance of multi class classifier could be made arbitrarily worse by adding those vehicle types to the test set that do not appear in the training set, however, since one-class classifiers can represent the concept 'none of the above', their performance should not deteriorate in these conditions.

Cabral et al. [173] propose a one-class nearest neighbour data description using the concept of structural risk minimization. KNN suffers with the drawback of storing all training samples as prototypes that would be used to classify an unseen sample. Their paper is based on the idea of removing redundant samples from the training set, thereby obtaining a compact representation aiming at improving generalization performance of the classifier. Their results on artificial and UCI datasets [50] have shown improved performance than the NN-d classifiers. Their method also achieved considerable reduction in number of stored prototypes. Cabral et al. [174] extended their work and presented another approach where they not only consider the 1 NN but all the k-nearest neighbours and arrive at a decision based on majority voting. In their experiments they observe that K nearest neighbour version of their classifier outperforms the 1 NN and is better than NN-d algorithms. They tested their algorithm on artificial data, biomedical data [37] and data from the UCI repository [50].

Gesù et al. [175] presents a one-class KNN and tested it on synthetic data that simulate microarray data for the identification of nucleosomes and linker regions across DNA. They presented a decision rule to classify an unknown sample X as:

$$j = \left\{ \begin{array}{ll} 1, & if\ |y \epsilon T_P \ \ such\ that \ \ \delta(y,x) \leq \varphi| \geq K \\ 0, & otherwise \end{array} \right\} \qquad \text{Equation 38}$$

where T_P is the training set for the patterns P representing positive instance, δ is the dissimilarity function between patterns. Also, j=1 means that x is positive. The above rule translates to that if there are at least K patterns in T_P dissimilar from x at most φ, then x is classified as a positive pattern, otherwise it is classified as negative. This KNN model depends on parameters K and φ and their values are chosen by using optimization methods.

Their results have shown good recognition rate on synthetic data for nucleosome and linker regions across DNA.

Haro-Garcia et al. [176] used one-class KNN along with other one-class classifiers for identifying plant/pathogen sequences. They find the suitability of above methods owing to the fact that genomic sequences of plant are easy to obtain in comparison to pathogens. They built one-class classifier based only on information from the sequences of the plant and presented a comparison of results.

4.4. Kernel-based One-class KNN classifier

We noted in Sections 4.2 and 4.3 that Kernel-based KNN and one-class KNN methods have been studied in various application domains. In Section 3.6.1 and 3.6.2 we presented two kernels (SLK and WSLK) that can be used as distance metrics to find similarity between spectra and they outperform other traditional similarity measures. The spectral library search similarity method searches for the closest match (similar in concept to 1-NN). The idea of using kernels as similarity metric can be translated in a one-class nearest neighbour classification framework wherein the traditional Euclidean distance measure is replaced by the kernels.

In this section, we propose a Kernel-based One-class NN Classification Method and investigates it applicability for the chemical spectral data. Our main contribution is to

- Replace the standard Euclidean metric with Kernel-based distance measures for estimating the similarity between spectra.
- Formulate an extended one-class Kernel-based KNN classifier that not only depends on target's j nearest neighbours but also on the k nearest neighbours of these j nearest neighbours.

In our research work, we implemented the following kernels:

- Polynomial Kernel of degree 1 (Poly1) $\Rightarrow$ Equivalent to Euclidean distance metric
- Polynomial Kernel of degree 2 (Poly1)
- RBF Kernel (RBF)
- Spectral Linear Kernel (SLK) [139]
- Weighted Spectral Linear Kernel (WSLK) [139]

These kernels will be used as distance metrics as described in Section 4.1.

In the subsequent subsections 4.4.1 and 4.4.2, we propose two variants of the above concept.

4.4.1. Kernel-based One-class KNN Algorithm (KOCKNN)

The Kernel-based One-class 1-NN Algorithm that uses kernel as a distance metric is presented diagrammatically in Figure 21.

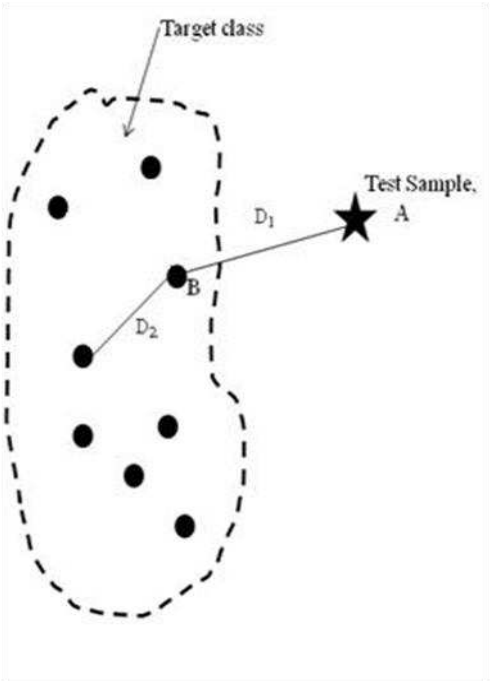


Figure 21: One-class 1-NN Classifier

The classification rule in this method is the same as suggested by Tax [2] and Munroe and Madden [137]. The distance from a test sample A to its nearest neighbour B is computed and called D_1. Then distance from B to its nearest neighbour in the target sample is computed and called D_2.If D_1/D_2 > threshold value then test sample is rejected as an outlier or else accepted as member of target sample.

A variant of above method is called Kernel Based One-class KNN. It works on the same principle except that the k nearest neighbours of B are determined and averaged out to give D_2 (see Figure 22).

The algorithmic steps of our algorithm are similar in concept with the work of Tax [2] and Munroe and Madden [137], the difference being the formulation of kernel as a distance metric. The algorithm can be summarized by following steps:

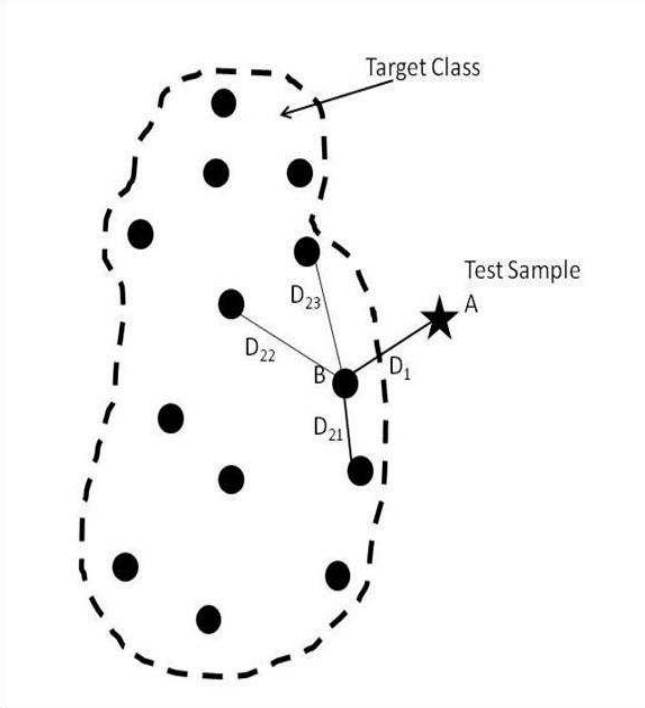


Figure 22: Kernel-based One-class KNN Classifier

Algorithm (KOCKNN):

Input: Target Data, Test sample A

Output: Class Label of test sample A

To classify a test sample, A as a member/not member of target class

1. Set a threshold value (e.g. 1.0) and choose the number of k neighbours
2. Find the nearest neighbour for A in the target class, call it B, compute their distance and call it D_1 (the distance used here will be one of the above defined Kernel-based distance metrics)
3. Find the k nearest neighbours of B in target class.
   3.1. Find the average distances of these k-nearest neighbours and call this distance D_2
4. If $D_1 / D_2 >$ threshold value
   4.1. Reject A as a target class, else
   4.2. Accept A as a target class

4.4.2. Kernel-based One-class J+KNN Classifier (KOCJKNN)

KOCNN is extended to not only consider the j^{th} nearest neighbour of a test sample to target, but to check similarity of k nearest neighbours of these j neighbours. The rationale is to consider the contribution of not one neighbourhood but many while arriving at classification

decision. The distance metric used will be based on kernels rather than Euclidean. In this method, first the j nearest neighbours of a test sample in target class are computed, then the k nearest neighbours of these j neighbours are computed in the target class and averaged out (See Figure 23). The overall results obtained for these j neighbours can be arrived at by using majority voting rule.

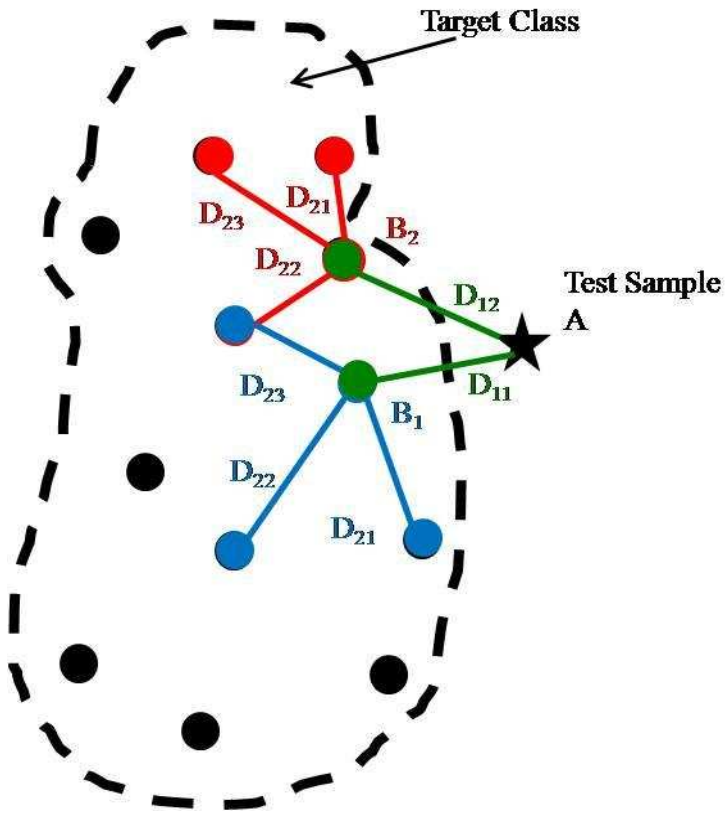


Figure 23: Kernel-based One-class J+KNN Classifier

The algorithmic steps are described below:

Algorithm (KOCJKNN):

Input: Target Data, Test sample A

Output: Class Label of test sample A

To classify a test sample, A as a member/not member of target class

1. Set a threshold value (e.g. 1.0), choose the number of j and k neighbours, set counter accept to zero (this counter will keep the number of acceptance of test sample as member of target class)

2. Find the j nearest neighbours of the test sample A in the target class, call it $B_1, B_2, \ldots B_j$, and compute their distance from A and call it $D_{11}, D_{12}, \ldots D_{1j}$. (the distance used here will be one of the above defined Kernel-based distance metrics)
3. For every j nearest neighbour (i=1,2,...j), repeat Step 4 to 5
4. Find k nearest neighbours for B_j in the target class, call it $C_1, C_2, \ldots C_k$, compute their distance from B_j and call this distance $D_{21}, D_{22}, \ldots D_{2k}$ (the distance used here will be one of the above defined Kernel-based distance metrics)
5. Find the average distances of the k nearest neighbours for B_j in the target class and call this distance D_2
   5.1. If $D_{1j} / D_2 <$ threshold value
   5.2. Increase the counter accept
6. If accept $\geq$ Ceiling(j/2) [majority voting rule], then
   6.1. Accept A as a member of target class, else
   6.2. Reject A as a member of target class

Note: When j is set to 1 and k is set to 1in KOCJKNN, it condenses to Kernel-based 1-NN, similarly when j is set to 1 it condenses to KOCKNN

In the next chapter we present classification results on the chlorinated solvents data using Kernel-based One-class nearest approaches proposed above.

Chapter 5

Experimentation and Results

This chapter describes the experimentation, results obtained, and their analysis on the chlorinated solvent data set, for the application of identifying chlorinated solvents using the kernel as distance metric applied to one-class nearest neighbour classification. At the end of the chapter, conclusions are presented and future directions for this research are discussed.

5.1. Experimentations

5.1.1. Dataset

The chlorinated solvent data is used to evaluate the performance of Kernel-based One-class nearest neighbour classifier. This data set is described in Section 3.8.1.

5.1.2. Setting Parameters

In the experiment KOCJKNN classifier (see Section 4.4.2) is implemented with values of j nearest neighbours set to 1, 3 and 5 and k nearest neighbours set to 1, 3, 5 and 7. This exercise is done to study the effect of varying number of nearest neighbours to the test sample in the target class and its nearest neighbours. The value of threshold to accept or reject a test sample as member of target or outlier class is set to 1. For the first 3 datasets, five one-class kernels were implemented as mentioned in Section 4.4. A fourth dataset is also created from the three main chlorinated solvent data sets, called ChlroinatedOrNot. This data contains the spectra of all those substances that contain one or more of the chlorinated solvents (in any of the three chlorinated solvent data sets) as one of its constituent. For this data, WSLK is not implemented as it only works for the case when we have the spectra of pure substances. As mentioned in Section 3.6.2, WSLK computes similarity between two spectra (at given wavenumber) by computing similarity between their peaks in a neighbourhood with providing more weights at positions where the corresponding pure substance has a peak of higher magnitude. Since ChlroinatedOrNot only contains information about whether chlorinated solvent is present or not and no information about individual pure chlorinated solvents, WSLK is omitted from implementation for this dataset. For kernels Poly1 and Poly2

default settings are used. For RBF kernel, kernel width of 1 is chosen. For SLK and WSLK the window size (neighbourhood) of 3 is used in the experiment.

5.1.3. Splitting into Training and Testing Sets

To perform an experiment, we randomly divide a dataset (i.e. target class) into 67% to form a training set and the remaining 33% to form a test set. An outlier dataset (equal to the number of test set samples) is also constructed by randomly selecting samples from the non-target class. This process is repeated 10 times and the average error is reported. The numbers of test set and outlier samples are kept equal for fair estimation of errors.

5.2. Performance Evaluation

The performance of the KOCJKNN is measured by first computing accuracy, which can be expressed as:

$$\text{accuracy} = \frac{T_{Accept} + O_{Re\,ject}}{T_{Accept} + T_{Re\,ject} + O_{Accept} + O_{Re\,ject}} \qquad \text{Equation 39}$$

where

T_{Accept} is the number of targets accepted as targets

$T_{Re\,ject}$ is the number of targets rejected as outliers

O_{Accept} is the number of outliers accepted as targets

$O_{Re\,ject}$ is the number of outliers rejected as outliers

Error is calculated as:

$$\text{error} = 1 - \text{accuracy} \qquad \text{Equation 40}$$

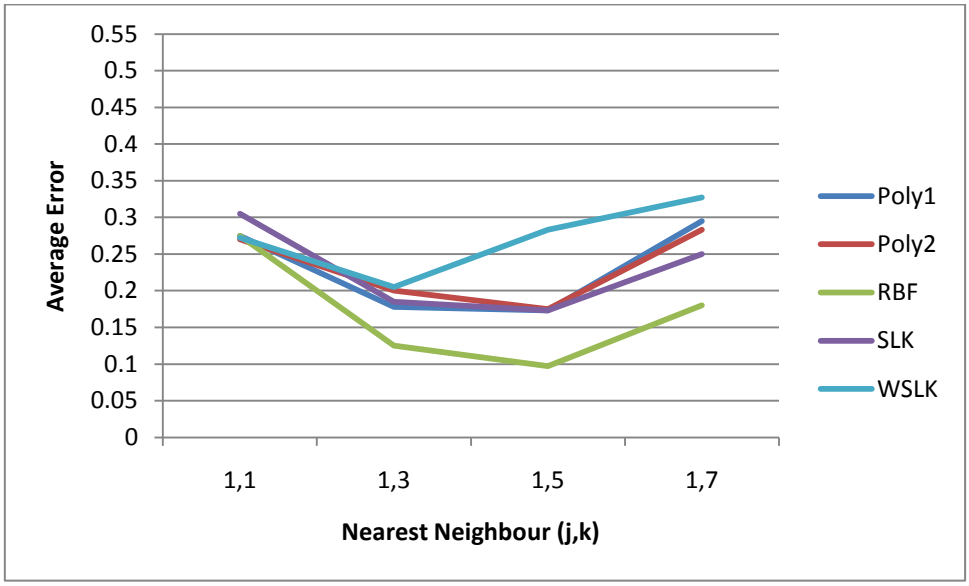
Error is used as performance metric to evaluate different kernels used as distance metric. In the following tables any entry in a cell can be read as average error for a particular Kernel (the row) and (j,k) nearest neighbour (column). The values in grey and bold emphasize the best results obtained.

5.2.1. Dichloromethane

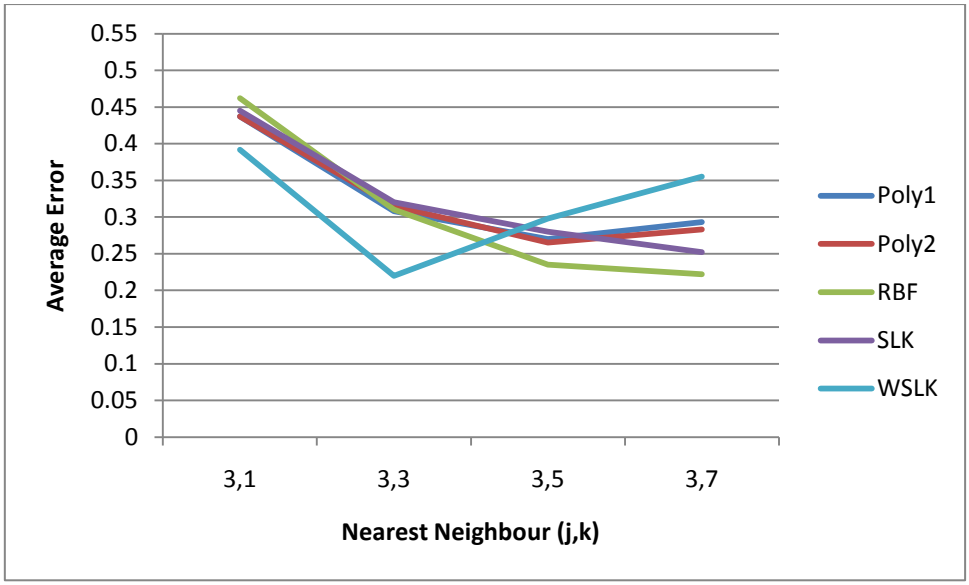
Kernels	Nearest Neighbour (j,k)											
	1,1	**1,3**	**1,5**	**1,7**	**3,1**	**3,3**	**3,5**	**3,7**	**5,1**	**5,3**	**5,5**	**5,7**
Poly1	0.275	0.178	0.173	0.295	0.437	0.308	0.27	0.293	0.487	0.397	0.3	0.305
Poly2	0.27	0.2	0.175	0.283	0.437	0.315	0.265	0.283	0.487	0.385	0.29	0.285
RBF	0.275	0.125	**0.097**	0.18	0.462	0.31	0.235	0.222	0.515	0.408	0.285	0.245
SLK	0.305	0.185	0.173	0.25	0.445	0.32	0.28	0.252	0.482	0.4	0.308	0.265
WSLK	0.272	0.205	0.283	0.327	0.392	0.22	0.298	0.355	0.497	0.335	0.332	0.342

Table 7: One-class Kernel-based j+kNN results for Dichloromethane Data

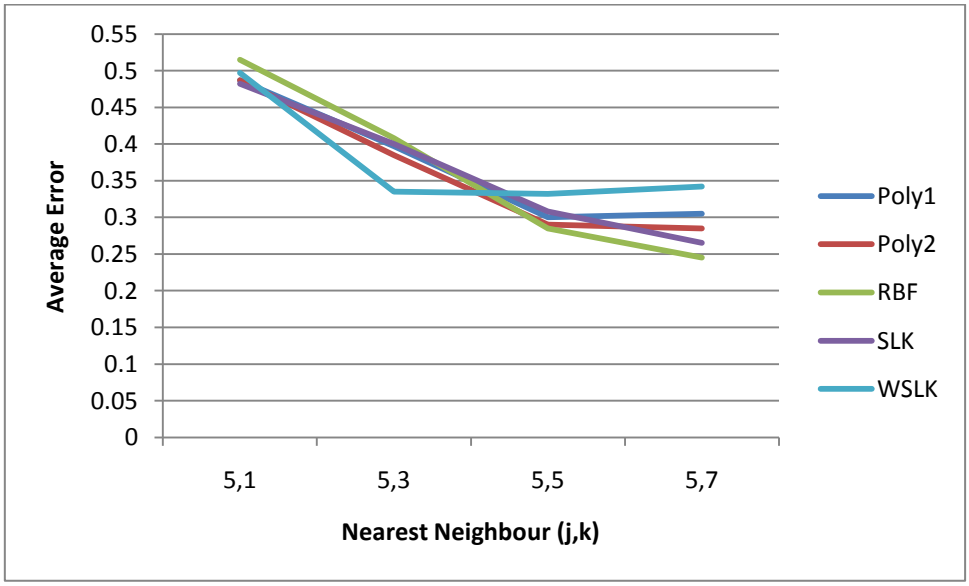
The above tabular results can be presented in graphical form as shown in Figure 24 (a), (b) and (c).



(a)



(b)



(c)

Figure 24: Effect of varying j and k Nearest Neighbours on different Kernels for Dichloromethane Data

Table 7 suggests that the lowest value of error is obtained for j=1 and k=5 for the one-class RBF Kernel. Figure 24 shows the effect of increasing k neighbours with fixed value of j. When the value of k is increased error initially decreases but after certain value of k it tends to increase. A different view is to look at error values by fixing k neighbours and increasing j. Doing so, in general, tend to increase error for almost all the kernels.

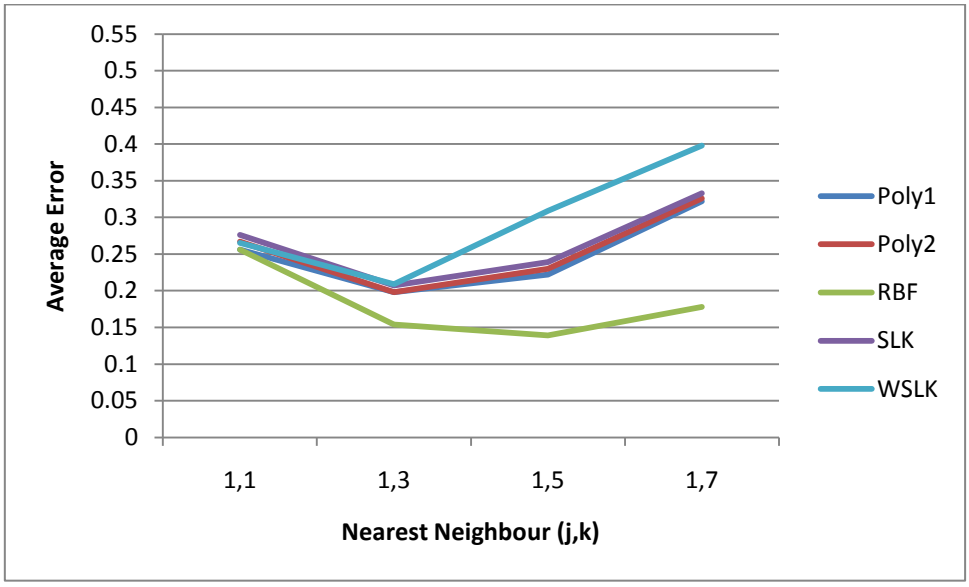
5.2.2. Trichloroethane

Table 8 shows the KOCJKNN results for Trichloroethane data.

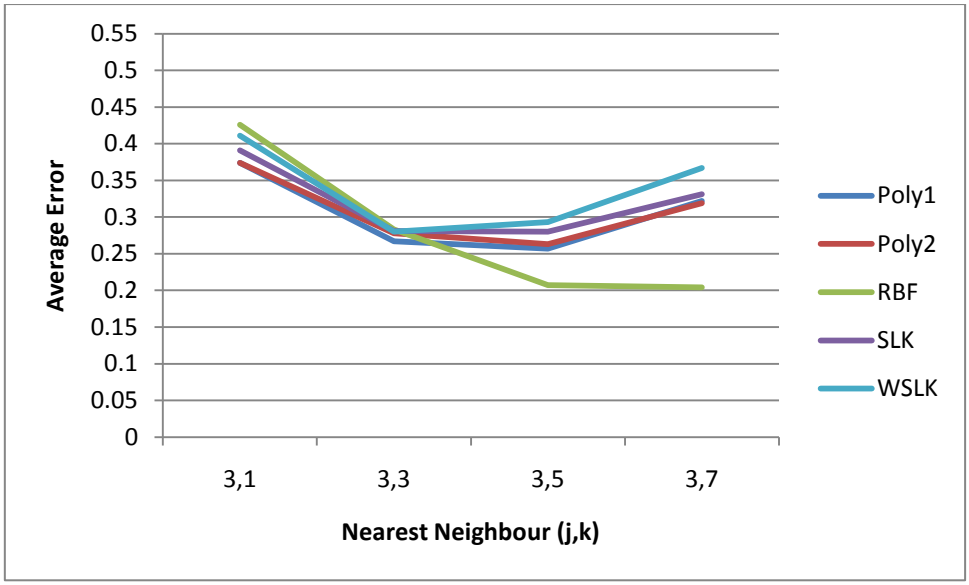
Kernels	Nearest Neighbours (j,k)											
	1,1	**1,3**	**1,5**	**1,7**	**3,1**	**3,3**	**3,5**	**3,7**	**5,1**	**5,3**	**5,5**	**5,7**
Poly1	0.256	0.198	0.222	0.322	0.374	0.267	0.257	0.322	0.485	0.374	0.339	0.335
Poly2	0.267	0.198	0.23	0.326	0.374	0.278	0.263	0.319	0.485	0.376	0.346	0.354
RBF	0.256	0.154	**0.139**	0.178	0.426	0.283	0.207	0.204	0.55	0.435	0.326	0.267
SLK	0.276	0.207	0.239	0.333	0.391	0.281	0.28	0.331	0.481	0.363	0.331	0.335
WSLK	0.265	0.209	0.309	0.398	0.411	0.28	0.293	0.367	0.487	0.394	0.326	0.346

Table 8: One-class Kernel-based j+kNN results for Trichloroethane

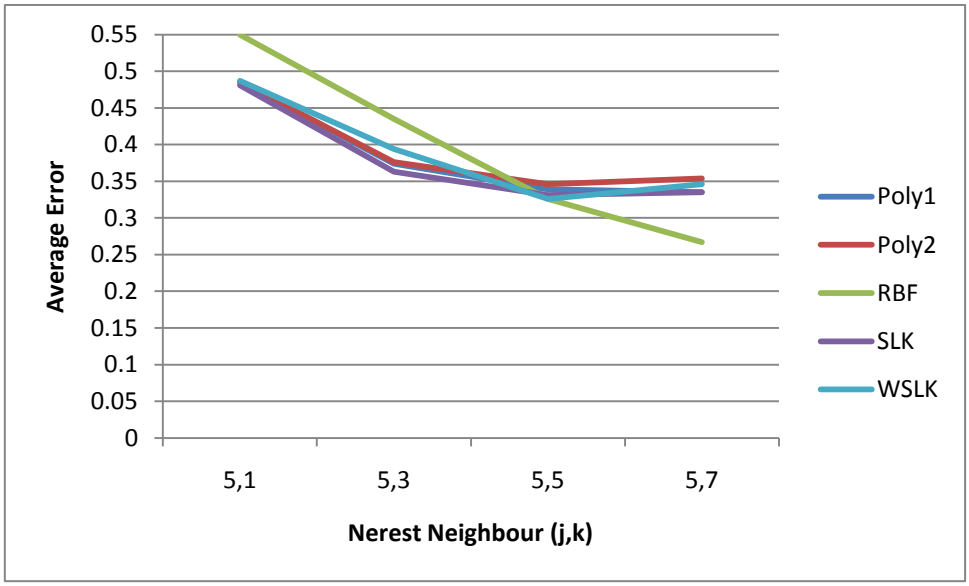
Figure 25 (a), (b) and (c) presents the above results in graphical form.



(a)



(b)



(c)

Figure 25: Effect of varying j and k Nearest Neighbours on different Kernels for Trichloroethane Data

From Table 8 it can be seen that RBF kernel gave the lowest error rates at j=1 and k=5. Figure 25 shows the effect of fixed j nearest neighbours with increasing k for all kernels. We observe that, for almost all kernels, increasing the value of k initially decreases the error but after certain value of k the error gradually increases.

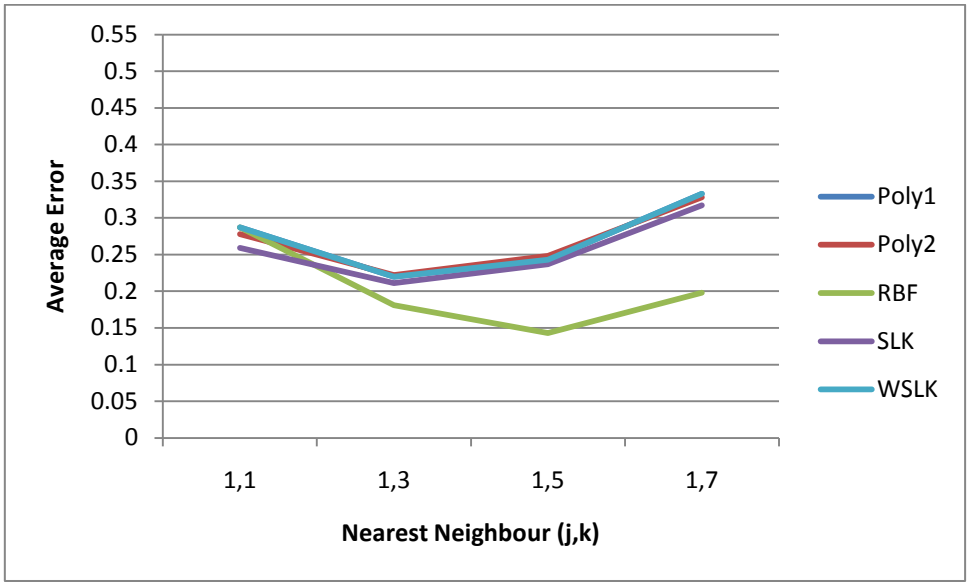
5.2.3. Chloroform

The classification results of KOCJKNN for chloroform data are shown in Table 9

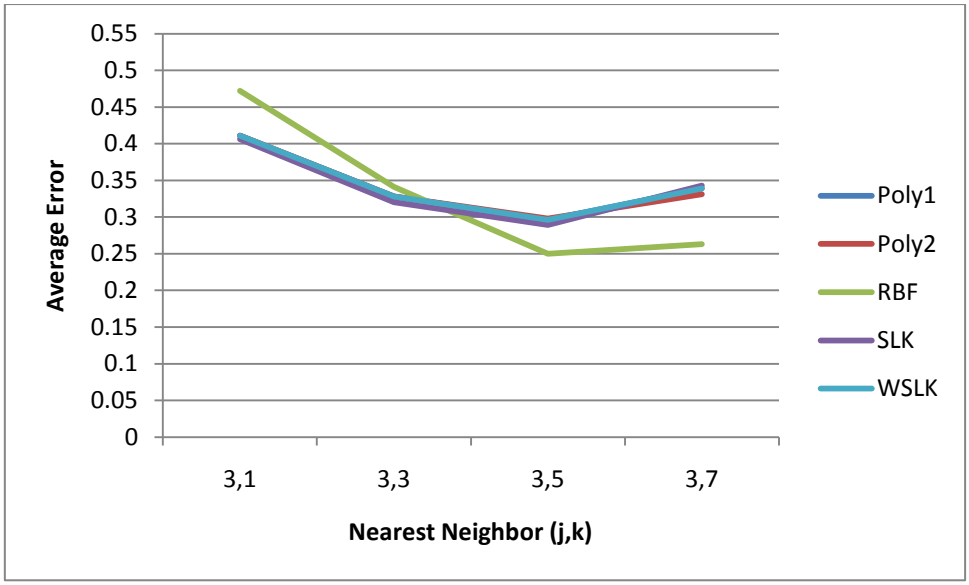
Kernels	Nearest Neighbour (j,k)											
	1,1	**1,3**	**1,5**	**1,7**	**3,1**	**3,3**	**3,5**	**3,7**	**5,1**	**5,3**	**5,5**	**5,7**
Poly1	0.287	0.22	0.243	0.333	0.411	0.328	0.296	0.339	0.48	0.385	0.35	0.363
Poly2	0.278	0.222	0.248	0.328	0.411	0.328	0.298	0.331	0.483	0.389	0.348	0.361
RBF	0.287	0.181	**0.143**	0.198	0.472	0.341	0.25	0.263	0.572	0.45	0.346	0.33
SLK	0.259	0.211	0.237	0.317	0.406	0.32	0.289	0.343	0.481	0.374	0.341	0.35
WSLK	0.287	0.22	0.243	0.333	0.411	0.328	0.296	0.339	0.48	0.385	0.35	0.363

Table 9: One-class Kernel-based j+kNN results for Chloroform Data

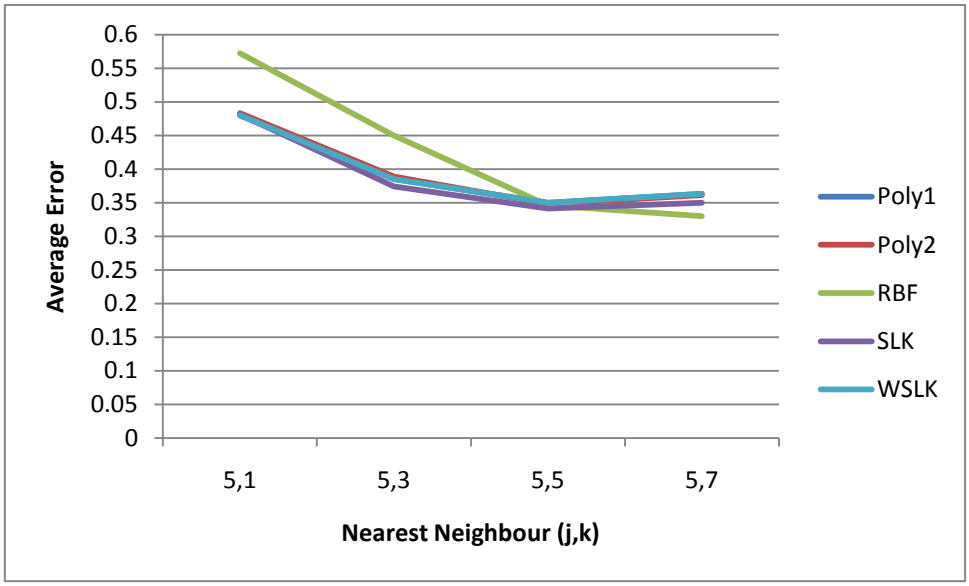
These tabular results are presented graphically in Figure 26 (a), (b) and (c)



(a)



(b)



(c)

Figure 26: Effect of varying j and k Nearest Neighbours on different Kernels for Chloroform Data

It can be seen from Table 9 that RBF kernel gave the lowest error rate at j=1 and k=5. Figure 26 shows that for fixed j neighbours and increasing k, the value of error initially reduces but as k increases, the error also increases. This trend is similar for all kernels.

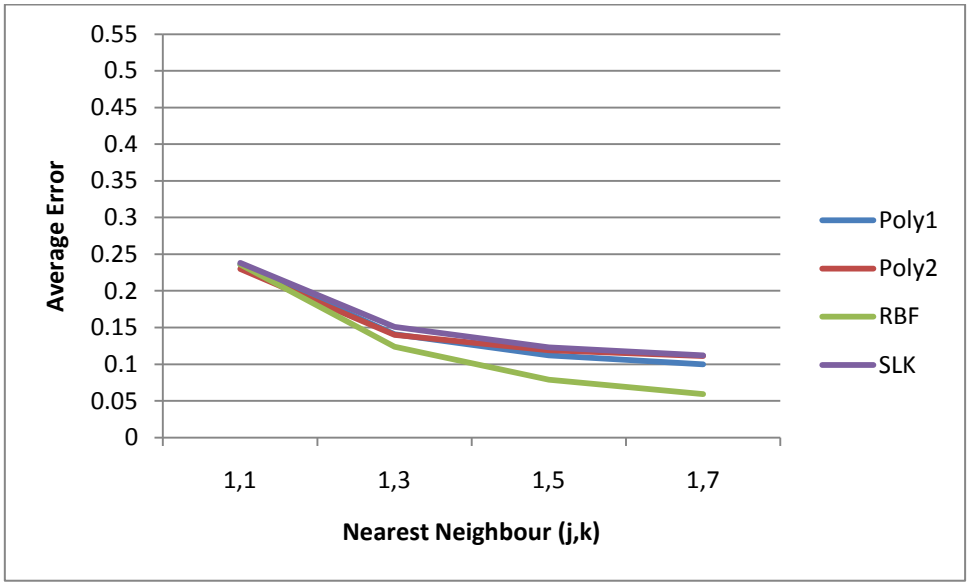
5.2.4. ChlorinatedOrNot

The classification results for ChlroinatedOrNot using KOCJKNN are shown in Table 10.

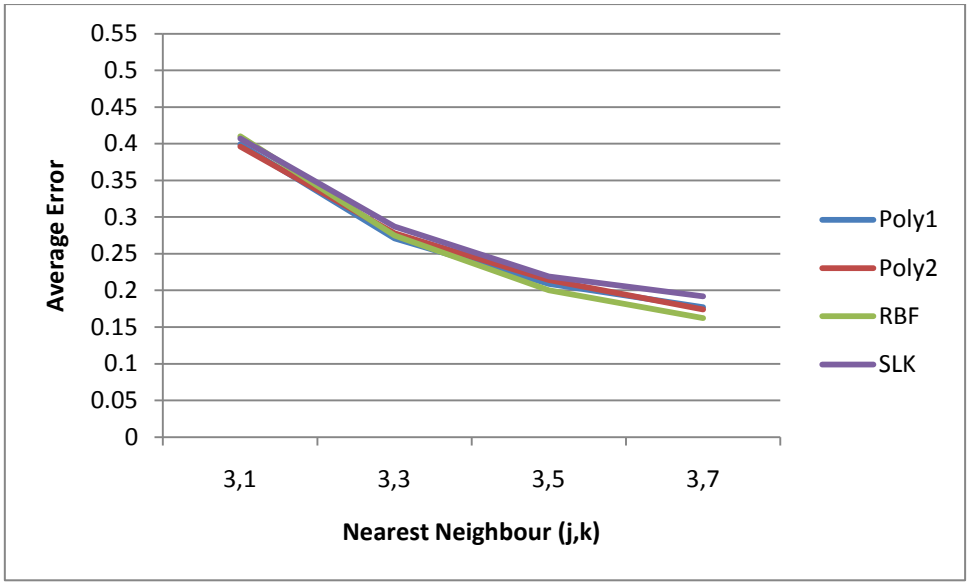
Kernels	Nearest Neighbours (k,j)											
	1,1	1,3	1,5	1,7	3,1	3,3	3,5	3,7	5,1	5,3	5,5	5,7
Poly1	0.236	0.141	0.112	0.1	0.399	0.271	0.209	0.177	0.479	0.378	0.306	0.251
Poly2	0.23	0.14	0.119	0.111	0.396	0.278	0.214	0.174	0.474	0.385	0.302	0.253
RBF	0.236	0.124	0.079	**0.059**	0.41	0.275	0.2	0.162	0.491	0.387	0.308	0.249
SLK	0.238	0.151	0.123	0.112	0.407	0.287	0.219	0.192	0.477	0.382	0.308	0.265

Table 10: One-class Kernel-based j+kNN results for ChlorinatedOrNot

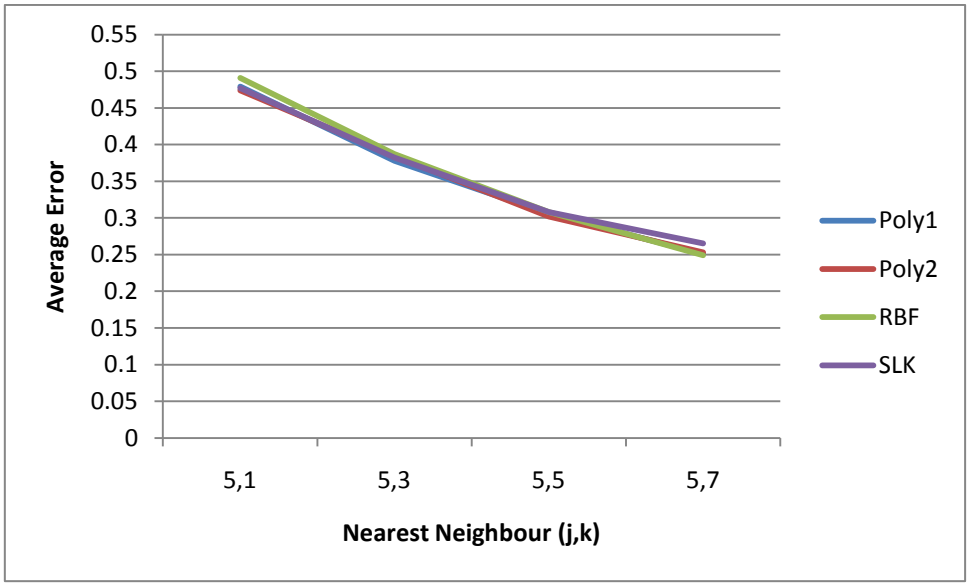
The above tabular results are presented in graphical form in Figure 27 (a), (b) and (c)



(a)



(b)



(c)

Figure 27: Effect of varying j and k Nearest Neighbours on different Kernels for ChlorintedOrNot data

Table 10 shows the results of ChlroinatedOrNot data set. The lowest value of error is obtained with RBF kernel for j=1 and k=7. Figure 27 shows the effect of fixed j neighbours with increasing value of k neighbours. As the value of k is increased the error shows a decreasing trend for all kernels with RBF kernel giving the lowest error rates. Alternatively, it can also be observed from Table 10 that by fixing k neighbours and increasing j neighbours, in all kernels, the error increases. The error rates for this dataset are very low in comparison to other three chlorinated solvent datasets, because here the task is much simpler to find only

the presence or absence of any chlorinated solvent in a mixture and not individual chlorinated solvents.

5.2.5. Analysis of Results

We present our analysis of results based on the following criteria:

- Increasing the number of k nearest neighbours

From Figure 24, Figure 25, Figure 26 and Figure 27 we observe a common trend that for any given j nearest neighbours (for almost all kernels), increasing the value of k nearest neighbour decreases the error rates till a particular value after which it error tends to increase. This is due to the fact that some of the nearest neighbours are quite close to each other, however when the number of neighbours are increased the classifier finds far away samples and this leads to decrease in accuracy.

- Increasing the number of j nearest neighbours

From Figure 24, Figure 25, Figure 26 and Figure 27 we observe that for any given kernel and k nearest neighbour, increasing j nearest neighbours increases the classification error. This trend is common almost all the data. The reason for this is that the classifier finds nearest neighbours that are farther away and lead to bad classification results.

- On Using Different Kernels

From Table 7, Table 8, Table 9 and Table 10 we observe that for any given k and j nearest neighbours, One-class RBF Kernel gave the lowest error rates for all the four datasets studied.

By looking at the overall results, we can infer that RBF Kernel when used as distance metric for implementing KOCJKNN gives the lowest values of errors at j=1 and k=5 or k=7. This experiment show that a one-class KOCJKNN approach performs better when j=1. Increasing the value of j neighbours is detrimental for this data set's classification accuracy. However increasing the value of k nearest neighbours to a certain limit may boost the accuracy. We also deduce that for KOCJKNN classifier, RBF Kernel is much better in performance in comparison to the Polynomial Kernel of degree 1 (which is equivalent to Euclidean metric) and other kernels considered. In all the chlorinated datasets studied, only the RBF Kernel performs significantly better than other kernels. In fact, the quadratic polynomial and spectral kernels perform no better than the linear kernel which is directly equivalent to the standard Euclidean metric. Moreover, the spectral kernels that give significantly better performance in

the spectral search setting in comparison to Euclidean metric, do not perform any better than it in the one-class KNN setting.

5.2.6. Effect of Varying Kernel Width in RBF Kernel

In Section 5.2.5 we observe that RBF kernel (on default setting) suits the most as a distance metric in the implementation of One-class Nearest Neighbour classifier for the chlorinated solvent data set. To study the effect of varying width of RBF kernel we extended our experiment and results are shown below.

In the following figures RBF1, RBF5, RBF25 and RBF100 corresponds to RBF kernel with width, σ=1, 5, 25 and 100.

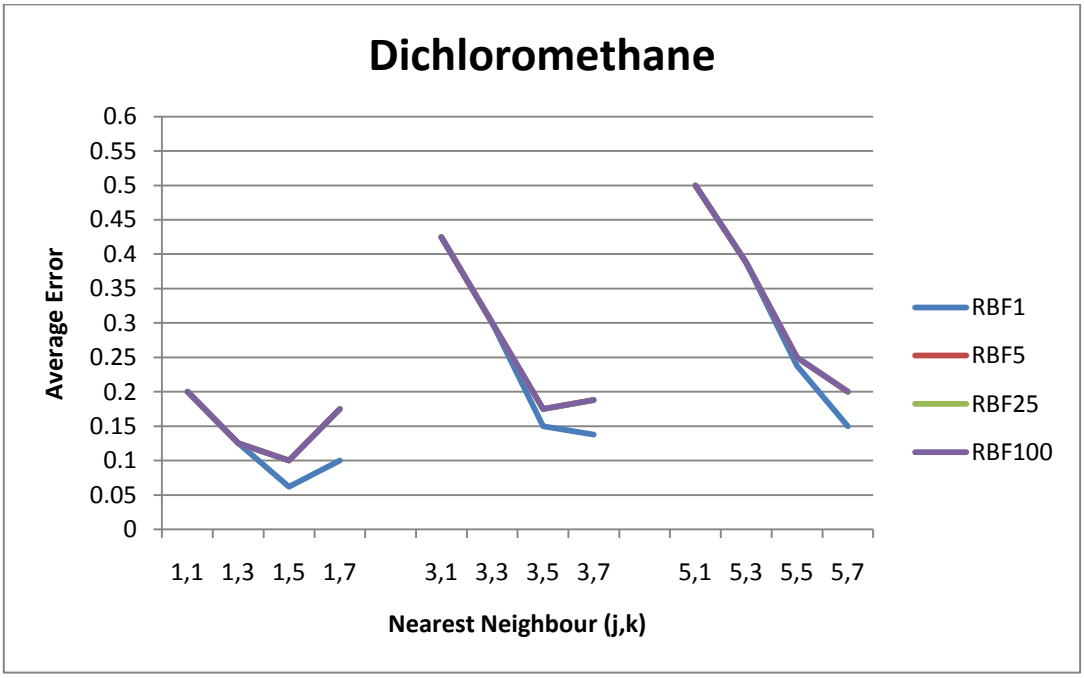


Figure 28: RBF Kernel with different widths for Dichloromethane

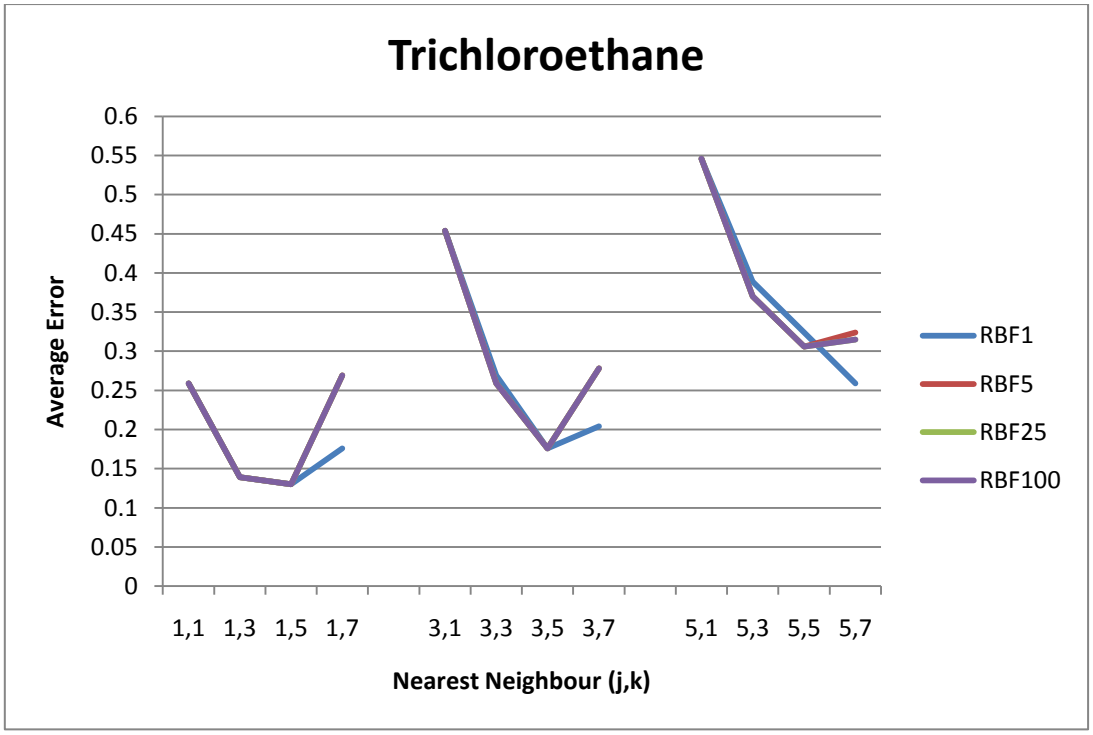


Figure 29: RBF Kernel with different widths for Trichloroethane

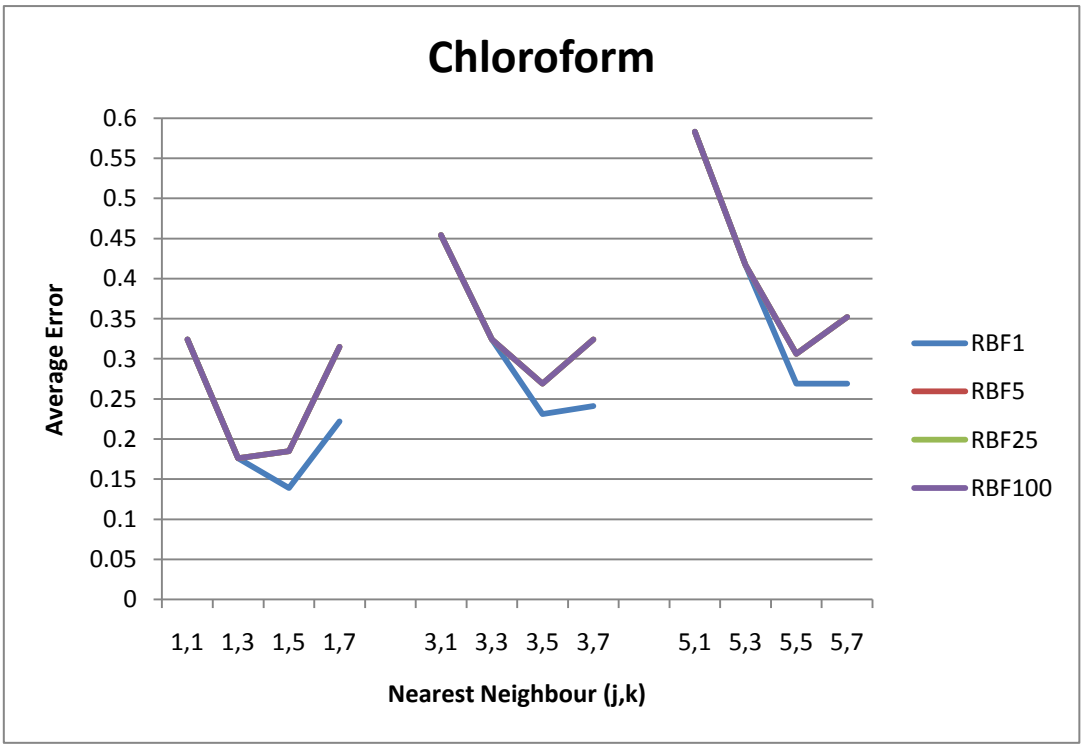


Figure 30: RBF Kernel with different widths for Chloroform

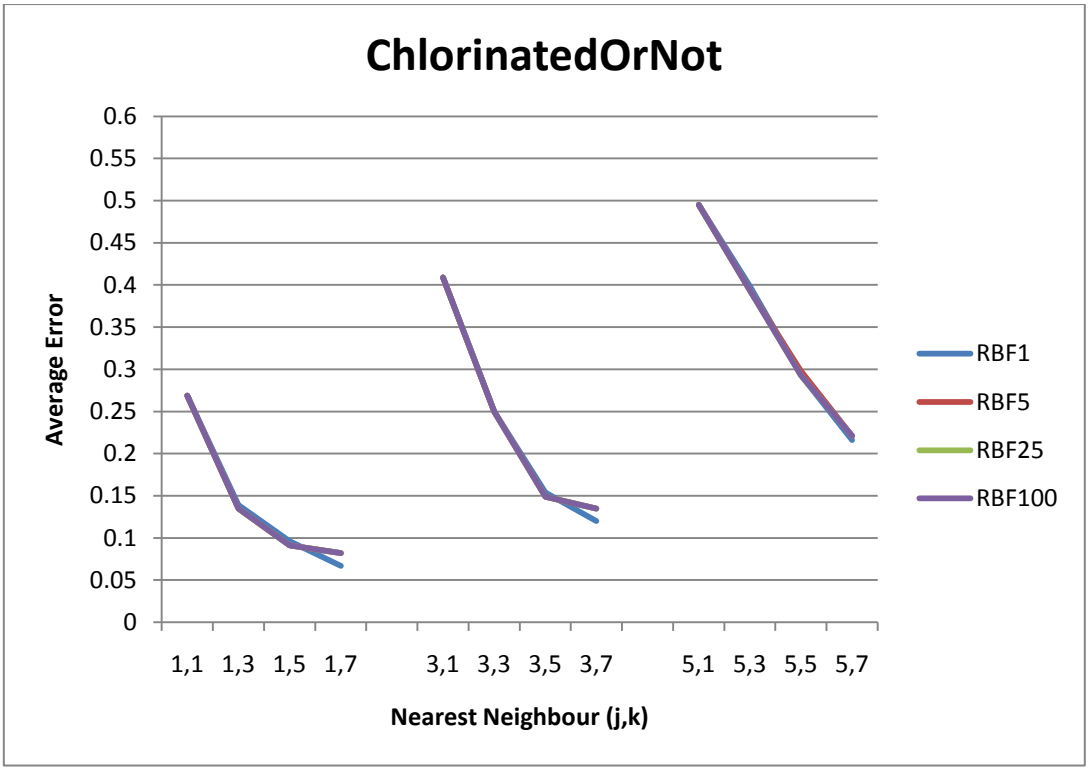


Figure 31: RBF Kernel with different widths for ChlorinatedORnot

The same inferences can be drawn by increasing k and j nearest neighbours. The best results came when j=1 and k=5 or 7. An important point to note is that increasing the kernel width does not necessarily improves the error rates. In fact, most of the time kernel width, σ=1 gave the lowest error rates. This behaviour may be because the chlorinated solvent data is dense in localized regions and beyond that it gets sparse.

5.3. Conclusions and Future Work

We can summarize our key research contributions as follows:

- Based on our survey of OCC literature, we provided a taxonomy for the study of OCC problems. This taxonomy is based on three categories i.e. availability of data, algorithms used, and applications. Researchers may find this taxonomy useful when exploring the broad range of publications on OCC. We hope that it may be enormously helpful to researchers and greatly reduce their time taken to do research. We also provided some guidelines for the study of OCC paradigm and flag certain open research areas in OCC that should be of interest to researchers working in this field.
- We studied various similarity metrics for effective spectral library search and proposed a new similarity measure by modifying the standard Euclidean metric that is

more specific to the spectroscopic data. We conducted our experiments on the real world Chlorinated Solvents data that contains Raman Spectra of various chlorinated solvents present in pure and mixture form. Our results suggest that domain specific (dis)similarity metrics perform much better than the standard search algorithms.

- We adapted the use of the kernels as distance metric to the task of One-class classification and use them to induce extended One-class j+k nearest neighbour classifier for the identification of chlorinated solvents. Our experiments showed that for j=1 and k=5 or 7 we get low error rates for the all four variants of chlorinated solvents we created. This indicates that in higher dimension data gets sparse and considering more neighbourhoods proves detrimental to classification accuracy. Moreover, RBF kernels proved to be the best choice. We further varied the kernel width,σ, of the RBF kernel in the proposed one-class nearest neighbour framework and deduce that low values of σ can provide low error rates.

A surprising finding arises from the experiments that the spectral kernels works well in the spectral search setting, however, they do not perform well in the one class KNN setting when used as distance metric. In future, we would like to investigate this deviation of behaviour of the spectral kernels.

We would like to test our proposed kernel-based nearest neighbour approach on other spectroscopic data. We would also like to explore new kernels, especially those which are specific to the domain of spectroscopy because our experiments show that domain specific kernels perform better than conventional ones. We would like to test our methodology on 'unexpected outliers' as studied by Glavin and Madden [103]. According to the authors, unexpected outliers can be defined as those outliers that do not come from the same distribution of data as in normal training and outlier data set. For example, for the chlorinated solvents data set, mixtures of sugars, salts etc can be considered 'unexpected outliers', because they do not come from the same set of chlorinated solvents.

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