One-Class Kernel Spectral Regression for Outlier Detection

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Abstract—The paper introduces a new efficient nonlinear one-class classifier formulated as the Rayleigh quotient criterion optimisation. The method, operating in a reproducing kernel Hilbert subspace, minimises the scatter of target distribution along an optimal projection direction while at the same time keeping projections of positive observations distant from the mean of the negative class. We provide a graph embedding view of the problem which can then be solved efficiently using the spectral regression approach. In this sense, unlike previous similar methods which often require costly eigen-computations of dense matrices, the proposed approach casts the problem under consideration into a regression framework which is computationally more efficient. In particular, it is shown that the dominant complexity of the proposed method is the complexity of computing the kernel matrix. Additional appealing characteristics of the proposed one-class classifier are: 1-the ability to be trained in an incremental fashion (allowing for application in streaming data scenarios while also reducing the computational complexity in a non-streaming operation mode); 2-being unsupervised, but providing the option for refining the solution using negative training examples, when available; Last but not least, 3-the use of the kernel trick which facilitates a nonlinear mapping of the data into a high-dimensional feature space to seek better solutions.

Extensive experiments conducted on several datasets verify the merits of the proposed approach in comparison with other alternatives.

Index Terms—One-class classification, graph embedding, spectral regression, Rayleigh quotient, Fisher analysis.

I. INTRODUCTION

ONE-class classification (OCC) deals with the problem of identifying objects, events or observations which conform to a specific behaviour or condition, identified as the target/positive class \( (\mathcal{T}) \), and distinguish them from all other objects, typically known as outliers or anomalies. More specifically, consider a set of points \( X = \{x_1, \ldots, x_n\} \) where \( x_i \in \mathbb{R}^d \) is a realisation of a multivariate random variable \( x \) drawn from a target probability distribution with probability density function \( p(x) \). In a one-class classification problem, the goal is to characterise the support domain of \( p(x) \) via a one-class classifier \( h(z) \) as

\[
h(z) = [q(z) \leq \tau] = \begin{cases} 1 & z \in \mathcal{T} \\ 0 & \text{otherwise} \end{cases}
\]

where function \( q(\cdot) \) is modelling the similarity of an observation to the target data and \([\cdot]\) denotes the Iverson brackets. Parameter \( \tau \) is optimised so that an expected fraction of observations lie within the support domain of the target distribution. One-class learning serves as the core of a wide variety of applications such as intrusion detection \([1]\), novelty detection \([2]\), fault detection in safety-critical systems \([3]\), fraud detection \([4]\), insurance \([5]\), health care \([6]\), surveillance \([7]\), etc. Historically, the first single-class classification problem seems to date back to the work in \([8]\) in the context of learning Bayes classifier. Later, with a large time gap, the term one-class classification was used in \([9]\). As a result of a widening spectrum of applications of one-class classification, other terminology has been adopted, including anomaly/outlier detection \([10]\), novelty detection \([11]\), concept learning \([12]\).

OCC techniques are commonly employed when the non-target/negative class is either not well defined, poorly sampled or totally missing, which may be due to the openness of the problem or due to the high cost associated with obtaining negative samples. In these situations, the conventional two-class classifiers are believed not to operate as effectively since they are based on the assumption that data from all classes are more or less equally balanced. OCC techniques are developed to address this shortcoming of the conventional approaches by primarily training on the data coming from a single class. Nevertheless, the lack of negative samples may pose serious challenges in learning one-class classifiers as the decision boundary can be estimated using only positive observations. As a result, the one-class problem is typically considered to be more difficult than the two-class counterpart. As observed in \([13]\), the challenges related to the standard two/multi-class problems, e.g. estimation of the error, atypical training data, the complexity of a solution, the generalisation capability, etc. are also present in OCC and may sometimes become even more severe.
Although there may exist a fine grain categorisation of one-class techniques \cite{14, 13, 15}, a general, overarching classification considers them to be either generative or non-generative \cite{16}. The generative approaches incorporate a model for generating all observations, whereas non-generative methods lack a transparent link to the data. In this context, the non-generative methods are best represented by discriminative approaches which partition the feature space in order to classify an object. As notable representatives of the generative approaches one may consider the parametric and non-parametric density estimation methods \cite{17, 18, 19} (using for example a Gaussian, a mixture of Gaussians or a Poisson distribution), neural-network based methods \cite{12, 20}, one-class sparse representation classification \cite{21, 22}, etc. Well-known examples of the non-generative methods include those based on support vector machines (SVDD/one-class SVM) \cite{23, 24}, linear programming \cite{25}, convex hull methods \cite{26}, \cite{27}, cluster approaches \cite{28}, deep-learning based methods \cite{29, 30} and subspace approaches \cite{31, 32, 33, 34, 35}. By virtue of the emphasis on classification, rather than modelling the generative process, the non-generative approaches tend to yield better performance in classification.

In practical applications where the data to be characterised is highly nonlinear and complex, linear approaches often fail to provide satisfactory performance. In such cases, an effective mechanism is to implicitly map the data into a very high dimensional space with the hope that in this new space the data become more easily separable, the prominent examples of which are offered by kernel machines \cite{36, 37, 38, 39}. Nevertheless, the high computational cost associated with these methods can be considered as a bottleneck in their usage. For instance, the one-class variants of kernel discriminant analysis \cite{33, 40, 34, 41} often require computationally intensive eigen-decompositions of dense matrices.

In this work, a new nonlinear one-class classifier formulated as optimisation of a Rayleigh quotient is presented which unlike previous discriminative methods \cite{31, 32, 33, 34, 35, 41} avoids costly eigen-analysis computations via the spectral regression (SR) technique. This solution has been shown to speed up the kernel discriminant analysis by several orders of magnitude \cite{42}. By virtue of bypassing the eigen-decomposition of large matrices via a regularised regression formulation, the proposed One-Class Kernel Spectral-Regression (OC-KSR) approach becomes computationally very attractive, with the dominant complexity of the algorithm being relegated to the computation of the kernel matrix. An additional appealing characteristic of the method is the amenability to be applied in an incremental fashion, allowing for the injection of additional training data into the system in a streaming data scenario, side-stepping the need to reinitialise the training procedure, while also reducing the computational complexity in a non-streaming operation mode. Additionally, the method can be operated in an unsupervised mode as well as by using some negative examples in the training set to further refine the solution.

A. Overview of the Proposed Approach

In the proposed one-class method, the strategy is to map the data into the feature space corresponding to a kernel and infer a direction in the feature space such that: 1-the scatter of the data along the projection direction is minimised; 2-the projected samples and the mean of negative class along the projection direction are maximally distant. The problem is then posed as one of graph embedding which is optimised efficiently using the spectral regression technique \cite{42}, thus avoiding costly eigen-analysis computations. In addition, an incremental version of the proposed method is also presented which reduces the computational complexity of the training phase even further. Although in an OCC problem negative training examples are not always expected to exist, if they do, the proposed method is able to utilise them to further refine the decision boundary. During the test phase, the decision criterion for the proposed approach involves projecting a test sample into an optimal feature subspace, followed by computing the distance between its projection and that of the mean of the training samples.

The main contributions of the present work are:

- A method of designing a nonlinear one-classifier (OC-KSR) developed from a graph embedding formulation of the problem;
- Efficient optimisation of the proposed formulation based on spectral regression;
- An incremental variant of the OC-KSR approach;
- An extension of the proposed OC-KSR method to benefit from possible negative samples in the training set in a supervised operating mode;
- An extensive evaluation of the proposed method and its comparison to the state-of-the-art one-class classification techniques on several datasets.

B. Outline of the Paper

The rest of the paper is organised as follows: In Section \[\text{II}\] the one-class methods which are closely related to the proposed method are reviewed. In doing so, the focus is on nonlinear methods posing the one-class classification problem as an optimisation of (generalised) Rayleigh quotient. In Section \[\text{III}\] the proposed one-class method (OC-KSR) is presented. An experimental evaluation of the proposed approach along with a comparison to other methods on several datasets is provided in Section \[\text{IV}\]. Finally, the paper is drawn to conclusions in Section \[\text{V}\].

II. RELATED WORK

As an example of the unsupervised methods using a Rayleigh quotient, the work in \cite{19} employs kernel PCA for novelty detection where a principal component in a feature space captures the distribution of the data and the reconstruction residual of a test sample with respect to the inferred subspace is employed as a novelty measure. Other work in \cite{43} describes a strategy to improve the convergence of the kernel algorithm for the iterative kernel PCA. A different study \cite{44} proposed a robustified PCA to deal with outliers in the training set.
In [31], [45], a one-class kernel Fisher discriminant classifier is proposed which is related to Gaussian density estimation in the induced feature space. The proposed method is based on the idea of separating the data from their negatively replicated counterparts and involved an eigenvalue decomposition of the kernel matrix. In this approach, the data are first mapped into some feature space, where a Gaussian model is fitted. Mahalanobis distance to the mean of this Gaussian is used as a test statistic to test whether the data is explained by the model. As pointed out in [45], for kernel maps which transform the input data into a higher-dimensional space, the assumption that the target data is normally distributed may not hold. If the deviation from normality is large, the method in [31], [45] may lead to unreliable results.

The work in [33] proposed a Fisher-based null space method where a zero within-class scatter and a positive between-class scatter are used to map all training samples of one class into a single point. The proposed method treats multiple known classes jointly and detects novelty with respect to the set of classes with the resulting single model by using a projection into a joint subspace where the training samples of all known classes are presumed to have zero variance. Checking for novelty involves computing a distance in the estimated subspace. The method requires eigen-decomposition of the kernel matrix. In a follow-up work [46], it is proposed to incorporate locality in the null space approach of [33] by considering only the most similar patterns to the query sample, leading to improvements in performance. In [41], an incremental version of the method in [33] is proposed to increase computational efficiency.

In [34], [47], a generalised Rayleigh quotient specifically designed for outlier detection is proposed. The method tries to find an optimal hyperplane which is closest to the target data and farthest from the outliers which requires building two scatter matrices: an outlier scatter matrix corresponding to the outliers and a target scatter matrix for the target data. While in [34], the decision boundary is found by a computationally intensive generalized eigenvalue problem, which limits the use of the method to medium sized datasets, in [47] the generalized eigenvalue problem is replaced by an approximate conjugate gradient solution to decrease the computational cost. The method presented in [34], [47] has certain shortcomings as the computation of the outlier scatter matrix requires the presence of atypical instances which is sometimes difficult to collect in some real applications. Another drawback is that the method is based on the assumption that the target population differs from the outlier population in terms of their respective densities which might not hold for real-world problems in general. A later study [40] tries to address these shortcomings via a null-space version of the method in [34], [47]. In order to overcome the limitation of the availability of outlier samples, it is proposed to separate the target class from the origin of the kernel feature space, which serves as an artificial outlier sample. The density constraint is then relaxed by deriving a joint subspace where the training target data population have zero covariance. The method involves eigen-computations of dense matrices.

While the majority of previous papers on one-class classification using a Rayleigh quotient formulation requires computationally intensive eigen-decomposition of large matrices, in this work, a one-class approach is proposed which replaces costly eigen-analysis computations by the spectral-regression technique [42]. In this sense, the present work can be considered as a one-class variant of the multi-class approach in [42] and the two-class, class-specific method of [48] with additional contributions discussed in the subsequent sections.

### III. One-Class Kernel Spectral Regression

Let us assume that there exist $n$ samples $x_1, x_2, \ldots, x_n \in \mathbb{R}^d$ and $\mathcal{F}$ is a feature space (also known as RKHS: reproducing kernel Hilbert space) induced by a nonlinear mapping $\phi : \mathbb{R}^d \to \mathcal{F}$. For a properly chosen mapping, an inner product $\langle \cdot, \cdot \rangle$ on $\mathcal{F}$ may be represented as $\langle \phi(x_i), \phi(x_j) \rangle = \kappa(x_i, x_j)$, where $\kappa(\cdot, \cdot)$ is a positive semi-definite kernel function. Our strategy for outlier detection is to map the data into a feature space induced by the nonlinear mapping $\phi(\cdot)$ and then look for an optimal projection direction (subspace) in the RKHS based on two criteria: 1-minimising the scatter of mapped target data in the RKHS along the projection direction, and 2-maximising their distances from the mean of non-target observations in this subspace. In doing so, the problem is formulated as one of graph embedding which is then posed as optimising a Rayleigh quotient. The optimisation problem is then efficiently solved using a spectral regression framework. The two criteria used in this work to find an optimal subspace are discussed next.

### TABLE I

| Notation | Description |
|---------|-------------|
| $T$     | The target class |
| $n$     | Total number of training samples |
| $n_0$   | Number of labelled negative examples in the training set |
| $x_i$   | The $i^{th}$ observation in the training set |
| $d$     | Dimensionality of observations in the input space |
| $\mathcal{F}$ | The feature (reproducing kernel Hilbert) space |
| $\phi(\cdot)$ | The nonlinear mapping function onto the feature space |
| $S(T)$  | Scatter of positive training observations along projection direction |
| $M$     | The mean of projected positive samples |
| $I(\cdot)$ | The projection function |
| $\mathbb{R}$ | The set of real numbers |
| $\mathbb{R}^d$ | The set of real vectors in the $d$-dimensional space |
| E       | Graph adjacency matrix |
| I       | The identity matrix |
| L       | A matrix of 1’s |
| M       | Graph Laplacian matrix |
| D       | Graph degree matrix |
| $B(T)$  | Sum of squared distances of positive training observations to the mean of the non-target class |
| $\alpha$ | The transformation vector |
| $\gamma$ | The vector of responses (projections) |
| $S_b$   | Between-class scatter |
| $S_w$   | Within-class scatter |
| $K$     | The kernel matrix |
| $\kappa(\cdot, \cdot)$ | The kernel function |
| $\tau$  | The threshold for deciding normality |
| $\delta$ | The regularisation parameter |
A. Scatter in the feature subspace

Let us consider a projection function \( f(\cdot) \) which maps each target data point \( x_i \) onto a feature subspace. For the reasons to be clarified later, \( f(\cdot) \) is assumed to be a one-dimensional mapping. The scatter of target data in the feature space along the direction specified by \( f(\cdot) \) is defined as

\[
S(T) = \sum_{i=1}^{n} (f(x_i) - \mathcal{M})^2
\]

(2)

where \( \mathcal{M} \) denotes the mean of all projections \( f(x_i) \)'s, i.e.

\[
\mathcal{M} = \frac{1}{n} \sum_{i=1}^{n} f(x_i)
\]

(3)

Note that as we are working in the feature space, \( f(\cdot) \) captures both a mapping from the original \( \mathbb{R}^d \) space onto the feature space as well as a projection onto a line in the RKHS. In order to detect outliers, it is desirable to find a projection function \( f(\cdot) \) which minimises dispersion of positive samples and forms a compact cluster, i.e. minimises \( S(T) \). \( f(\cdot) \) can be written in terms of real numbers \( \alpha_i \)'s and a positive semi-definite kernel function \( \kappa(\cdot, \cdot) \) defining an \( n \times n \) kernel matrix \( \mathbf{K} \) (where \( K_{ij} = \kappa(x_i, x_j) \)) according to the following proposition:

**Proposition.**

\[
f(z) \in \{ \sum_{i=1}^{n} \alpha_i \kappa(z, x_i) | \alpha_i \in \mathbb{R} \}
\]

(4)

cf. [49] for a proof.

Assuming that the kernel function \( \kappa(\cdot, \cdot) \) is chosen and fixed, the problem of minimising \( S(T) \) with respect to \( f(\cdot) \) boils down to finding \( \alpha^{opt} \):

\[
\min_{\alpha} S(T) = \min_{f(\cdot)} \sum_{i=1}^{n} (f(x_i) - \mathcal{M})^2
\]

\[
= \min_{\alpha} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \kappa(x_i, x_j) - \frac{1}{n} \sum_{k=1}^{n} \sum_{j=1}^{n} \alpha_j \kappa(x_k, x_j)^2
\]

(5)

1) **Graph Embedding View:** Let us now augment the dataset \( (x_i)^n \) with an additional point \( x_{n+1} \) satisfying \( f(x_{n+1}) = \mathcal{M} \). Let us also define the \( (n+1) \times (n+1) \) matrix \( \mathbf{E} \) as

\[
\mathbf{E} = \begin{pmatrix}
0 & \ldots & 0 & 1 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \ldots & 0 & 1 \\
1 & 1 & 1 & 0
\end{pmatrix}
\]

(6)

The scatter \( S(T) \) in Eq. 2 can now be written as

\[
S(T) = \frac{1}{2} \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} (f(x_i) - f(x_j))^2 E_{ij}
\]

(7)

where \( E_{ij} \) denotes the element of \( \mathbf{E} \) in the \( i^{th} \) row and \( j^{th} \) column. The latter formulation corresponds to a graph embedding view of the problem where the data points are represented as vertices of a graph and \( \mathbf{E} \) is the graph adjacency matrix, encoding the structure of the graph. That is, if \( E_{ij} = 1 \), then the two vertices \( i \) and \( j \) of the graph are connected by an edge. With this perspective and \( \mathbf{E} \) given by Eq. 6 each data point \( x_i \), for \( i = 1, \ldots, n \) is connected by an edge to \( x_{n+1} \), resulting in a star graph structure, Fig. 2. The purpose of graph embedding is to map each node of the graph onto a subspace in a way that the similarity between each pair of nodes is preserved. In view of Eq. 7, the objective function encodes a higher penalty if two connected vertices are mapped to distant locations via \( f(\cdot) \). Consequently, by minimising \( S(T) \), if two nodes are neighbours in the graph (i.e. connected by an edge), then their projections in the new subspace are encouraged to be located in nearby positions. Defining the diagonal matrix \( \mathbf{D} \) such that \( D_{ii} = \sum_{j=1}^{n+1} E_{ij} \) would yield

\[
\mathbf{D} = \begin{pmatrix}
1 & 0 & \ldots & 0 \\
0 & \ddots & \vdots & \vdots \\
\vdots & \vdots & 1 & 0 \\
0 & 0 & \ldots & n
\end{pmatrix}
\]

(8)

Assuming \( y = (f(x_1), \ldots, f(x_{n+1})) \), Eq. 7 can now be written in matrix form as

\[
S(T) = \frac{1}{2} \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} (f(x_i) - f(x_j))^2 E_{ij}
\]

\[
= \sum_{i=1}^{n+1} f(x_i) D_{ii} f(x_i) - \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} f(x_i) E_{ij} f(x_j)
\]

(9)

Defining matrix \( \mathbf{L} \) as \( \mathbf{L} = \mathbf{D} - \mathbf{E} \), Eq. 9 becomes

\[
S(T) = y^\top \mathbf{L} y
\]

(10)

In the graph embedding literature, \( \mathbf{D} \) is called degree matrix, the diagonal elements of which counts the number of times an edge terminates at each vertex while \( \mathbf{L} \) is graph Laplacian [50], [51]. Since our data points are connected to an auxiliary point \( x_{n+1} \) in the star graph representation, minimising the scatter given by Eq. 10 with respect to projections of target observations (i.e. with respect to \( y_i \) for \( i = 1, \ldots, n \)) forces the mapped data to be located in nearby positions to \( f(x_{n+1}) \). As \( f(x_{n+1}) = \mathcal{M} \) is the mean of data in the subspace, by minimising \( S(T) \) all target data are encouraged to be as close as possible to their mean on a line defined by \( f(\cdot) \) in the feature space. The optimum of the objective function \( S(T) \)
would be reached if all target data are exactly mapped onto a single point, i.e. $\mathcal{M}$.

B. Origin as an artificial outlier

The idea of using the origin as an exemplar outlier has been previously used in designing one-class classifiers such as OC-SVM [24] and others [40], [33], [41]. In essence, such a strategy corresponds to the assumption that novel samples lie around the origin while target objects are farther away. In [24], it is shown that using a Gaussian kernel function, the data are always separable from the origin. In this work, a similar assumption is made and target data points are mapped onto locations in a feature subspace such that they are distant from the origin. In order to encourage the mapped data points to lie at locations far from the origin in the subspace, we make use of sum of squared (Euclidean) distances between the projected data points to the projection of the origin. In order to encourage the mapped data points to lie around the origin while target objects are farther away. In [24], it is shown that using a Gaussian kernel function, the data are always separable from the origin. In this work, a similar assumption is made and target data points are mapped onto locations in a feature subspace such that they are distant from the origin. In order to encourage the mapped data points to lie at locations far from the origin in the subspace, we make use of sum of squared (Euclidean) distances between the projected data points to the projection of the origin. In order to encourage the mapped data points to lie around the origin while target objects are farther away. In [24], it is shown that using a Gaussian kernel function, the data are always separable from the origin. In this work, a similar assumption is made and target data points are mapped onto locations in a feature subspace such that they are distant from the origin. In order to encourage the mapped data points to lie at locations far from the origin in the subspace, we make use of sum of squared (Euclidean) distances between the projected data points to the projection of the origin. In order to encourage the mapped data points to lie around the origin while target objects are farther away. In [24], it is shown that using a Gaussian kernel function, the data are always separable from the origin. In this work, a similar assumption is made and target data points are mapped onto locations in a feature subspace such that they are distant from the origin. In order to encourage the mapped data points to lie at locations far from the origin in the subspace, we make use of sum of squared (Euclidean) distances between the projected data points to the projection of the origin.

Thus, the numerator needs to be expressed in $y_\sim$. Regarding

$y^\top Ey$ we have

$$y^\top Ey \equiv (y_1, \ldots, y_{n+1}) \begin{pmatrix} 0 & \ldots & 0 & 1 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \ldots & 0 & 1 \\ 1 & \ldots & 1 & 0 \end{pmatrix} (y_1, \ldots, y_{n+1})^\top$$

$$= (y_1, \ldots, y_{n+1})(y_{n+1}, \ldots, y_1, \sum_{i=1}^{n} y_i)^\top$$

$$= y_{n+1} \sum_{i=1}^{n} y_i + y_{n+1} \left( \sum_{i=1}^{n} y_i \right)^\top$$

$$= \frac{2}{n} \left( \sum_{i=1}^{n} y_i \right) \left( \sum_{i=1}^{n} y_i \right)$$

$$= \frac{2}{n} (y_-^\top 1^{n \times 1}) (1^{1 \times n} y_-)$$

$$= \frac{2}{n} y_-^\top 1^{n \times n} y_-$$

(14)

where $1^{n \times n}$ denotes an $n \times n$ matrix of 1’s.

Due to the special structure of $D$ given in Eq. 8 for $y^\top Dy$, one obtains

$$y^\top Dy = y_-^\top y_- + n(f(x_{n+1}))^2 = y_-^\top y_- + n(\sum_{i=1}^{n} y_i)^2$$

$$= y_-^\top y_- + \frac{1}{n} \left( \sum_{i=1}^{n} y_i \right)^2$$

$$= y_-^\top y_- + \frac{1}{n} (y_-^\top 1^{n \times 1}) (1^{1 \times n} y_-)$$

$$= y_-^\top y_- + \frac{1}{n} y_-^\top 1^{n \times n} y_-$$

(15)

As a result, Eq. 13 can be purely written in terms of $y_\sim$ as

$$y_-^\top y_- + \frac{1}{n} (y_-^\top 1^{n \times n} y_-) - \frac{2}{n} (y_-^\top 1^{n \times n} y_-)$$

$$= \arg \min_{y_-} \frac{y_-^\top y_- + \frac{1}{n} (y_-^\top 1^{n \times n} y_-) - \frac{2}{n} (y_-^\top 1^{n \times n} y_-)}{y_-^\top y_-}$$

$$= \arg \min_{y_-} \frac{y_-^\top 1^{n \times n} y_-}{y_-^\top y_-}$$

(16)

The relation above is known as the Rayleigh quotient. It is well known that the optimum of the Rayleigh quotient is attained at the eigenvector $\nu$ corresponding to the largest eigenvalue of the matrix in the numerator. That is, $y_-^\top y_- = \nu$, where in this case $\nu$ corresponds to the eigenvector corresponding to the largest eigenvalue of $1^{n \times n}$. It can be easily shown that matrix $1^{n \times n}$ has a single eigenvector $\nu$ corresponding to the non-zero eigenvalue of $n$, where $\nu = \left( \frac{1}{\sqrt{n}}, \ldots, \frac{1}{\sqrt{n}} \right)^\top$. Note that the Rayleigh quotient is constant under scaling $y_- \rightarrow cy_-$. In other words, if $y_-^\top y_-$ maximises the objective function in Eq. 16 then any non-zero scalar multiple $cy_-^\top y_-^\top$ also maximises Eq. 16. As a result, one may simply choose $y_-^\top y_-$ as $y_-^\top = (1, \ldots, 1)^\top$ which would lead to $M = 1$.

D. Relation to the Fisher null-space methods

We now establish the relationship of our formulation in Eq. 16 to the null-space Fisher discriminant analysis using...
the origin as an artificial outlier. For this purpose, first, it is shown that the criterion function in Eq. 16 is, in fact, the Fisher ratio and then its relation to the null-space approaches is established.

The Fisher analysis maximises the ratio of between-class scatter $S_w$ to the within-class scatter $S_b$. As the negative class is represented by only a single sample (i.e. the origin), it would have a zero scatter and thus the within-class scatter in this case would be $S_w = S(T)$, and hence

$$S_w = y_\top y_- - \frac{1}{n}(y_\top 1_{n\times n}y_-)$$

(17)

The between-class scatter when the origin is considered as mean of the negative class along the direction specified by $f(.)$ is

$$S_b = (M - 0)\top (M - 0) = \frac{1}{n} \sum_{i=1}^{n} f(x_i))^2$$

$$= \frac{1}{n^2}(y_\top 1_{n\times 1})(1_{1\times n}y_-)$$

$$= \frac{1}{n^2}y_\top 1_{n\times n}y_-$$

(18)

The Fisher analysis maximises the ratio $\frac{S_w}{S_b}$ or equivalently minimises the ratio $\frac{S_b}{S_w}$ and thus

$$y_-^{opt} = \arg\min_{y_-} \frac{S_w}{S_b} = y_- - \frac{1}{n}y_\top 1_{n\times n}y_-$$

$$= \arg\min_{y_-} \frac{y_-y_-}{y_-1_{n\times n}y_-}$$

$$= \arg\max_{y_-} \frac{y_-1_{n\times n}y_-}{y_-y_-}$$

(19)

which shows that when the negative class is represented by the origin, our criterion function in Eq. 16 is in fact the Fisher criterion.

Next, it is shown that the proposed approach is in fact a null-space Fisher analysis. The null projection function 41, 33 is defined as a function leading to zero within-class scatter while providing positive between-class scatter. Thus, one needs to show that $y_-^{opt} = (1, \ldots, 1)\top$ leads to $S_w = 0$ and $S_b > 0$. As all the elements of $y_-^{opt}$ are equal, it is clear that the proposed formulation corresponds to a zero scatter for the target class. The conjecture can be also verified by substituting $y_-^{opt} = (1, \ldots, 1)\top$ in the relation for the within-class scatter as

$$S_w|_{y_-^{opt}=(1,\ldots,1)\top} = y_-y_- - \frac{1}{n}(y_-1_{n\times n}y_-) = 0$$

(20)

Next, as all positive training observations are mapped onto point 1 in the feature subspace while the exemplar outlier is at the origin, the between-class scatter would be 1. This can be confirmed by substituting $y_-^{opt} = (1, \ldots, 1)\top$ in the relation for the between-class scatter as:

$$S_b|_{y_-^{opt}=(1,\ldots,1)\top} = \frac{1}{n^2}y_-1_{n\times n}y_- = 1$$

(21)

As a result, the proposed approach corresponds to a projection function (i.e. $f(.)$) leading to $S_w = 0$ and $S_b = 1$ and hence is a null-space Fisher analysis similar to 41, 33.

E. Extension to the supervised case: the use of counter-examples

Up to this point, it is assumed that the training data solely consists of positive samples. Although in a one-class classification problem, negative samples are not expected to be available abundantly, nevertheless, in case some negative observations exist, they might be used to refine the solution. In this section, the proposed method is extended to benefit from the availability of labelled non-target observations in the training set in a supervised operating mode. In this respect, two transformations shall be applied to the criterion function in Eq. 16 to reflect the existence of negative training samples. Recall that we are minimising the scatter of positive training samples while keeping them far from the centre of the negative class in the feature subspace. As a result, if some negative samples are available, first, the centre of the negative class which was assumed to be the origin, needs to be modified to the mean of the non-target training samples. Next, in the computation of the scatter $S(T)$, as per definition, only positive training observations shall be included. These two modifications to the optimisation problem in Eq. 16 are discussed next.

Without loss of generality, let us assume that the last $n_0$ samples in the training set $\{x_i \in \mathbb{R}^d | i = 1, \ldots, n\}$ correspond to the non-target training observations. The mean of the non-target training samples is

$$\mathcal{O} = \frac{1}{n_0} \sum_{i=n_0+1}^{n} x_i$$

(22)

Next, let us define the $(n - n_0) \times n$ matrix $T$ as a concatenation of an $(n - n_0) \times (n - n_0)$ identity matrix and an $(n - n_0) \times n_0$ zero matrix as

$$T = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & \vdots & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 0 & 1 & \ldots & 0 \end{pmatrix}$$

(23)

Using $\mathcal{O}$ and $T$, the transformed $y_-$, denoted as $y_-^t$, which corresponds to the positive samples of the training set shifted by the mean of the negative training samples can be written as

$$y_-^t = Ty_- - \frac{1}{n_0} \sum_{i=n_0+1}^{n} x_i$$

$$= (T - \frac{1}{n_0} \sum_{i=n_0+1}^{n} x_i) y_-$$

(24)

where $G = T - \frac{1}{n_0} \sum_{i=n_0+1}^{n} x_i$.

Applying the above transformation to the numerator and denominator of Eq. 16 the transformed problem becomes

$$y_-^{opt} = \arg\max_{y_-} \frac{y_-^\top T \sum_{i=n_0+1}^{n} x_i y_-}{y_-^\top G y_-}$$

(25)
If no negative training samples are available, i.e. \( n_0 = 0 \), the solution above would be simplified to the solution of Eq. (16), i.e. \( y_{\alpha}^* = (1, 1, \ldots, 1) \), as it must.

### F. Spectral Regression

Once \( y_{\alpha}^* \) is determined, the relation \( y_{\alpha}^* = K^T \alpha_{\alpha} \) may be used to determine \( \alpha_{\alpha} \). This approach is called spectral regression in [42]. Rewriting Eq. (25) in a general form as

\[
\begin{align*}
\text{min} & \quad y_{\alpha}^* W y_{\alpha} - y_{\alpha}^* Q y_{\alpha}
\end{align*}
\]

the spectral regression involves two steps to solve for \( \alpha \):

1) Solve \( W \nu = \lambda Q \nu \) for \( \nu \);

2) Solve \( K \alpha = \nu \) for \( \alpha \).

The method is dubbed spectral regression as it involves spectral analysis for the problem \( W \nu = \lambda Q \nu \), which is equivalent to a regularised regression problem [42]. However, in our formulation, due to the special structures of \( W \) and \( Q \), the leading eigenvector could be directly found.

Solving \( y_{\alpha}^* = K^T \alpha_{\alpha} \) for \( \alpha_{\alpha} \) can be performed using the Cholesky factorisation and forward-back substitution. In this case, if \( K \) is positive definite, then there exists a unique solution for \( \alpha \). If \( K \) is singular, it is approximated by the positive definite matrix \( K + \delta I \) where \( I \) is the identity matrix and \( \delta > 0 \) is a regularisation parameter. As a widely used kernel function, the radial basis kernel function, i.e. \( K_{ij} = \kappa(x_i, x_j) = e^{-||x_i - x_j||^2/2\sigma^2} \), leads to a positive definite kernel matrix [42], [38] for which \( \delta = 0 \) and the spectral regression finds the exact solution. Considering a Cholesky factorisation of \( K \) as \( K = R^T R \), \( \alpha \) may be found by first solving \( R^T \theta = \nu \) for \( \theta \) and then solving \( R \alpha = \theta \) for \( \alpha \). Since in the proposed approach there is only one eigenvector associated with the equation \( K \alpha = \nu \), only a single vector, i.e. \( \alpha_{\alpha} \), is computed.

### G. Outlier Detection

Once \( \alpha_{\alpha} \) is determined, the projection of a probe \( z \) onto the optimal feature subspace can be obtained as \( f(z) = \sum_{i=1}^{n} c_i \kappa(z, x_i) = k_z^T \alpha_{\alpha} \), where \( k_z \) is a vector collection of the elements \( \kappa(z, x_i) \). The decision rule is now defined as the distance between the mean of projections of positive training observations in the subspace, i.e. \( M \) and \( f(z) \). As \( M = 1 \), the decision rule becomes

\[
\begin{align*}
|k_z^T \alpha_{\alpha} - 1| > \tau \quad & \text{z is an outlier} \\
|k_z^T \alpha_{\alpha} - 1| \leq \tau \quad & \text{z is a target object}
\end{align*}
\]

where \( \tau \) is a threshold for deciding normality. Two observations regarding the decision rule and the decision threshold are in order. First, as the Rayleigh quotient is constant under scaling, the value of \( y_{\alpha}^* \) (and consequently \( M \)) can be chosen arbitrarily as long as all the elements of \( y_{\alpha}^* \) are equal.

This freedom is reflected in the decision rule as choosing a different \( y_{\alpha}^* \) (leading to a different \( M \) other than \( 1 \)) would only introduce a scaling (e.g. \( c \)) due to the relation \( K \alpha_{\alpha}^* = y_{\alpha} \). In this case, the same scaling effect (i.e. \( c \)) would be applied to \( f(z) = k_z^T \alpha_{\alpha} \). As a result, the same decision rule in Eq. (29) would still be valid by using the new threshold \( \tau/c \). In other words, the choice of a particular value for the elements of \( y_{\alpha}^* \) only introduces a scaling effect on the threshold and does not affect the performance as long as numerical errors due to finite precision of computations do not occur. Second, since there is only one single point on the feature subspace corresponding to the projection of positive training samples and another single point corresponding to the projection of negative training instances, a threshold can be set to reject all negative training samples while accepting all positive training observations. However, finding a threshold to reject an arbitrary proportion of training samples when they are all utilised for training is not feasible. Nevertheless, if an arbitrary proportion of the training data shall be rejected, an leave-one-out training scheme on the training set may be followed to produce \( n \) possibily distinct scores for the training samples on which a threshold to reject a desired proportion of the data might be set experimentally.

The pseudo-codes for the training and testing stages of the proposed OC-KSR approach are summarised in the Algorithms 1 and 2.

#### Algorithm 1 Training

1: Set \( n = \# \text{total samples} \) & \( n_0 = \# \text{negative examples} \)
2: Set \( \nu = (1, 1, \ldots, 1, n_0 - n_0, \ldots, n_0 - n_0) \)
3: Calculate \( K \)
4: Form the Cholesky decomposition of \( K \):
   \[
   K = R^T R
   \]
5: Solve \( R^T \theta = \nu \) for \( \theta \)
6: Solve \( R \alpha = \theta \) for \( \alpha \)
7: output \( \alpha \)

#### H. Incremental OC-KSR

In the proposed OC-KSR method, a high computational cost is associated with the Cholesky decomposition of the kernel matrix \( K \), the batch computation of which requires \( O(n^3) \) arithmetic operations. However, as advocated in [52], a Cholesky decomposition may be obtained more efficiently using an incremental approach. In the incremental scheme, the goal is to find the Cholesky decomposition of an \( m \times m \) matrix given the Cholesky decomposition of its \((m - 1) \times (m - 1) \) submatrix. Hence, given the Cholesky decomposition of the kernel matrix \( K^{(m-1) \times (m-1)} \) of \( m - 1 \) samples we want to compute the Cholesky factorisation of the kernel matrix \( K^{m \times m} \) for the augmented training set where a single sample \((x_m) \) is injected into the system. The incremental Cholesky
If in the KPCA approach one uses the eigenvector corresponding to the smallest eigenvalue for projection, a small variance on the projection direction is expected. Note that in KPCA one may obtain at most $n$ ($n$ being the number of training samples) distinct eigenvalues using the kernel matrix. As the smallest eigenvalue of a general kernel matrix need not be zero, the variance along the corresponding eigenvector would not necessarily be zero. As a widely used kernel function, an RBF kernel results in a positive positive-definite kernel matrix which translates into strictly positive eigenvalues. In contrast, in the proposed method, the variance along the projection direction is zero even when using an RBF kernel function.

As discussed previously, the proposed method is similar to the null-space methods for anomaly detection presented in [IV-D] in the sense that all methods employ the Fisher criterion for estimation of a null feature space. However, the proposed approach, as will be discussed in [IV-D] is computationally attractive by virtue of avoiding costly eigen-decompositions. Other work in [40] tries to optimise the ratio between the target scatter and outlier scatter which is different from the Fisher ratio utilised in this work. As illustrated, the proposed approach can be implemented in an incremental fashion which further reduces the computational complexity of the method while allowing for application in streaming data scenarios. Moreover, the proposed OC-KSR method can employ possible labelled negative training observations to refine the decision boundary.

Algorithm 2 Testing probe $z$
1: compute $k_z = \kappa(z_1, z), \ldots, \kappa(z_n, z)^\top$
2: compute $f(z) = k_z \alpha_{opt}$
3: if $|f(z)| \leq \tau$ then
4: $z$ is a target object
5: else
6: $z$ is an outlier
7: end if

Algorithm 3 Incremental Cholesky decomposition
1: Set $R^2 = \sqrt{\kappa(x_1, x_1)}$
2: for $m=2:n$ do
3: $k_{1m} = \kappa(x_1, x_m), \ldots, \kappa(x_{m-1}, x_m)^\top$
4: $k_{1m} = R^{(m-1)\times(m-1)}^\top r_{1m}$
5: $k_{mm} = \kappa(x_m, x_m)$
6: $r_{mm} = \sqrt{k_{mm} - r_{1m}^\top r_{1m}}$
7: $R^{(m-1)\times(m-1)} = \begin{pmatrix} R^{(m-1)\times(m-1)}^\top & 0 \\ 0 & r_{mm} \end{pmatrix}$
8: end for
9: output $R = R_m$

IV. EXPERIMENTAL EVALUATION

In this section, an experimental evaluation of the proposed approach is provided to compare the performance of the OC-KSR method to those of several state-of-the-art approaches in terms of the area under the ROC curve (AUC). Ten different datasets which include relatively low to medium and high dimensional feature set are used for this purpose. A summary of the statistics of the datasets used is provided in Table I. A brief description regarding the datasets used in the experiments is as follows.

- **Arcene**: The task in this dataset is to distinguish cancer versus normal patterns from mass-spectrometric data. The dataset was obtained by merging three mass-spectrometry datasets with continuous input variables to obtain training and test data. The dataset is part of the 2003 NIPS variable selection benchmark. The original features indicate the abundance of proteins in human sera having a given mass value. Based on these features one must separate cancer patients from healthy patients. The dataset is part of the UCI machine learning datasets [53].
- **AD** includes EEG signals from 11 patients with a diagnosis of a probable AD and 11 controls subjects. The task in this dataset is to discriminate between healthy and Alzheimers (AD) patients. AD patients were recruited from the Alzheimers Patients Relatives Association of Valladolid (AFAVA), Spain for whom more than 5 minutes of EEG data were recorded using Oxford Instruments Profile Study Room 2.3.411 (Oxford, UK) [54]. As suggested in [54], in this work the signal associated with the O2 electrode is used.
- **Face** consists of face images of different individuals where the task is to recognise a subject among others.
For each subject, a one-class classifier is built using the data for the same subject while all other subjects are considered as outliers with respect to the built model. The experiment is repeated in turn for all of the subjects in the dataset. The features used for image representation are obtained via the GoogleNet deep CNN \([55]\). We have created this dataset out of the real-access data of the Replay-Mobile dataset \([56]\) and included ten subjects in the experiments.

- **Caltech256** is a challenging set of 256 object categories containing 30607 images in total \([57]\). Each class of images has a minimum of 80 images representing a diverse set of backgrounds, poses, lighting conditions and image sizes. In this experiment, the 'American-flag is considered as the target class and the samples associated with the 'boom-box', 'bulldozer' and 'cannon' classes as outliers. Bag-of-visual-words histograms from densely sampled SIFT features are used to represent images \([1]\).

- **MNIST** is a collection of 28 \(\times\) 28 pixel images of handwritten digits 0-9 \([58]\). Considering digit '1' as the target digit, 220 images are used as target data and 293 images corresponding to other digits are used as negative samples. Raw image intensities are used for the experiments on this dataset.

- **Delft pump** includes 5 vibration measurements taken under different normal and abnormal conditions from a submersible pump. The 5 measurements are combined into one object, giving a 160-dimensional feature space. The dataset is obtained from the one-class dataset archive of Delft university \([59]\).

- **Sonar** is composed of 208 instances of 60 attributes representing the energy within a particular frequency band, integrated over a certain period of time. There are two classes: an object is a rock or a mine. The task is to discriminate between sonar signals bounced off a metal cylinder and those bounced off a roughly cylindrical rock. The Sonar dataset is from the undocument databases from UCI.

- **Vehicle** dataset is from Statlog, where the class van is used as a target class. The task is to recognise a vehicle from its silhouette. The dataset is obtained from the one-class dataset archive of Delft university \([59]\).

- **Vowel** is an undocumented dataset from UCI. The purpose is speaker independent recognition of the eleven steady state vowels of British English using a specified training set of lpc derived log area ratios. Vowel 0 is used as the target class in this work.

- **Balance-scale** was generated to model psychological experimental results. Each example is classified as having the balance scale tip to the right, tip to the left, or be balanced. The attributes are the left weight, the left distance, the right weight, and the right distance. The dataset is part of the UCI machine learning repository \([53]\).

The methods included in the comparison are as follows.

- **OC-KSR** is the proposed one-class spectral regression when negative training samples are not present in the training set.

- **SVDD** is the Support Vector Data Description approach to solve the one class classification problem \([22]\). As a widely used method, it provides a baseline for comparison.

- **OC-KNFST** The one-class kernel null Foley-Sammon transform presented in \([33]\) which operates on the Fisher criterion. This method is chosen due to its similarity to the proposed approach.

- **KPCA** is based on the kernel PCA method where the reconstruction residual of a sample in the feature space is used as the novelty measure \([19]\).

- **GP** is derived based on the Gaussian process regression and approximate Gaussian process classification \([60]\) where in this work the predictive mean is used as one class score.

- **LOF** Local outlier factor (LOF) \([61]\) is a local measure indicating the degree of novelty for each object of the dataset. The LOF of an object is based on a single parameter k, which is the number of nearest neighbours used in defining the local neighbourhood of the object.

- **K-means** is the k-means clustering based approach where k centres are assumed for the target observation. The novelty score of a sample is defined as the minimum distance of a query to data centres.

- **KNDD** The k-nearest neighbours data description method (KNDD) is proposed in terms of the one class classification framework \([13]\). The principle of KNDD is to associate to each data a distance measure relative to its neighbourhood (k-neighbours).

In all the experiments that follow, the positive samples of each dataset are divided into training and test sets of equal sizes randomly. Each experiment is repeated 100 times and the average area under the ROC curve (AUC) and the standard deviation of the AUC’s are reported. No pre-processing of features is performed other than normalising all features to have a unit L2-norm. For the methods requiring a neighbourhood parameter (i.e. LOF, K-means and KNDD), the neighbourhood parameter is set in the range \([3, \ldots, 10]\) to obtain the best performance. Regarding the methods operating in the RKHS space (i.e. SVDD, OC-KNFST, GP, KPCA and OC-KSR), a common Gaussian kernel is computed and shared among all methods.

### A. Comparison to other methods

A comparison of the proposed OC-KSR approach to other methods is provided in Tables \([III]\) and \([IV]\) for the datasets with medium to high dimensional features and datasets with relatively lower dimensional features, respectively. From Tables \([III]\) and \([IV]\) one may observe that in 4 out of 10 datasets, the proposed OC-KSR method achieves leading performance and on 3 others is placed second in terms of average AUC. The results over different datasets are summarised in Tables \([V]\ \[VI]\ and \[VII]\ in terms of average AUC over medium to high dimension, relatively lower dimension and all datasets, respectively. As can observed from Table \([V]\) the best performing methods on
the medium to high dimensional datasets in terms of average AUC are the proposed OC-KSR and the OC-KNFST method with an average AUC of 89.54%, closely followed by KPCA and K-means with average AUC’s of 89.38% and 88.84%, respectively. It is worth noting that the performances of both OC-KSR and the OC-KNFST methods do exactly match. As previously discussed, this is expected since both approaches are equivalent theoretically, optimising the Fisher criterion for classification.

Regarding the lower dimensional datasets, the best-performing methods in terms of average AUC are the proposed OC-KSR approach and the OC-KNFST method with an average of 92.64% AUC, Table VII. The second best performing method, in this case, is GP with an average AUC of 90.66% followed by KPCA with an average AUC of 90.24%.

Table VII reports the average AUC’s for all the evaluated methods over all datasets regardless of the dimensionality of feature vectors. The best performing methods of OC-KSR and OC-KSR achieve an average AUC of 91.09% while the next best performing methods are KPCA and GP with average AUC’s of 89.81% and 89.75%, respectively.

| Dataset          | # Positive Instances | # Negative Instances | d   |
|------------------|----------------------|----------------------|-----|
| Arcene           | 88                   | 112                  | 10000 |
| AD               | 263                  | 400                  | 1280 |
| Face             | 10×290               | 10×290               | 1024 |
| Caltech256       | 97                   | 304                  | 1000 |
| MNIST            | 220                  | 293                  | 784  |
| Pump             | 189                  | 531                  | 160  |
| Sonar            | 111                  | 97                   | 60   |
| Vehicle          | 199                  | 647                  | 18   |
| Vowel            | 48                   | 480                  | 10   |
| Balance-scale    | 49                   | 576                  | 4    |

B. Training sample size

In this experiment, the effect of training sample size on the performance of the proposed approach is compared to other methods. For this purpose, the training sample size is gradually decreased from 100% of total training observations to 50% in decrements of 2%. As the LOF method is found to perform much worse compared to others, it is excluded from this experiment. The results are presented in Fig. 5 and Fig. 6 for the medium to high and relatively lower dimensional datasets, respectively. As expected, for all the datasets, with the exception of the AD and MNIST, a reduction in training sample size deteriorates the performance of all systems. Regarding the AD dataset, an oscillatory behaviour is observed whereas for the MNIST dataset the performance of some methods (including the proposed OC-KSR approach) even slightly improves as the training set size decreases. This spurious behaviour will be the subject of future research.

Most importantly, the ranking of the proposed OC-KSR method in terms of average AUC as a function of training sample size is typically preserved. In particular, the proposed method achieved leading performance on 4 out the 10 datasets examined when using 100% of the training data and continues to do so even when the training set is shrunk by up to \( \approx 50\% \). A similar observation can be made regarding the datasets on which the proposed OC-KSR method ranked second, except for the AD dataset where an oscillation in performance is observed for the majority of the methods. It can be concluded that, although a reduction in the training sample size may degrade the performance of the proposed approach, it maintains its relative ranking position on the majority of the datasets.

C. Using negative examples

In this experiment, the effectiveness of the proposed approach in making use of counter-examples in the training set is examined. For this purpose, labelled negative samples are gradually included in the training set and the performances on different datasets are examined. On each dataset, the negative training examples are obtained from the negative samples of the corresponding dataset, the proportion of which relative to the initial positive sample set is increased from 0% to 50% in increments of 2%. Each experiment is repeated 100 times and the average AUC’s are plotted. As among other methods only SVDD provides an explicit built-in mechanism for using negative examples in the training set, the methods included in this experiment are SVDD, the OC-KSR method without using negative examples (denoted as OC-KSR) and the OC-KSR method using counter-examples (denoted as OC-KSR\(^+\)). The results of this evaluation are depicted in Fig. 5 and Fig. 6 for the medium to high and relatively lower dimensional datasets, respectively. From the figures, the following observations can be made. Initially when negative examples are relatively much fewer than the positive samples, the OC-KSR\(^+\) method does not seem to provide an advantage over OC-KSR. In fact, it may even deteriorate the performance. As more negative examples become available, the performance of the OC-KSR\(^+\) method tends to improve. This is expected since when very few numbers of counter-examples are available (less than 10% of the initial positive training set), their mean is not a good representative of the negative class. Increasing the number of negative examples, they may better represent the non-target class and hence the OC-KSR\(^+\) method outperforms OC-KSR in the majority of the datasets. Moreover, typically when more negative examples are available the proposed OC-KSR\(^+\) method also outperforms SVDD. The merits of the proposed OC-KSR\(^+\) method over SVDD become more prominent as more and more negative examples are included in the training set.

D. Computational complexity

In this section, the computational complexity of the proposed OC-KSR method in the training and test phases is discussed.

1) Computational complexity in the training stage: An analysis regarding the computational complexity of the proposed method in the training stage is as follows. As with all the kernel methods, the computation of the kernel matrix has a time complexity of \( O(n^2d) \). Computing the additional
TABLE III
Mean AUCs (+- std) (%) over 100 repetitions for datasets with medium to high dimensional feature vectors

| Method   | Arcene  | AD       | Face     | Caltech256 | MNIST   |
|----------|---------|----------|----------|------------|---------|
| OC-KSR   | 82.44+2.68 | 69.49+1.72 | 99.13+2.66 | 97.90+0.95 | 98.75+0.27 |
| SVDD     | 75.09+2.35 | 69.86+1.95 | 99.33+3.07 | 97.90+0.94 | 98.32+0.27 |
| OC-KNFSF | 82.44+2.68 | 69.49+1.72 | 99.13+2.66 | 97.90+0.95 | 98.75+0.27 |
| KPCA     | 82.44+2.68 | 70.53+1.50 | 97.08+3.45 | 97.33+1.07 | 99.56+0.24 |
| GP       | 81.39+2.69 | 69.09+1.49 | 98.70+2.86 | 97.61+1.13 | 97.44+0.42 |
| LOF      | 55.11+2.88 | 30.12+1.52 | 54.25+6.61 | 57.80+3.39 | 52.64+2.13 |
| KMEANS   | 79.94+2.81 | 67.85+1.33 | 98.81+2.83 | 97.42+1.07 | 99.53+0.20 |
| KNNDD    | 77.20+2.96 | 67.57+1.25 | 99.04+4.66 | 97.00+1.09 | 99.57+0.19 |

TABLE IV
Mean AUCs (+- std) (%) over 100 repetitions for datasets with relatively lower dimensional feature vectors

| Method   | Delft pump | Sonar mines | Vehicle van | Vowel 0 | Balance-scan |
|----------|------------|-------------|-------------|---------|--------------|
| OC-KSR   | 99.32+0.24 | 82.79+3.55 | 92.38+1.61 | 99.47+1.38 | 89.24+3.54  |
| SVDD     | 99.49+0.61 | 77.38+3.29 | 93.43+1.46 | 67.57+4.22 | 73.19+5.45  |
| OC-KNFSF | 99.32+0.24 | 82.79+3.55 | 92.38+1.60 | 99.47+1.38 | 89.24+3.94  |
| KPCA     | 99.32+0.24 | 81.81+3.59 | 81.24+2.01 | 99.44+1.41 | 89.43+3.95  |
| GP       | 99.34+0.26 | 81.35+3.56 | 84.47+1.28 | 99.47+1.38 | 88.67+4.22  |
| LOF      | 53.02+1.68 | 51.78+2.61 | 55.44+1.38 | 73.03+2.76 | 69.31+3.50  |
| KMEANS   | 98.93+0.32 | 73.56+4.73 | 85.76+1.77 | 97.44+2.17 | 77.12+5.25  |
| KNNDD    | 98.59+0.35 | 66.57+3.51 | 88.53+1.67 | 90.18+6.42 | 66.27+5.44  |

TABLE V
Summary of performances on datasets with medium to high dimensional feature vectors

| Method       | Mean AUC(%) |
|--------------|-------------|
| OC-KSR (this work) | 89.54       |
| SVDD         | 88.10       |
| OC-KNFSF     | 89.54       |
| KPCA         | 89.38       |
| GP           | 88.84       |
| LOF          | 49.98       |
| KMEANS       | 88.71       |
| KNNDD        | 87.07       |

TABLE VI
Summary of performances on datasets with relatively lower dimensional feature vectors

| Method       | Mean AUC(%) |
|--------------|-------------|
| OC-KSR (this work) | 92.64       |
| SVDD         | 81.85       |
| OC-KNFSF     | 92.64       |
| KPCA         | 90.24       |
| GP           | 90.66       |
| LOF          | 60.51       |
| KMEANS       | 86.56       |
| KNNDD        | 82.02       |

part of the kernel matrix in the incremental scheme requires $O(dn\Delta n + d\Delta n^2)$ compound arithmetic operations each consisting of one addition and one multiplication (flam \[52\]), where $\Delta n$ is the number of additional training samples. The incremental Cholesky decomposition requires $1/6(n+\Delta n)^3 - 1/6n^3$. Given the Cholesky decomposition of $K$, the linear equations $K\alpha^opt = y^opt$ can be solved within $(n + \Delta n)^2$ flamns. As a result, the computational cost of training the incremental OC-KSR approach in the updating phase is

$$O(dn\Delta n + d\Delta n^2) + \frac{1}{6}(n+\Delta n)^3 - \frac{1}{6}n^3 + (n + \Delta n)^2$$

$$= O(dn\Delta n + d\Delta n^2) + \frac{1}{2}n^2\Delta n + \frac{1}{2}n\Delta n^2 + \frac{1}{6}\Delta n^3$$

assuming $\Delta n \ll n$, the cost can be approximated as

$$\left(\frac{\Delta n}{2} + 1\right)n^2$$ (32)

In the initial training stage, the computation of the kernel matrix, the Cholesky decomposition of the kernel matrix and solving $n$ linear equations are required. Noting that even in the initial stage the Cholesky decomposition can be performed in an incremental fashion (we assume $\Delta n = 1$ during the initial training phase), the total cost in the initialisation stage can be approximated as

$$O(n^2d) + \frac{3}{2}n^2$$ (33)
Fig. 3. The effect of training sample size on performance on datasets with medium to high dimensional feature vectors. (from top to bottom: Arcene, AD, Face, Caltech256 and MNIST)

Fig. 4. The effect of training sample size on performance on datasets with relatively lower dimensional feature vectors. (from top to bottom: Pump, Sonar mines, Vehicle van, Vowel-0, Balance-scale)
As a result, if \( d \gg 3 \) (which is often the case), the proposed algorithm would have a time complexity of \( O(n^2d) \) in the training stage. That is, the computation of the kernel matrix has the dominant complexity in the training phase of the proposed approach.

2) Computational complexity in the Test stage: In the test phase, the OC-KSR method requires computation of \( k_z \), which has a time complexity of \( O(nd) \) followed by the computation of \( f(z) \) requiring \( n \) flms. Hence the dominant computational complexity in the test phase is \( O(nd) \). As the classification performance of the proposed approach is provably identical with the OC-KNFST method of [33], in the test phase the two methods are comparable.

Recently, an incremental variant of the OC-KNFST approach was proposed in [41] which reduces the computational complexity of the original KNFST algorithm in the training stage. Specifically, the incremental OC-KNFST algorithm requires \( O(n^2d) + O(n^3) \) for the computation of the kernel matrix, its eigen-decomposition and matrix multiplications. As the computation of the kernel matrix is common for both the OC-KSR and the incremental OC-KNFST, the relative computational advantage of the OC-KSR over the incremental OC-KNFST in the training stage is \( \approx \frac{2}{3} O(n^3) \). In other words, the computational superiority of the OC-KSR approach with respect to the incremental OC-KNFST increases almost linearly with the number of training samples, \( n \). This is due to the fact that the method in [41] uses eigen-decomposition, whereas OC-KSR solves the optimisation problem by regression.

The computational complexity of the method in [41] in the updating phase of the training stage is \( O(\Delta n^3 + an\Delta n) \approx O(an\Delta n) \) where \( a \) is the number of eigen-bases, upper bounded by \( n \). As a result, in common scenarios where e.g. \( \Delta n > 10 \), if the number of eigen-bases \( a \) for the incremental OC-KNFST method exceeds 60% of \( n \), the proposed OC-KSR method would be more efficient. In summary, in the initial training phase, the proposed OC-KSR approach is computationally more efficient than the incremental OC-KNFST method of [41]. In the updating phase, under mild conditions, it would be more efficient too.

V. Conclusion

A new nonlinear one-class classifier built upon the Fisher criterion was presented while providing a graph embedding view of the problem. The proposed OC-KSR approach operated by mapping the data onto a one-dimensional feature subspace where the scatter of training data is minimised while keeping positive samples far from the centre of the negative class. It was shown that positive and negative training observations were projected onto two distinct points in a feature subspace the locations of which could be determined up to a multiplicative constant. The proposed method, unlike previous similar approaches, casts the problem under consideration into a regression framework optimising the criterion function via the efficient spectral regression method thus avoiding costly eigen-decomposition computations. It was illustrated that the dominant complexity of the proposed method in the training phase is the complexity of computing the kernel.
matrix. The proposed OC-KSR approach offers a number of appealing characteristics such as the ability to be trained in an incremental fashion and the operability in an unsupervised mode. Moreover, it was shown that in the presence of non-target training observations, such samples can be directly used to further refine the decision boundary for classification in a supervised mode. Extensive experiments conducted on several datasets with varied dimensions of features verified the merits of the proposed approach in comparison with some other alternatives.

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