Generalized Reference Kernel for One-class Classification

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Abstract—In this paper, we formulate a new generalized reference kernel hoping to improve the original base kernel using a set of reference vectors. Depending on the selected reference vectors, our formulation shows similarities to approximate kernels, random mappings, and Non-linear Projection Trick. Focusing on small-scale one-class classification, our analysis and experimental results show that the new formulation provides approaches to regularize, adjust the rank, and incorporate additional information into the kernel itself, leading to improved one-class classification accuracy.

Index Terms—One-class classification, kernel methods, Support Vector Data Description, One-class Support Vector Machine

I. INTRODUCTION

One-class classification aims at building a model for a class by using data from this target class only. During inference, the model may also see outliers not belonging to the target class and it should be able to recognize that they do not fit to the model. This kind of methods are suitable for anomaly detection, where only samples of the normal situation are available, while any kind of anomaly should be detected [1].

Traditional well-known one-class classification techniques include One-class Support Vector Machine (OC-SVM) [2] and Support Vector Data Description (SVDD) [3], which are commonly applied as non-linear models exploiting the kernel trick. Various extensions of both methods have been proposed (e.g., [4]–[6]), and recently also deep neural network-based variants have been proposed [7]–[9]. Some recent works have shown that also the traditional methods used on top of deep features may be useful. In [10], both SVDD and OC-SVM were used to improve the classification accuracy of very small classes on top of deep classification. In [11], OC-SVM applied on top of features obtained via self-supervised representation learning was shown to yield better results than end-to-end trained deep learning approaches.

In this work, we focus on small-scale one-class classification tasks that do not provide enough training data for deep models. Thus, we focus on traditional one-classification methods and specifically on the kernel used with the methods. Previous works have attempted to improve the kernels for one-class classification by applying multikernel approaches that combine multiple kernels [12], [13] or have applied approximate features to allow distributed implementation [14]. We take a different approach and formulate a new generalized reference kernel hoping to improve the original base kernel using a set of reference vectors. Depending on the selected reference vectors, our formulation shows similarities to approximate kernels, random mappings, and Non-linear Projection Trick (NPT). It also reveals ways to regularize, adjust the rank, and incorporate additional information into the kernel itself.

The rest of the paper is organized as follows: Section II first briefly introduces the one-class classification methods, SVDD and OC-SVM, used in the experiments and then reviews works on kernel-based methods, in particular different approximate kernel methods, random features, and NPT, which all have similarities to our proposed kernel formulation. Section III introduces the proposed generalized reference mapping and kernel formulations. Section IV provides our experimental results and Section V concludes the paper.

II. RELATED WORK

A. One-class Classification

In this paper, we focus a one-class classification scenario with a training set \( X = [x_1, \ldots, x_n] \in \mathbb{R}^{D \times N} \) and a test set \( \hat{X} = [\hat{x}_1, \ldots, \hat{x}_N] \in \mathbb{R}^{D \times N} \), where \( D \) is the data dimension and \( N, \hat{N} \) are the number of training and testing data samples. All the samples in the training set belong to same class of interest or a target class, and the goal is to use this data to build a model that can predict whether an unseen test sample belongs to the target class or is an outlier.

SVDD [3] aims at enclosing the training data inside a minimum hypersphere by minimizing the following objective function:

\[
\min_{R, \mathbf{c}} F(R, \mathbf{c}) = R^2 + C \sum_{i=1}^{N} \xi_i \\
\text{s.t. } ||x_i - \mathbf{c}||_2^2 \leq R^2 + \xi_i, \\
\xi_i \geq 0, \quad \forall i \in \{1, \ldots, N\},
\]

where \( R \) is the radius of the hypersphere and \( \mathbf{c} \in \mathbb{R}^D \) is the center of the hypersphere. The hyperparameter \( C > 0 \) and the slack variables, \( \xi_i \), are used for controlling the trade-off between the volume of the hypersphere and the amount of target.
samples allowed outside the hypersphere. The Lagrangian dual of (1) (for derivation, see [3]) can be given as

\[
\max L = \sum_{i=1}^{N} \alpha_i x_i^T x_i - \sum_{i}^{N} \sum_{j}^{N} \alpha_i \alpha_j x_i^T x_j,
\]

s.t. \( 0 \leq \alpha_i \leq C. \) \( \quad \) (2)

Solving (2) gives a value \( \alpha_i \) for each training sample \( x_i \). These values define which values are inside the hypersphere (\( \alpha_i = 0 \)), support vectors on the boundary (\( 0 < \alpha_i < C \)), and outliers (\( \alpha_i = C \)). This, in turn, allows to solve \( R \) and \( c \) and use these to classify unseen samples.

OC-SVM [2] aims at separating all the training data from the origin and maximizes the distance \( \rho \) from the hyperplane to the origin:

\[
\begin{align*}
\min & \frac{1}{2} \|w\|^2 + \frac{1}{\nu N} \sum_{i=1}^{N} \xi_i - \rho \\
\text{s.t.} & \quad w^T x_i \geq \xi_i - \rho, \\
& \quad \xi_i \geq 0, \quad \forall i \in \{1, \ldots, N\},
\end{align*}
\]

where \( w \) is a weight vector, slack variables \( \xi_i \) allow some data points to lie within the margin, and hyper-parameter \( \nu \) sets an upper bound on the fraction of training samples allowed within the margin. The dual of (3) can be given as:

\[
\begin{align*}
\min L &= \frac{1}{2} \sum_{i=1}^{N} \alpha_i \alpha_j x_i^T x_j, \quad \text{s.t.} \quad 0 \leq \alpha_i \leq \frac{1}{\nu N}, \sum_{i=1}^{N} \alpha_i = 1.
\end{align*}
\]

Now samples on the hyperplane have \( 0 < \alpha_i < \frac{1}{\nu N} \) and they can be used to solve \( \rho \).

B. Kernel-based Methods

Non-linear versions of various pattern recognition techniques can be obtained by using the kernel trick. The kernel trick was introduced already in 1960s for kernel perceptrons [15] and became popular in 1990s along with Support Vector Machines (SVMs) [16], and has been combined also with state-of-the-art convolutional neural networks (CNNs) [17], [18] with promising results.

The main idea of kernel methods is to non-linearly map the input data to a feature space employing a mapping function \( \phi(\cdot) : x_i \in \mathbb{R}^D \rightarrow \phi(x_i) \in \mathcal{F} \) and then apply the original linear method in that space. The feature space \( \mathcal{F} \) usually has the properties of Hilbert spaces [19], [20] and it is often selected to be higher or even infinite-dimensional space leading to the classes to be more likely linearly separable. While this makes it infeasible to operate directly on the mapped samples, many pattern recognition techniques use only inner products of the input samples, not the samples by themselves (as examples, see SVDD (2) and OC-SVM (4)). Thus, if the inner products are known, the mapped samples \( \phi(x_i) \) and even the function \( \phi(\cdot) \) are not needed. This is the basis of the kernel trick: the inner products of the mapped samples are obtained using a kernel function:

\[
\kappa(x_i, x_j) \triangleq \phi(x_i)^T \phi(x_j)
\]

without explicitly using the function \( \phi(\cdot) \). An example of the kernel function is the widely used Radial Basis Function (RBF):

\[
\kappa(x_i, x_j) = \exp \left( -\frac{\|x_i - x_j\|^2}{2\sigma^2} \right),
\]

where \( \sigma \) is a hyperparameter. The kernel trick has been used to create many widely-used non-linear variants of originally linear pattern recognition techniques, such as Kernel Principal Component Analysis (KPCA) [21] from Principal Component Analysis (PCA), Kernel Discriminant Analysis (KDA) [22], [23] from Linear Discriminant Analysis (LDA), and non-linear SVDD [3].

An inherit drawback of kernel methods for large datasets is the fact that they require the calculation of the so-called kernel matrix \( K_{XX} \in \mathbb{R}^{N \times N} \), having elements \( K_{XX}(i,j) = \kappa(x_i, x_j) \), and the exploitation of \( K_{XX} \) in order to learn the model parameters. For example, KPCA and KDA solve a (generalized) eigendecomposition problem defined on \( K_{XX} \) and, thus, their time complexity is a function of \( N^3 \). For large scale problems, such a time complexity is prohibitive and, thus, approximate kernel approaches have been proposed to overcome this issue [24]–[26]. They aim at constructing a low-rank approximation of the kernel matrix \( K_{XX} \) to reduce the computational complexity of applying the main algorithm.

Some of well-known techniques to generate approximate kernels include random sampling methods (e.g., [26]–[29]), random projection methods (e.g., [30]), and random Fourier features (e.g., [31]–[33]). Random sampling or Nyström methods sample a subset of the columns of \( K_{XX} \) to construct the approximate matrix. An important aspect in this process is the distribution used to sample the columns. While it would be possible to simply use a uniform distribution (vanilla Nyström), other distributions have been shown to be more efficient [27]. Random projection methods multiply the original kernel matrix with a random data-independent projection matrix, thus selecting linear combinations of the columns of \( K_{XX} \). Random Fourier features take a different approach. Unlike random sampling and random projection methods that try to approximate the kernel matrix \( K_{XX} \), they try to approximate the kernel function \( \kappa(x_i, x_j) \) using a data-independent approach. It was demonstrated in [26], [34] that the data-dependent Nyström methods can lead to better kernel approximations than data-independent random projection methods or random Fourier features.

To give a more mathematical explanation, random sampling methods approximate the full kernel matrix \( K_{XX} \) by randomly selecting a subset of \( n \) samples, \( \mathbf{X} = [\hat{x}_1, \ldots, \hat{x}_n] \in \mathbb{R}^{D \times n} \), among the original \( N \) samples and then constructing the low-rank matrix as

\[
\hat{K}_{XX} = K_{XX} \hat{K}_{xx}^+ K_{xx}^T K_{XX},
\]

where \( K_{XX} = [\kappa(x_i, x_j)]_{ij} \in \mathbb{R}^{N \times N} \), \( K_{xx} = [\kappa(\hat{x}_i, \hat{x}_j)]_{ij} \in \mathbb{R}^{n \times n} \), and \( (\cdot)^+ \) denotes a pseudo inverse. Besides random sampling, the vector in \( \mathbf{X} \) can
be selected, e.g., via clustering the input vectors and using the cluster centroids [35].

As derived in [31], [32], random Fourier features are based on the knowledge that for shift invariant kernel functions, i.e., kernel functions of form $\kappa(x_i, x_j) = \kappa(x_i - x_j)$ having $\kappa(0) = 1$, there is a probability distribution $p_\kappa(\cdot)$ such that

$$\kappa(x_i, x_j) = \int_{\mathbb{R}^d} e^{-2\pi i \eta^T (x_i - x_j)} p_\kappa(\eta) d\eta, \quad (8)$$

i.e., the inverse Fourier transform of a kernel function $\kappa(\cdot, \cdot)$ is a probability distribution $p_\kappa(\cdot)$. Drawing $\eta_1, \ldots, \eta_M$ from $p_\kappa(\cdot)$ and defining

$$\phi_\eta(x_i) = \frac{1}{\sqrt{M}} [e^{-2\pi i \eta_1^T x_i}, \ldots, e^{-2\pi i \eta_M^T x_i}]^T, \quad (9)$$

leads to

$$\kappa(x_i, x_j) = \mathbb{E}_{\eta} [\phi_\eta(x_i)^T \phi_\eta(x_j)]. \quad (10)$$

For the RBF kernel in (6), the corresponding probability distribution $p_{\kappa}(\cdot)$ is $\mathcal{N}(0, \sigma^2 I)$ [34] and, thus, random Fourier features can be generated by sampling vectors $\eta_1, \ldots, \eta_M$ from this distribution and computing $\phi_\eta(x_i)$ according to (9). The mapped representations $\phi_\eta(x_i)$ can be then used as new features for $x_i$, which can be used with the original linear methods, or they can be used to construct a low-rank approximation (assuming $M < N$), of the kernel matrix as $K_{xx} = [\phi_\eta(x_1)^T, \ldots, \phi_\eta(x_N)^T]_{ij}$.

The optimal low-rank approximations in terms spectral or Frobenius norms can be obtained using eigenvalue decomposition [36], but it has prohibitive cubic complexity. Furthermore, it is not clear what is the best way to measure the optimality of the transformation. Therefore, most of the research on approximate kernels focuses on the following aspects: 1) How to evaluate the optimality of the approximation? [26], [33], [34], [37]. 2) How to construct more efficiently more optimal approximations? [36], [38], [39]. Some works focus on analyzing the performance of the approximate kernels in a specific application [29], [40], and some works study the rank of the low-rank approximations [40], [41]. Interestingly, all this research assumes that the original kernel is optimal or contains all the relevant information that can be extracted. However, this assumption has not been justified.

While the kernel trick can be used in numerous applications, there are also methods that cannot be presented in terms of inner products only (e.g., Ellipsoidal Support Vector Data Description (ESVDD)). In such cases, the mapping function $\phi(\cdot)$ would be directly needed to first map the input vectors to the feature space and then apply the method directly on these new features. However, for many kernel functions the corresponding feature space can be infinite dimensional and/or the mapping function can be unknown. The problem can be approached by mapping the inputs $x_i$ to their pre-images $\hat{x}_i$ [42], [43], which satisfy $\hat{x}_i^T \phi_j(\cdot) = \kappa(x_i, x_j)$. Random Fourier features (9) can be directly used as pre-images as $\hat{x}_i = \phi(x_i)$. When the computational complexity of obtaining the pre-images is not a concern, NPT [44] provides an alternative solution, while its approximate version can be used for large-scale problems [45].

NPT maps the data to the effective subspace $\mathcal{P}$ of the feature space $\mathcal{F}$ by as follows: First, the original kernel matrix $K_{xx} \in \mathbb{R}^{N \times N}$ is computed and centered (see Appendix (A.4)). Then, the eigendecomposition of the centered kernel matrix $K$ is computed as

$$K_{xx} = U \Sigma U^{-1} = U \Lambda U^T = U \Lambda_r U_r^T, \quad (11)$$

where $U$ contains as its columns the eigenvectors, $\Lambda$ is a diagonal matrix with the eigenvalues on its diagonal, the second equality follows from the symmetry, and in the last step only the non-zero eigenvalues and the corresponding eigenvalues are kept, i.e., $U_r \in \mathbb{R}^{N \times r}$ and $\Lambda_r \in \mathbb{R}^{r \times r}$, where $r$ is the rank of $K_{xx}$. Finally, the matrix containing the pre-images, $\Phi = [\phi_1, \ldots, \phi_N] \in \mathbb{R}^{r \times N}$, is computed as

$$\Phi = \Lambda_r^\frac{1}{2} U_r^T. \quad (12)$$

In the test phase, the pre-image or a test vector $\hat{x}_j$ is computed as follows: First the kernel vector $k_{xx_j} = [\kappa(x_i, x_j)]_{i \in N}$ is computed and centered (see Appendix (A.5)). Finally, the pre-image of the test vector is computed as

$$\hat{\phi}_j = \Lambda_r^{-\frac{1}{2}} U_r^T k_{xx_j}, \quad (13)$$

where $k_{xx_j}$ is the centered kernel vector. As computing the pre-images via NPT requires the eigendecomposition of $K_{xx}$, it suffers from the inherent problem of standard kernel methods related to their computational cost. Therefore, it is most suitable for smaller problem that cannot be solved using the kernel trick. An approximate version of NPT [45] uses a Nyström approximation of the full kernel matrix, making the computational cost of the eigendecomposition of the kernel matrix lower. Since both NPT and its approximate version are based on the kernel matrix, they still rely on a similar assumption of the original kernel matrix being the optimal solution.

III. GENERALIZED REFERENCE MAPPING AND KERNEL

As discussed above, a lot of research from different perspectives has been done to construct better kernel approximations in large-scale problems. While it is known that approximate methods can lead to implicit regularization of the methods for noisy data [46], most of the above discussed research shares the same underlying assumption that the original kernel function or kernel matrix is optimal and worth approximating as closely as possible. While some studies focus on kernel function selection [47]–[49], and hyperkernels or multikernels have been proposed to combine different kernel functions to create better kernels [13], [48], the optimality of the kernel functions has received surprisingly little attention in general. In this paper, we take a different approach from the works discussed in Section II-B and, instead of attempting to approximate the original kernel, we formulate a new kernel definition using a set of selected reference vectors. We focus on small-scale one-class classification problems, where the
computational complexity is not a concern but rather the lack of training samples. We hope to use our new kernel as an implicit data augmentation for such problems.

In our kernel definition, we use the following notations: We consider a training set \( X = \{x_1, \ldots, x_n\} \in \mathbb{R}^{D \times N} \) and a test set \( \tilde{X} = \{\tilde{x}_1, \ldots, \tilde{x}_N\} \in \mathbb{R}^{D \times N} \). As we focus on one-class classification, the training set is assumed to contain samples from a single class only. Both training and test sets are assumed standardized using the training set mean and standard deviation. Furthermore, our kernel uses a set of reference vectors \( R = \{r_1, \ldots, r_M\} \in \mathbb{R}^{D \times M} \), where \( M \) can be less, equal, or greater than \( N \). We will later return the selection of \( M \) and the reference vectors.

Our kernel definition is built on an original kernel to which we refer to as the base kernel. We use a tilde to denote all the related terms (kernel matrix \( \tilde{K} \), kernel vector \( \tilde{k} \), and kernel function \( \tilde{\kappa} \)), whereas the terms referring to proposed reference kernel do not have tildes. Furthermore, we use subscripts with kernel matrices and vectors to denote the data over which they have been computed as follows:

\[
K_{XX} = [\kappa(x_i, x_j)]_{ij} \in \mathbb{R}^{N \times N},
\]

where \( x_i \in X \) and \( \tilde{x}_j \in \tilde{X} \), and

\[
k_{XX} = [\kappa(x_i, \tilde{x}_j)]_{ij} \in \mathbb{R}^{N \times 1},
\]

where \( x_i \in X \).

To formulate a new kernel using a base kernel function \( \kappa(\cdot, \cdot) \) and a set of reference vectors \( R \), we first compute the reference base kernel matrix \( \tilde{K}_{RR} \) and center it (see Appendix (A.4)). Then, we calculate the eigendecomposition of the centered base kernel matrix as \( \tilde{K}_{RR} \):

\[
\tilde{K}_{RR} = U \Lambda U^{-1} = U \Lambda U^T = U_r \Lambda_r U_r^T,
\]

where \( U \) contains its columns the eigenvectors and \( \Lambda \) is a diagonal matrix with the eigenvalues on its diagonal. We keep only the \( r \) non-zero eigenvalues \( \lambda_r \) and the corresponding eigenvectors \( u_r \), where \( r \) is the rank of \( \tilde{K}_{RR} \).

We now define our generalized reference mapping function \( \phi(\cdot) \):

\[
[\phi(x_i)]_t = \frac{1}{\lambda_t} \int u_{tm} \tilde{k}(x_i, r_m) = \frac{1}{\lambda_t} u_{tm}^T \tilde{\Phi} \tilde{r}_{X},
\]

\[
\rightarrow [\phi(x_i)] = \Lambda_r^{-1} U_r^T \tilde{\Phi} \tilde{r}_{X},
\]

where \( \phi(x_i) \in \mathbb{R}^r \) and \( \tilde{r}_{X} \) is the centered version (using Appendix (A.5)) of the base kernel vector \( k_{RX} \). Using the defined mapping function \( \phi(\cdot) \), we can either map all the samples into the corresponding feature space and apply the linear methods on the new features or compute the kernel matrices using the corresponding kernel function:

\[
\kappa(x_i, x_j) = \phi(x_i)^T \phi(x_j) = \tilde{k}_{RX}^T U_r \Lambda_r^{-1} U_r^T \tilde{\Phi} \tilde{r}_{X},
\]

where \( \tilde{k}_{RX} = U \Lambda^{-1} U^T \) is the pseudo inverse of \( \tilde{K}_{RR} \). Using this kernel function, the kernel matrix \( K_{XX} \) becomes

\[
K_{XX} = \phi(X)^T \phi(X) = \tilde{k}_{RX}^T \tilde{K}_{RR} \tilde{k}_{RX} = \tilde{k}_{X} \tilde{K}_{RR} \tilde{k}_{RX}.
\]

Similarly, the test kernel matrix \( K_{XX} \) becomes

\[
K_{XX} = \tilde{k}_{X} \tilde{K}_{RR} \tilde{k}_{RX}.
\]

As can be seen, the above definitions for reference mapping and reference kernel function are not following the typical approach, where only the kernel function is known, while \( \phi(\cdot) \) is possibly both undefined and infinite-dimensional. Instead, we now have an explicit formula for \( \phi(\cdot) \in \mathbb{R}^r \), where \( r \) is the rank of \( \tilde{K}_{RR} \), and the formula depends on the selected reference vectors. Here, it should be noted we see the reference vectors as hyperparameters of the mapping/kernel function. They can be either data-dependent or data-independent as discussed below, but both cases are common also for the common kernel function. For example, the value of \( \sigma \) in the RBF kernel function is often scaled according to the training data. Despite the unusual definition, kernel function in (18) fulfils the definition of a proper kernel function [50]: A necessary and sufficient condition for a function \( \kappa(\cdot, \cdot) \) to be a valid kernel is that the kernel matrix \( K_{XX} \) is positive semidefinite. Our kernel matrix is Gram matrix by definition (19) and, thus, it is always positive semidefinite.

We call our new definitions generalized reference mapping and kernel, because different selection of the reference vectors \( R \) produces kernels, which are equivalent to different approximate solutions discussed in Section II-B. In particular, we consider the following seven cases:

1) \( R = X \in \mathbb{R}^{D \times N} \): Here, the target class training samples are used as reference vectors, and the mapping function \( \phi(\cdot) \) in (17) is equivalent to NPT in (12) and (13). The kernel function \( \kappa(\cdot, \cdot) \) in (18) is almost equal to the base kernel function with some difference coming from the centering operations.

2) \( R = N \in \mathbb{R}^{D \times N} \sim N(0, 1) \): Here, \( N \) random reference vectors are drawn from the normal distribution. As the training data is standardized and contains samples from the target class only, the reference vectors come approximately from the training distribution. This may have a regularizing effect. With this reference vector selection, the generalized reference mapping has connections with the mappings used by randomized single hidden-layer feedforward network one-class classifiers, e.g., [51], [52], with two differences, i.e., the centering of the base kernel vector \( \tilde{k}_{RX} \) and the normalization of the mapping \( \phi(x_i) \), which follows from the projection and normalization with the eigenpairs of \( \tilde{K}_{RR} \) in (17).

3) \( R = X^* \in \mathbb{R}^{D \times M}, M < N \): Here, we pick randomly a subset of the training samples. This option corresponds to the vanilla Nystöm approximate kernel approach (7). Using this reference vector selection along with the mapping function in (17) can be seen as an approximate variant of NPT.
We experimentally compared the seven cases of our proposed generalized reference approach, both by using the proposed kernel function (18) to create the corresponding kernel matrix to be used in the kernel implementation of the one-class classification techniques and by using the proposed mapping function in (17) to generate new features to be used in the linear implementation of the one-class classification techniques. The kernel approach was compared against the base kernel and the mapping approach was compared against NPT using the base kernel function. The base kernel function in all experiments was the RBF kernel (6) and the one-class classification techniques and by using the proposed kernel matrix to be used in the kernel implementation of the approximate generalized reference approach, both by using the proposed kernel function (17) to generate new features to be used in the approximate kernel method to the NPT setting.

5) \( \mathbf{R} = [\mathbf{X}, \mathbf{X}_{\text{neg}}] \in \mathbb{R}^{D \times (N+T)} \): Here, the reference vectors are the target class training samples augmented with some of the non-target class training samples. This approach can be seen as an implicit data augmentation scheme for non-linear one-class classification.

6) \( \mathbf{R} = [\mathbf{X}, \mathbf{N}] \in \mathbb{R}^{D \times (N+T)} \): Here, the reference vectors are the target class training vectors augmented by \( T \) random vectors drawn from normal distribution. This approach can be seen as an implicit data augmentation scheme for non-linear one-class classification.

7) \( \mathbf{R} = [\mathbf{N}] \in \mathbb{R}^{D \times (N+T)} \sim \mathcal{N}(0, 1) \): Here, we draw \( N+T \) random reference vectors from the normal distribution for direct comparison against the previous two cases.

IV. EXPERIMENTS

A. Experimental Setup

We experimentally compared the seven cases of our proposed generalized reference approach, both by using the proposed kernel function in (18) to create the corresponding kernel matrix to be used in the kernel implementation of the one-class classification techniques and by using the proposed mapping function in (17) to generate new features to be used in the linear implementation of the one-class classification techniques. The kernel approach was compared against the base kernel and the mapping approach was compared against NPT using the base kernel function. The base kernel function in all experiments was the RBF kernel (6) and the one-class classification techniques used in the experiments were SVDD and OC-SVM. The codes for linear SVDD and both linear and kernel OC-SVM were obtained from LIBSVM library.

We selected for our experiments six different small-scale datasets from UCI machine learning repository [55] shown in Table I. For each class in these datasets, we created a different one-class classification task by considering this class as the target class and all the other classes as outliers. Thus, we had a total of 14 different tasks as shown in Table I. For each task, we selected randomly 70% of the samples as our training set and the remaining 30% as the test set. This was repeated five times and the same splits were used to test the performance of all methods. For each split, the experiments were also repeated five times. Thus, each reported result is an average of 25 different runs. For each run, the hyperparameters were selected using a random 5-fold cross-validation approach within the training set. Thus, also for non-random kernel/mappings variants, there may be differences between the repetitions due to the differences in validation splits that may lead to different hyperparameter selection.

We experimented with the cases 3-4 listed in Section III by setting \( M = \lceil \frac{N}{2} \rceil \) and with cases 5-7 by setting \( T = \min(N, N_{\text{neg}}) \), i.e., in these cases we doubled the number of reference vectors, if the number of negative samples allowed it. While the number of negative samples is not relevant for cases 6-7, we used the same \( T \) to allow direct comparison. The number of training samples, \( N \), and the value of \( T \) used for cases 5-7 are also shown in Table I. When forming \( \Upsilon_r \) and \( \Lambda_r \) in (16) we consider values \( < 10^{-6} \) as zeros. The hyperparameter values selected by cross-validation included \( \sigma \) for RBF kernel, \( C \) for SVDD, and \( \nu \) for OC-SVM. Hyperparameter \( \sigma \) was set as \( \sqrt{s \text{aver}} \), where \( d \text{aver} \) is the average squared distance between the training samples and \( s \) is selected from the following options: \( 10^{-3}, 10^{0}, 10^{1}, 10^{2}, 10^{3} \). Hyperparameters \( C \) and \( \nu \) are selected from \( [0.1, 0.2, 0.3, 0.4, 0.5, 0.6] \). As the performance metric, we use Geometric Mean (Gmean), because it takes into account both True Positive Rate (TPR) and True Negative Rate (TNR) as \( \text{Gmean} = \sqrt{\text{TPR} \times \text{TNR}} \).

B. Experimental Results and Discussion

The experimental results in terms of Gmean are given in Table II-V. Table II shows SVDD results using the base kernel matrix along with the seven cases of our proposed

| Dataset | \( C \) | \( N_{\text{tot}} \) | \( D \) | Task | Target | \( N \) | \( T \) |
|---------|-------|--------|-------|------|-------|------|------|
| Iris1   | 3     | 150    | 4     | Iris1 | Setosa | 35   | 35   |
| Iris2   | 3     | 210    | 7     | Iris2 | Versicolor | 35   | 35   |
| Iris3   | 3     | 250    | 6     | Iris3 | Virginica | 35   | 35   |
| Seeds   | 3     | 208    | 60    | Seeds1 | Kama | 68   | 68   |
| Seeds2  | 3     | 502    | 60    | Seeds2 | Rosa | 68   | 68   |
| Seeds3  | 3     | 100    | 60    | Seeds3 | Canadian | 49   | 49   |
| Ionosphere | 3   | 250    | 60    | Ion1 | Bad | 88/89 | 88/89 |
| Ionosphere | 3   | 250    | 60    | Ion2 | Good | 157/158 | 88/89 |
| Sonar   | 2     | 208    | 60    | Son1 | Rock | 68   | 68   |
| Sonar   | 2     | 208    | 60    | Son2 | Mines | 78   | 68   |
| Qualitative bankruptcy | 2 | 502 | 60 | Bank1 | Bankr. | 74/75 | 74/75 |
| Qualitative bankruptcy | 2 | 502 | 60 | Bank2 | No bankr. | 100/101 | 74/75 |
| Somerville happiness | 2 | 100 | 60 | Happ1 | Happy | 54 | 47 |
| Somerville happiness | 2 | 100 | 60 | Happ2 | Unhappy | 47 | 47 |

\( C \) - number of classes, \( N_{\text{tot}} \) - total number of samples, \( D \) - dimensionality, Task - subtask abbreviation, Target - target class in the subtask, \( N \), \( T \) - as defined in Section III

1. https://www.csie.ntu.edu.tw/~cjlin/libsvm/
2. https://www.tudelft.nl/ewi/over-de-faculteit/afdelingen/intelligent-systems/pattern-recognition-bioinformatics/pattern-recognition-bioinformatics/data-and-software/dd-tools
3. https://github.com/JenniRaitoharju/GeneralizedReferenceKernel
### Table II
Average Gmean values (and kernel matrix ranks) for SVDD with the base kernel function and the seven cases of our proposed generalized reference function

| Data | $M = N$ | $M = N/2$ | $M = N + 1$ |
|------|---------|-----------|-------------|
| Case 1 | 90.0-1.3 (34.0) | 89.0-1.0 (34.0) | 88.8-0.8 (34.0) |
| Case 2 | 89.0-1.0 (34.0) | 88.8-0.8 (34.0) | 88.8-0.6 (34.0) |
| Case 3 | 88.8-0.8 (34.0) | 88.8-0.6 (34.0) | 88.8-0.4 (34.0) |
| Case 4 | 88.8-0.6 (34.0) | 88.8-0.4 (34.0) | 88.8-0.2 (34.0) |
| Case 5 | 88.8-0.4 (34.0) | 88.8-0.2 (34.0) | 88.8-0.0 (34.0) |
| Case 6 | 88.8-0.2 (34.0) | 88.8-0.0 (34.0) | 88.6-0.0 (34.0) |
| Case 7 | 88.8-0.0 (34.0) | 88.6-0.0 (34.0) | 88.6-0.0 (34.0) |

### Table III
Average Gmean values (and feature space dimensions) for SVDD with NPT using the base kernel function and the seven cases of our proposed generalized reference mapping function

| Data | $M = N$ | $M = N/2$ | $M = N + T$ |
|------|---------|-----------|-------------|
| Case 1 | 89.8-1.4 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |
| Case 2 | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |
| Case 3 | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |
| Case 4 | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |
| Case 5 | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |
| Case 6 | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |
| Case 7 | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) | 89.8-1.1 (18.5) |

### Table IV
Average Gmean values (and kernel matrix ranks) for OC-SVM with the base kernel function and the seven cases of our proposed generalized reference kernel function

| Data | $M = N$ | $M = N/2$ | $M = N + T$ |
|------|---------|-----------|-------------|
| Case 1 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
| Case 2 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
| Case 3 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
| Case 4 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
| Case 5 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
| Case 6 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
| Case 7 | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) | 88.6-1.4 (34.3) |
generalized kernel matrix (19) via kernel implementation and Table III shows the results using NPT along with the seven cases of our proposed generalized kernel mapping (17) via linear implementation. Tables IV and Tables V have the corresponding results for OC-SVM. The tables also give the average kernel matrix ranks or feature space dimensions for the mappings. In each table, the best performance for each number of reference vectors is bolded.

First, we see that the results for the base NPT and for the case 1 of the proposed mapping are indeed almost identical. For the kernel setting, the difference is larger in particular for OC-SVM. Our additional experiments verify that the differences indeed follow mainly from the centering operation and, in most cases, OC-SVM suffers from the centering, while for SVDD centering slightly improves the results. Also in general, we see that the conclusions for SVDD and OC-SVM are similar. In particular, the results are consistent with the kernel properties with respect to a specific algorithm.

For SVDD, the random cases 2, 4, and 7 quite consistently improve the results compared to the base method or to using training vectors as reference vectors. In particular, there are few cases (Ion1, Bank2), where the base methods clearly fail, but the proposed kernel and mapping with random reference vectors leads to clearly improved results. The random reference vectors indeed seem to provide implicit regularization and, thus, a more robust performance. The results are on average slightly better when there are more reference vectors, but the differences are quite insignificant. Thus, using the proposed generalized reference kernel as an implicit data augmentation ($M > N$) may slightly help, but it is more beneficial to replace the training samples with random data than to augment the training samples with random data (case 6).

Looking at the kernel matrix ranks, we see that the proposed implementation with the case 2 often leads to lower ranks but better results than the original method. On the hand, in the tasks where the random reference vectors lead to significant improvements do not have lower rank. This gives some indication that the random reference vector variant can adapt the rank to the task at hand. For the base NPT, ranks are lower than for the base kernel, whereas for the proposed approach the ranks are more similar between the kernel and mapping, while for the mapping the variance in ranks is higher.

For OC-SVM, as mentioned already, centering clearly harms the performance. Thus, the base kernel performs much better than the base NPT, while most of the proposed generalized reference kernel variants also achieve a lower performance than the corresponding variant for SVDD. A very interesting exception for both generalized reference kernel and mapping with OC-SVM is the case 5 that uses also negative samples as reference vectors. The case 5 results are consistently outperforming all the other cases and also all the SVDD results. While it should be remembered that comparing this directly with the other cases is unfair, because the basic assumption of not having negative examples is violated, the results still open interesting future work opportunities either as a result still open the case 5 as a way to exploit some negative samples within the regular one-class implementation or as an indication that for OC-SVM it may be more beneficial to pick reference vectors outside the training data distribution. Furthermore, it is interesting that only OC-SVM with generalized reference kernel and mapping can exploit the negative data efficiently, while the same is not true for SVDD with the proposed approaches. Further analyzing this difference may lead to better understanding how to select most suitable kernels for different algorithms.

V. CONCLUSIONS

In this paper, we proposed a new kernel formulation based on a base kernel and reference vectors that can be applied in different ways. Different cases (i.e., different ways to select the reference vectors) of our generalized reference mapping and kernel have links to different prior works including approximate kernels and NPT. Our formulation also provides a
way to extend random sampling and random projection-based approximate kernel methods into an NPT-like setting. In this paper, we considered the new formulation in the context of small-scale one-class classification and with RBF kernels, but in the future it can be used also in different tasks and with different kernels.

Our experimental results show that the new formulation can help to implicitly regularize and adjust the rank of the kernel matrices. It also allows to incorporate additional information into the kernel itself, leading to improved one-class classification accuracy. For SVDD, random reference vectors led to best classification results and more robust performance indicating that this approach provides implicit regularization.

For OC-SVM, using negative samples as references vectors led to significant classification performance improvements. While this approach violates the assumption that one-class classification cannot use negative examples for training, it can be considered in the future in the class-specific classification context or in one-class classification with few negative examples. It may also indicate that for OC-SVM it would be more beneficial to select random reference vector outside the training distribution.

As the conclusions for SVDD and OC-SVM are quite different, this suggests that the new kernel formulation should be further studied with respect to a specific method. On the other hand, further analyzing the causes for the observed differences may help to understand how to optimize the reference vectors for the method and task at hand.

APPENDIX

In NPT, the training data needs to be centered in $\mathcal{F}$, i.e. $\sum_{i=1}^{N} \phi(x_i) = 0$. If this assumption is not met, $\mathcal{P}$ is a manifold in $\mathcal{F}$ and not a subspace of $\mathcal{F}$, since $0$ does not necessarily belong to $\mathcal{P}$ [44]. In our formulation, $\mathcal{F}$ is spanned by function $\phi(\cdot)$, meaning that the centering operation is not mandatory. Nevertheless, in practice we apply KPCA for the reference data with the base kernel $\hat{K}_{RR}$ and, therefore, we also opt to center our reference data in the base kernel space $\mathcal{F}$ by aligning the corresponding kernel function $\hat{K}_{RR}$. To align our training and testing data, we also center $\hat{K}_{RR}$ and $\hat{K}_{RX}$ with respect to the center of the reference data $\hat{R}$.

Let us denote by $\mu$ the mean of the $M$ uncentered reference vectors $\hat{\Phi}(\hat{R}) = [\phi(r_1), \ldots, \phi(r_M)] \in \mathcal{F}$:

$$
\hat{\mu} = \frac{1}{M} \sum_{i=1}^{M} \phi(r_i) = \frac{1}{M} \hat{\Phi}(\hat{R}) 1_M, \quad (A.1)
$$

where $1_M \in \mathbb{R}^M$ is a vector of ones. The centered reference vectors in $\mathcal{F}$ are given by

$$
\hat{\Psi}(\hat{R}) = \hat{\Phi}(\hat{R}) - \hat{\mu} 1_M^T = \hat{\Phi}(\hat{R})(I - \frac{1}{M} 1_M 1_M^T) = \hat{\Phi} C_M, \quad (A.2)
$$

where we denote by $C_M = I - \frac{1}{M} 1_M 1_M^T$ the centering matrix for the reference vectors. The training vectors $\hat{X}$ (and test vectors $\hat{X}$ accordingly) can be centered with respect to $\hat{\mu}$ in $\mathcal{F}$ as follows:

$$
\hat{\Psi}(\hat{X}) = \hat{\Phi}(\hat{X}) - \hat{\mu} 1_N^T = \hat{\Phi}(\hat{X}) - \frac{1}{M} \hat{\Phi}(\hat{R}) 1_M 1_N^T = \hat{\Phi}(\hat{X}) - \hat{\Phi}(\hat{R}) C_N, \quad (A.3)
$$

where $C_N = \frac{1}{M} 1_N 1_N^T$. By using $\hat{\Psi}(\hat{R})$ and $\hat{\Phi}(\hat{X})$ (or $\hat{\Psi}(\hat{X})$), the centered kernel matrices $\hat{K}_{RR}$ and $\hat{K}_{RX}$ (or $\hat{K}_{RX}$) can be calculated as follows:

$$
\hat{K}_{RR} = \hat{\Psi}(\hat{R})^T \hat{\Psi}(\hat{R}) = C_M \hat{K}_{RR} C_M \quad (A.4)
$$

and

$$
\hat{K}_{RX} = \hat{\Psi}(\hat{R})^T \hat{\Psi}(\hat{X}) = C_M (\hat{K}_{RR} - \hat{K}_{RX} C_N), \quad (A.5)
$$

Note that the centering formulas for NPT can be obtained by setting $\hat{R} = \hat{X}$ and by using the kernel at hand as the base kernel in the formulas.

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