Generalized Likelihood Ratio Test
With One-Class Classifiers

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Abstract—One-class classification (OCC) is the problem of deciding whether an observed sample belongs to a target class or not. We consider the problem of learning an OCC model when the dataset available at the learning stage contains only samples from the target class. We aim at obtaining a classifier that performs as the generalized likelihood ratio test (GLRT), which is a well-known and provably optimal (under specific assumptions) classifier, when the statistics of the target class is available. To this end, we consider both the multilayer perceptron neural network (NN) and the support vector machine (SVM) models. They are trained as two-class classifiers using an artificial dataset for the alternative class, obtained by generating random samples, uniformly over the domain of the target-class dataset. We prove that, under suitable assumptions, the models converge (with a large dataset) to the GLRT. Moreover, we show that the one-class least squares SVM (OCLSSVM) at convergence performs as the GLRT, with a suitable transformation function. Lastly, we compare the obtained solutions with the autoencoder (AE) classifier, which does not in general provide the GLRT.

Index Terms—Generalized likelihood ratio test, One-class classification, One-class support vector machine, Neural network, and Support vector machine.

I. INTRODUCTION

One-class classification (OCC) is the problem of deciding whether an observed sample belongs to a target class or not. When using machine learning (ML) approaches, it is assumed that only samples from the target class are available during the learning phase. 1 In a statistical framework, the equivalent hypothesis testing problem is denoted as composite hypothesis testing, when only the distribution of samples from the target class is available. In both meanings, several other assumptions on the alternative class have been considered, including the possibility that only very few alternative-class samples are available (with their label), or that the dataset is polluted with few wrongly labeled samples from the alternative class (outliers), as better described in Section II.

Here we focus on the case wherein no sample is available from the alternative class. Such condition occurs in several contexts, and a relevant application domain is security, where OCC has been applied to several problems, including authentication in underwater acoustic networks [1], intrusion detection in industrial networks security [2], in-region location verification using radio signals [3], and global navigation satellite system (GNSS) spoofing detection [4], [5]. The considered OCC problem is also known under different names, e.g., outlier and novelty/anomaly detection.

1When samples from both the target and alternative classes are available, we have a two-class classification problem.

In such a scenario, within the ML domain, several architectures for OCC have been investigated in the literature (see Section II for a detailed report), and the main solutions are the one-class support vector machine (OSVM) and the autoencoder (AE). In the statistical domain, instead, the main tool is the generalized likelihood ratio test (GLRT), which provides a solution for composite hypothesis testing when the alternative class is partially known, i.e., samples may come from many possible distributions, rather than a single one. The GLRT has been well characterized and proved to be optimal under relevant assumptions, as better detailed in Section II. In this paper, we focus on the case where no knowledge of the alternative class is available and denote the resulting test as the GLRT with undefined alternative (GLRT-UA).

In this paper we aim at bringing a bridge between the ML and statistical approaches, by introducing learning strategies for the multilayer perceptron neural network (NN) and support vector machine (SVM) models that implement GLRT-UA. We propose to generate an artificial dataset containing random samples uniformly distributed in the domain of the target-class dataset. Then, either a NN or a least-square SVM (LS-SVM) is applied on the two datasets in a supervised manner. By leveraging existing results showing that NNs and LS-SVM converge to the likelihood ratio test (LRT) when two labeled datasets are available, we prove that the proposed models and learning strategies provide classifiers equivalent to the GLRT-UA for large training datasets. Moreover, we show that the one-class least squares SVM (OCLSSVM) at convergence performs as the GLRT-UA with a large dataset and using a suitably designed transformation function. We also prove that a classifier based on the AE does not provide the GLRT-UA.

The rest of the paper is organized as follows. Section II presents the related state of the art and our contribution. Section III describes the OCC problem, analyzing it from both the statistical decision theory and the ML points of view. Section IV introduces the GLRT-UA and the proposed learning strategy for NN and OCLSSVM. In Section VI we present performance results of the proposed techniques, which are also compared to the GLRT-UA and the AE. Finally, Section VII draws the conclusions.

II. RELATED STATE-OF-THE-ART AND CONTRIBUTION

When the statistics of samples belonging to both classes of a binary classification problem are known, the LRT provides the minimum misdetection (MD) probability for a given false alarm (FA) probability, as shown in the Neyman and Pearson
theorem \[6\]. When the statistics of samples of either one or both classes depend on unknown parameters, a widely used test is the GLRT \[7\]. The GLRT has been proved to be asymptotically optimal (with \(n \to \infty\)) for several parametric distributions \[8\] when performed jointly on \(n\) independent identically distributed (i.i.d.) samples (from an unknown class). Another test to be used in case of partially unknown statistics is the Hoeffding test \[9\], which is a modified GLRT that estimates the distribution for the alternative class from the samples: such test is proven to be asymptotically optimal when the test is performed jointly on \(n \to \infty\) i.i.d. samples. However, in this paper we consider tests and classifiers on single samples (on which it is not meaningful to obtain a sampling distribution), thus GLRT, and its special case GLRT-UA, is our reference statistical test, as no assumption on the alternative class is done.

When statistics are not known, but sample datasets are available, ML solutions should be considered. For two-class classification, when labeled datasets from both classes are available during training, supervised training for classifications can be applied on several models, including deep NN and SVM. In \[3\] it has been proven that NNs and LS-SVMs \[10\] performs as the LRT, when the training dataset is large enough and the models are complex enough.

When samples are available only from one class, the OCC problem arises, and typical solutions are based on AE \[11\] and OSVM \[12\]. Several variations of such approaches have been considered. In \[13\], the input data is embedded into the dissimilarity space then represented by weighted Euclidean graphs, used to compute the entropy of the data distribution in the dissimilarity space and obtain decision regions. In \[14\], it is observed that the mean square error (MSE) loss function for the training of OSVM is robust to the Gaussian noise but less effective against large outliers, and a robust maximum correntropy loss function is proposed. For surveys of one-class classification techniques see also \[11, 15\].

When dataset vector samples are realizations of \(n\) i.i.d. variables and an NN is used for OCC, asymptotically (for \(n \to \infty\)) we obtain the performance of the optimal Hoeffding test \[16\]. However, when samples are not large vectors of i.i.d. variables, no result on the optimality of classifiers is available.

A. Contributions

In this paper we aim at identifying ML solutions that implement the GLRT-UA. First, we propose to train NN and LS-SVM models with samples for two labeled datasets: one is the target-class dataset, while the alternative-class dataset is artificially generated with samples uniformly distributed in the (estimated) domain of the target-class dataset. As a second solution, we consider the OCLSSVM and prove that, with a suitable choice of the transformation function and for a large dataset, performs at convergence as the GLRT-UA.

Note that artificial datasets for training classification models have been already considered in the literature, however under different assumptions and with different generation techniques. In \[17\], a two-class classifier is used for OCC, where the dataset for the alternative class is randomly generated with the same distribution of the available dataset, obtained with a probability density function (PDF) estimation technique. We instead consider a uniform distribution. In \[18\], few samples of the available dataset are considered as belonging to the alternative class, and the samples that have the least fit with the one-class model are passed to an expert for labeling and then used for two-class training. We instead do not assume neither a prior knowledge on the statistics nor availability of samples from the alternative class. In \[19\], it is proposed to create dataset for the two classes in binary classification (or classification with unknown parameters), instead of computing the LRT or GLRT, when the alternative class is described by a PDF with unknown parameters and the equivalence between GLRT and the ML techniques is supported only by a simulation campaign. In our paper instead we assume no knowledge of the alternative class statistics (and no dataset availability) and we prove that under specific conditions the models with proper training converge to the GLRT. In \[20\], an AE is used to extract the features of the target class, then a zero-mean Gaussian noise is applied in the latent space to generate samples of the alternative class; datasets are then used to train a NN. The generation of the artificial dataset is different from our approach, as we aim at obtaining the GLRT-UA. Lastly, generative models (see the survey \[15\]) also include the generation of artificial datasets. With such approaches, two models are trained, the discriminator and the generator: the discriminator aims at distinguishing inputs belonging to the target class from other inputs, while the generator aims at generating random samples that fed to the discriminator are accepted as belonging to the target class. Also in this case, the obtained solution has not been proved to be equivalent to the GLRT-UA.

In summary, the main contributions of this paper with respect to the existing literature are the following:

- We resort to the generation of an artificial dataset to train the NN and LS-SVM models as two-class classifiers. The artificial dataset contains random samples, uniformly distributed in the domain of the target class.
- We prove that the proposed solutions based on NN and LS-SVM converge to GLRT-UA for complex enough models and a large-enough target-class training set.
- We prove that OCLSSVM using a specific transformation function and a large-enough target-class training set at convergence performs as the GLRT-UA.

III. ONE-CLASS CLASSIFICATION AND COMPOSITE HYPOTHESIS TESTING

Consider a system that observes sample vectors of \(M\) elements \(x = [x_1, \ldots, x_M]^T\), where \(^T\) denotes the transpose operator, and elements \(x_j \in \mathbb{R}, j = 1, \ldots, M\), are real numbers. The sample vectors belong to a domain \(\mathcal{X} \subseteq \mathbb{R}^M\). We assume that any sample vector can be generated from two possible PDFs, denoted as \(\{p_0(a)\}\) and \(\{p_1(a)\}\), with \(a \in \mathcal{X}\) when generated according to \(\{p_0(a)\}\), \(x\) is said to belong to 2

\[\text{Here we consider real-valued vectors, but other cases can be easily accommodated in the same framework, e.g., when the vector elements are either discrete or complex.}\]
the target class $\mathcal{H}_0$, and we write $C(x) = \mathcal{H}_0$. When generated from $\{p_1(a)\}$, $x$ is said to belong to the alternative class $\mathcal{H}_1$, and we write $C(x) = \mathcal{H}_1$. Note that we are considering non-separable classes, as the same sample vector can be observed in both classes with non-zero probability. Still, we assume that PDFs $\{p_0(a)\}$ and $\{p_1(a)\}$ are different, thus each sample vector has a different (differential) probability of belonging to each class.

We address the problem of deciding if a given sample $x$ belongs to class $\mathcal{H}_0$ or $\mathcal{H}_1$. To this end, we resort to a classifier $f(x)$ that, after suitable training, gives for each possible value of $x$ one of the two classes as output, i.e.,

$$f(x) \in \{\mathcal{H}_0, \mathcal{H}_1\}. \quad (1)$$

Since we are dealing with non-separable classes, in general, the decision taken by the classifier is not always correct, as either FA or MD errors may occur. An FA occurs when the decision is for the alternative class $\mathcal{H}_1$ (i.e., $f(x) = \mathcal{H}_1$), while $x$ has been generated from $\{p_0(a)\}$. Similarly, an MD occurs when the decision is for the target class $\mathcal{H}_0$ (i.e., $f(x) = \mathcal{H}_0$), while $x$ was actually generated from $\{p_1(a)\}$. We denote the FA and MD probabilities as

$$P_{\text{FA}}(f) = P[f(x) = \mathcal{H}_1 | C(x) = \mathcal{H}_0]$$

$$= \int_{a: f(a) = \mathcal{H}_1} p_0(a) da, \quad (2)$$

$$P_{\text{MD}}(f) = P[f(x) = \mathcal{H}_0 | C(x) = \mathcal{H}_1]$$

$$= \int_{a: f(a) = \mathcal{H}_1} p_1(a) da, \quad (3)$$

where we have highlighted the dependency of both probabilities on the classifier $f(x)$. Therefore, when designing the classifier $f(x)$, both probabilities should be considered, as discussed in the following.

In the rest of this section, we describe the design of the classifier $f(x)$, within both the statistical and ML frameworks. In all cases, the classifier at the end compares a real value $u$, obtained from the sample vector $x$, with a suitable threshold $\delta$. Therefore, we introduce the decision function

$$\Delta(u, \delta) = \begin{cases} 
\mathcal{H}_0 & u > \delta, \\
\mathcal{H}_1 & u \leq \delta,
\end{cases} \quad (4)$$

that decides for the target class $\mathcal{H}_0$ when $u > \delta$, and for the alternative class $\mathcal{H}_1$ otherwise.

A. ML and Statistical Frameworks

Since in this paper we aim at connecting the classification problem (in an ML framework) to the hypothesis testing problem (in a statistical framework), we define here the two settings.

In the statistical framework, $\mathcal{H}_0$ and $\mathcal{H}_1$ are also denoted as null and alternative hypothesis, respectively. Here we will always use the class nomenclature.

$\text{Statistical Framework:}$ In the statistical framework, either one of both the PDFs $\{p_0(a)\}$ and $\{p_1(a)\}$ are available at the design time, while no dataset is available. A two-class classification problem is denoted as hypothesis testing problem and is based on the assumptions that the PDFs for both classes, $\{p_0(a)\}$ and $\{p_1(a)\}$, are available. In OCC, only the target-class PDF $\{p_0(a)\}$ is available and the problem is denoted as composite hypothesis testing (as discussed in more details in the following). Classifiers are denoted as tests in the statistical framework and $f(x)$ is a function obtained from the available PDFs.

$\text{ML Framework:}$ In the ML framework, the PDFs $\{p_0(a)\}$ and $\{p_1(a)\}$ are not available, but a dataset containing vector samples from one or both classes is available during the training. In two-class classification, a dataset with (correctly) labeled samples is available, while in OCC a dataset with only vector samples belonging to the target class is available.

In OCC the target-class dataset available for training has $N_0$ samples and is denoted as

$$\mathcal{D}_0 = \{x_1, \ldots, x_{N_0}\}. \quad (5)$$

B. LRT and GLRT in the Statistical Framework

We briefly summarize here the most important results for the two-class classification problem and OCC with partially known statistics of the alternative class in the statistical framework, that will be useful to better understand OCC in the ML framework.

Two-Class Classification: In the statistical framework, the test for two-class classification typically aims at minimizing the MD probability, while ensuring a target FA probability $\epsilon$. Thus, the test is designed as

$$f(x) = \arg \min_{g \in \mathcal{G}} P_{\text{MD}}(g), \text{ s.t. } P_{\text{FA}}(g) \leq \epsilon, \quad (6)$$

where $\mathcal{G}$ is the set of all possible test functions. The test solving (6), when the PDFs for both classes are available, is the LRT, which first computes the log-likelihood ratio on the sample $x$

$$\Gamma(x) = \log \frac{p_0(x)}{p_1(x)}, \quad x \in \mathcal{X}, \quad (7)$$

and then performs the test by comparing $\Gamma(x)$ with a threshold $\delta$,

$$f_{\text{LRT}}(x) = \Delta(\Gamma(x), \delta), \quad (8)$$

where threshold $\delta$ is chosen to ensure the constraint on the FA probability, i.e., $P_{\text{FA}}(f_{\text{LRT}}) \leq \epsilon$.

Composite Hypothesis Testing with Unknown Parameters: Composite hypothesis testing $[1]$, refers to a classification problem where a partial knowledge of the PDF of the alternative-class samples is available. This typically occurs when the PDF of the alternative-class samples can be written as $\{p_1(a, \theta)\}$, where $\theta$ is a vector of unknown parameters. For example, it can be assumed that in the alternative class, $x$ is a Gaussian vector with unknown mean $\theta$ and given covariance matrix. In such scenarios, a widely considered test function is the GLRT, that first computes

$$A(x) = \log \frac{p_0(x)}{\max_{\theta} p_1(x, \theta)}, \quad (9)$$
and the maximum at the denominator is taken in the set of all possible values of the unknown parameter vector $\theta$; then the test function is defined as

$$f_{\text{GLRT}}(x) = \Delta(\Lambda(x), \delta),$$

where threshold $\delta$ is chosen to ensure a constraint on the FA probability, i.e., $P_{\text{FA}}(f_{\text{GLRT}}) \leq \epsilon$.

The GLRT does not solve problem (6), but it has been proven to solve an asymptotic version of (6). In particular, consider a collection of $n$ vector samples $x(n) = \{x_1, \ldots, x_n\}$, where each vector $x_i$ is independently drawn from the same class: we consider the following optimization problem

$$\min_{\theta} \lim_{n \to \infty} \frac{1}{n} \log P_{\text{MD}}(g_n),$$

s.t.

$$\lim_{n \to \infty} \frac{1}{n} \log P_{\text{FA}}(g_n) < -\epsilon,$$

where $g_n$ is the set of all test functions on $x(n)$. In words, we aim at finding a sequence of test functions $\{g_n, n = 1, \ldots\}$ that asymptotically minimizes the MD probability, while satisfying asymptotically a constraint on the FA probability. A GLRT defined as in (10), but now on $x_n$ rather than $x$, solves (11) under specific conditions on $g_n$, as proven in [8]. In other words, when the GLRT is performed on a collection of $n$ i.i.d. vector samples from the same class, it becomes asymptotically optimum (according to (6)) as the number of vector samples $n$ grows to infinity. Hence, at the moment, the GLRT is the best known test (in the sense described above) in case of partial knowledge of the PDF $\{p_1(a, \theta)\}$.

C. Composite Hypothesis Testing With Unknown Alternative Hypothesis Statistics

We now focus on the OCC problem (under the statistical framework), when the statistics of the samples under the alternative hypothesis is unknown.

Such scenario can be seen as an extreme case of composite hypothesis testing, where $\{p_1(a, \theta)\}$ can represent any PDF, according to the value taken by the (large) vector of parameters $\theta$. For example, a mixture of multiple multivariate Gaussian variables well models a wide class of multivariate PDFs. In this case, the denominator of (9), $\max_{\theta} p_1(x, \theta)$, can be very large for any value of $x$, as the parameter vector $\theta$ can be appropriately chosen. Thus, we can assume that the same (large) value of denominator is taken, i.e.,

$$p_{\text{max}} = \max_{\theta} p_1(x, \theta), \forall x \in \mathcal{X}. \tag{12}$$

Under condition (12), the denominator of $\Lambda(x)$ becomes irrelevant for the decision function (10), and the GLRT boils down to what we denote as the GLRT-UA, i.e.,

$$f_{\text{GLRT-UA}}(x) = \Delta(p_0(x), \delta). \tag{13}$$

Note that in (13) we have neglected the log function, which is irrelevant for the decision process, as it can be included in the choice of the threshold $\delta$. Also in this case, threshold $\delta$ is chosen to ensure the constraint on the FA probability $P_{\text{FA}}(f_{\text{GLRT-UA}}) \leq \epsilon$, as we note that this constraint does not depend on the statistics of the alternative class.

D. OCC in The ML Framework

In the ML framework, the dataset $\mathcal{D}_0$ is used to train a model $\mu(x)$, having as input the samples $x$ and providing a soft real number $\mu(x)$, which is then thresholded to make OCC, i.e.,

$$f_{\text{ML}}(x) = \Delta(\mu(x), \delta), \tag{14}$$

where also in this case threshold $\delta$ is chosen to ensure the constraint on the FA probability $P_{\text{FA}}(f_{\text{ML}}) \leq \epsilon$. This choice can be performed for example using the test dataset and computing the sampling FA probability on it.

What distinguishes the various solutions of OCC is the kind of used model $\mu(\cdot)$ and the way it is trained, still using the dataset $\mathcal{D}_0$. In the following, we recall two OCC solutions, namely the AE and the OSVM.

Autoencoder (AE) Classifier: An AE is an unsupervised multilayer perceptron trained to replicate its input to the output. The AE can be decomposed into two sub-networks, the encoder providing output in the latent space, and the decoder, giving as output a vector of the same size of the encoder input. The encoder NN $f_e(x, w_e, b_e)$ (with weights $w_e$ and biases $b_e$) aims at projecting the $M$-dimensional input, $x$, into the $K$-dimensional space modeled by the latent vector, $\mathbf{y} \in \mathbb{R}^K$. The representation of the input in the latent space is then given as input to the decoder NN, $f_d(\mathbf{y}, w_d, b_d)$ (with weights $w_d$ and biases $b_d$), which aims at replicating the original input, computing the reconstructed vector $\hat{x} = f_d(f_e(x_n, w_e, b_e), w_d, b_d)$. Thus, for each sample vector, the AE is trained to minimize the MSE loss function, i.e.,

$$\min_{w, b} \rho_{\text{AE}}(\mathcal{D}_0, w) = \min_{w, b} \frac{1}{N_0} \sum_{n=1}^{N_0} ||x_n - \hat{x}_n||^2,$$

where $\mathbf{w} = [w_e^T, w_d^T]^T$ and $\mathbf{b} = [b_e^T, b_d^T]^T$. We remark that the latent space typically has a smaller dimension than the input vector, i.e., $M > K$ and in general, the reconstruction process is not perfect. Thus, to replicate the input, the AE must learn the statistical properties of the input. More details about the AE design can be found in [21].

In this framework, the model used for OCC provides as output the MSE between the input sample $x$ and the AE output $\hat{x}$, i.e.,

$$\mu(x) = ||x - \hat{x}||^2, \tag{16}$$

which is then used in (14) to obtain the AE classifier. The idea behind the use of an AE for OCC is that, by training the NN using only the $\mathcal{D}_0$ dataset, only input samples with the same (or similar) statistical distribution of the samples in $\mathcal{D}_0$ itself are expected to be reconstructed with low MSE during the test phase, [3, 22].

One-class least squares SVM (OCLSSVM) Classifier: During training, the two-class SVM finds the boundary that better separates the samples of the two classes. The OCLSSVM model instead is trained only on the $\mathcal{D}_0$ dataset and finds the hyper-surface that best contains the samples in $\mathcal{D}_0$. In details, consider a proper feature-space transformation
function $\phi : \mathbb{R}^M \rightarrow \mathbb{R}^P$. Then, the OCLSSVM \[(10)\] is trained by solving the following optimization problem
\[
\min_{w, b} \rho_{\text{OCLSSVM}}(D_0, w, b),
\]
with \[
\rho_{\text{OCLSSVM}}(D_0, w, b) = \frac{1}{2} w^T w + b + \frac{1}{2} \sum_{n=1}^{N_0} e_n^2
\]
\[(17a)\]
\[
e_n = -w^T \phi(x_n) - b \quad n = 1, \ldots, N_0,
\]
\[(17b)\]
where $w$ is the $P$-size weight column vector, $b$ is a bias parameter, and $C$ is a hyper-parameter, whose value is tuned depending on the learning dataset itself \cite{23}.

The model used for OCC \cite{14} in this case is \[
\mu(x) = w^T \phi(x) + b.
\]
\[(18)\]
Note that the shape of the surface that envelops the samples in $D_0$ significantly depends on the choice of the transformation function $\phi(x)$.

IV. GLRT-UA WITH NEURAL NETWORKS AND SUPPORT VECTOR MACHINES

We now propose models with suitable training to perform the GLRT-UA. To this end, we a) show how the GLRT-UA can be described as a two-class classifier, with suitably defined statistics for the alternative hypothesis; b) define a training and properly selected models to be used in the ML classifier \cite{14} that, using properly selected model, performs as GLRT-UA.

A. GLRT-UA As Two-Class Classifier

Starting from the statistical framework, we first describe the OCC problem as a two-class classification problem, with a properly designed alternative-class PDF.

The following result links the LRT of two-class classification with the GLRT-UA for OCC.

Lemma 1. When the PDF of the alternative class is constant on the domain of the target class, i.e.,
\[
p_1^*(a) = \begin{cases} \frac{1}{|\mathcal{X}|}, & a \in \mathcal{X}, \\ 0, & \text{otherwise}, \end{cases}
\]
\[(19)\]
where $|\mathcal{X}|$ is the volume of $\mathcal{X}$, the GLRT-UA \[(13)\] is equivalent to the LRT \[(8)\], i.e., for each threshold $\delta_1$ there exists a threshold $\delta_2$ such that
\[
\Delta(\Gamma(x), \delta_1) = \Delta(p_0(x), \delta_2), \quad \forall x \in \mathcal{X}.
\]
\[(20)\]
Proof. By inserting the definition \[(19)\] of $p_1^*(a)$ into the log-likelihood ratio \[(7)\], we have
\[
\Gamma(x) = \log |\mathcal{X}| + \log p_0(x), \quad x \in \mathcal{X}.
\]
\[(21)\]
Considering the LRT of \[(8)\], from \[(3)\] we have
\[
\Delta(\Gamma(x), \delta) = \begin{cases} \mathcal{H}_0 & \log |\mathcal{X}| + \log p_0(x) > \delta \\ \mathcal{H}_1 & \log |\mathcal{X}| + \log p_0(x) \leq \delta \end{cases}
\]
\[
\mathcal{H}_0 \quad p_0(x) > \exp[\delta - \log |\mathcal{X}|]
\]
\[
\mathcal{H}_1 \quad p_0(x) \leq \exp[\delta - \log |\mathcal{X}|]
\]
\[(22)\]
with $\delta' = \exp[\delta - \log |\mathcal{X}|]$. Note that the last line of \[(22)\] is the GLRT-UA \[(13)\], thus the tests are equivalent in the sense of \[(20)\].

Therefore, GLRT-UA can also be seen as a binary hypothesis test, where the statistic of samples under the alternative hypothesis is uniform over the target-class sample domain $\mathcal{X}$.

B. GLRT-UA-Based OCC

Moving now to the ML framework, we consider here one-class classifiers implemented as follows:

1) Generate an artificial dataset
\[
D'_1 = \{v_1, \ldots, v_{N'_1}\}
\]
\[(23)\]
of samples randomly generated according to \cite{19}.

2) Train a model $\mu(x)$ as a two-class classifier on the two-class labeled dataset of size $N = N_0 + N'_1$
\[
D = \{D_0, D'_1\} = \{q_1, \ldots, q_N\},
\]
\[(24)\]
with labels $t_n = -1$ for samples $q_n \in D_0$ and $t_n = 1$ for $q_n \in D'_1$.

3) Use the trained model in the classifier \cite{14} to obtain the one-class classifier.

We will show that, when using the NN and the LS-SVM as models $\mu(x)$, this approach implements the GLRT-UA.

We consider a NN trained with either the MSE loss function
\[
\min_w \rho_{\text{NN}}(D, w) = \min_{w} \sum_{n=1}^{N} |\mu(q_n) - t_n|^2,
\]
\[(25)\]
or the cross-entropy loss function
\[
\min_w \rho'_{\text{NN}}(D, w) = -\sum_{n=1}^{N} t_n \log \mu(q_n) + (1 - t_n) \log[1 - \mu(q_n)],
\]
\[(26)\]
where $w$ is the vector of the weights of the NN. The LS-SVM instead an SVM trained using the least-square (LS) function, i.e., solving the optimization problem
\[
\min_{w, b} \rho_{\text{LS-SVM}}(D, w, b) = \min_{w, b} \frac{1}{2} w^T w + C \frac{1}{N} \sum_{n=1}^{N} e_n^2,
\]
\[
e_n = 1 - t_n \log \phi(q_n) + b \quad n = 1, \ldots, N,
\]
\[(27a)\]
\[(27b)\]
where $w$ is the weight column vector, $b$ is a bias parameter, and $C$ is an hyper-parameter. We remark that, differently from the one-class optimization problem of \[(17)\], here the bias parameter does not appear in the optimization function itself.

We now show that the procedure described above with these models provides the GLRT-UA.

Theorem 1. Consider a NN $\mu_{\text{NN}}(x)$ (trained with either the MSE or cross-entropy loss function) or an LS-SVM $\mu_{\text{LS-SVM}}(x)$ (trained with the LS loss function) over the two-class labeled dataset $D = \{D_0, D'_1\}$, obtained from the artificial dataset. When using such models in \cite{14}, we obtain one-class classifiers equivalent to the GLRT-UA, when a) the NN is complex enough, and b) the training converges to the configuration minimizing the loss functions of the two models.
Proof. We resort to the results of [3] Theorems 2 and 3], where it has been shown that, under the hypotheses of the theorem, classifier \([14]\) implements the LRT, when using as model \(\mu(x)\) either the multilayer perceptron NN or the LS-SVM. Then, using the artificial dataset for the alternative class and leveraging the result of Lemma 1 we conclude that the classifier defined by the theorem is equivalent to the GLRT-UA.

C. NN Training With Modified Gradient

Since the artificial dataset has a very simple distribution (uniform), we now consider an alternative approach, where we modify the loss function used for training the NN to incorporate the effects of the artificial dataset, without the need of explicitly generating it.

In round \(n\), \(n = 1, \ldots, N\), of the steep gradient descent (SGD) algorithm used for training [21], the weights are updated as follows

\[
w_{n+1} = w_n - \lambda \nabla \rho_{NN}(D_0, q_n, w)|w_n,
\]

(28)

where \(\lambda\) is the learning rate and \(\nabla \rho_{NN}(D_0, q_n, w)|w_n\) is the gradient operator with respect to the NN weights, computed for weight values \(w_n\).

Now, let us define the average gradient when \(x\) belongs to the artificial alternative class with PDF \(\{p^1(a)\}\), i.e., using [19],

\[F(\hat{w}) = \mathbb{E}_{x,C(x) \in H_1} \left[ \nabla \rho_{NN}(D_0, x, w)|\hat{w}\right] = \frac{1}{|X|} \int_X \nabla \rho_{NN}(D_0, x, w)|\hat{w} dx.\]

(29)

Note that function \(F(w)\) depends on the structure of the NN and not on the target-class dataset \(D_0\). Thus, we can compute such function offline and store it either in a look-up table or as a model itself.

Then, during training we only use the target-class dataset \(D_0\) and update the weights as follows, now for \(n = 1, \ldots, N_0\),

\[w_{n+1} = w_n - \lambda \left[ \nabla w|w_n \rho_{NN}(D_0, x_n, w) + F(w_n) \right].\]

(30)

With this choice we replicate the average behavior of the update [23] when the input belongs to the alternative class, without explicitly generating the dataset. The main advantage of this approach is that we do not need to generate the artificial dataset and half iterations are needed for training, while the disadvantage is that we must obtain the multivariate function \(F(\hat{w})\) offline and we must compute it at each iteration of the training algorithm. Lastly, we note that if the domain \(X\) changes, the average gradient \(F(\hat{w})\) must be recomputed accordingly.

D. On The Domain \(X\)

The knowledge of the domain \(X\) to generate the artificial dataset may not be trivial.

A first possibility is that the domain is available, because of known properties of the sample vectors. For example, sample vectors obtained by digital sampling of a analog signals, usually are clipped within an acquisition range. Such condition typically occurs in the security problems operating on samples obtained from receivers, as mentioned in the Introduction.

A second possibility occurs when we know that the domain of samples in the alternative class is the same of those in the target class. In this case, following the ML approach, to learn the domain from the dataset \(D_0\) as \(X\). This approach works well when dataset \(D_0\) covers all points of the domain, i.e., domain \(X\) is a discrete set. When the domain \(X\) is a continuous set of points, we may interpolate samples of \(D_0\) to obtain a continuous domain.

A third case occurs when we assume to have no prior knowledge on the alternative class, including its domain, which in general is assumed to be different from that of the target class. In this scenario, two cases should be considered, when a) the domain points of the target class do not belong to the domain of the alternative class, and b) the domain points of the alternative class do not belong to the domain of the alternative class.

Case a) is not problematic, since if we consider \(\{p^1(a)\}\) still uniform but over a larger domain, Lemma 1 still holds, and we still obtain a classifier equivalent to the GLRT-UA. Case b) is instead problematic, since points of the alternative class domain not belonging to the target class will not be explored in the training phase, while they may occur in the training phase. Since the model has not been trained for these points, its behavior is hardly predictable. In this case, we may extend the domain of the artificial dataset over which the uniform samples are generated, to consider possible external points. Again, considering a larger domain for the artificial dataset even beyond the domain of the alternative class does not alter the resulting classifier; however, drawbacks of the domain extensions are the need of generating a larger dataset, a slower convergence rate of the model, and a potentially more complex model (more layers and neurons) to obtain a classifier equivalent to the desired GLRT-UA also for the new input points.

E. On The AE Classifier

AE classifiers have not shown good performance [24] and several patches have been proposed. Here we confirm these deficiencies by the following result that compare the AE classifier to the GLRT-UA.

Theorem 2. The AE classifier is not equivalent to a GLRT-UA, i.e., it will make in general different classifications for the same input.

Proof. It has been shown [25] that any non-linear AE, with enough layers and trained with the MSE loss function, will perform as a three-layer AE with linear activation functions, and the resulting structure only projects the input into a subspace (the latent domain). The GLRT-UA instead performs in general a non-linear transformation of the observation through the PDF \(\{p(\alpha)\}\) (see [13]), thus the AE classifier does not implement (always) the GLRT-UA. Note that an alternative proof the same result was provided also in [3].

V. One-Class Classification With OCLSSVM

The GLRT-UA can also be implemented by the OCLSSVM classifier described in Section [III-D] with a suitable transformation function, as we show in the following Theorem.

**Theorem 3.** Consider an OCLSSVM model using a transformation function that maps different samples of \( D_0 \) into orthonormal vectors, i.e.,

\[
\phi^T(x)\phi(y) = 0, \quad \forall x \neq y, x \in D_0, y \in D_0, \tag{31}
\]

\[
||\phi(x)||^2 = 1, \quad \forall x \in D_0, \tag{32}
\]

Training this model to the global minimum of \( \beta \) and using the resulting model \( \beta \) in the classifier \( \beta \), provides a classifier equivalent to the GLRT, when the target-class dataset is large enough \( (N_0 \to \infty) \).

To prove the theorem, we first consider the following Lemma.

**Lemma 2.** Given a \( \mathbb{R} \to \mathbb{R} \) invertible function \( h(u) \), with \( h(u) \geq 0, \forall u \), and \( h(u) \) invertible. Given two models \( \mu_1(x) \) and \( \mu_2(x) \) satisfying

\[
\mu_1(x) = h(\mu_2(x)), \tag{33}
\]

the classifiers obtained using \( \beta \) with both models are equivalent.

In particular, for any model \( \mu(x) \) satisfying

\[
\mu(x) = h(p_0(x)), \tag{34}
\]

the resulting test is equivalent to GLRT-UA.

**Proof.** From the definition of the decision function \( \beta \), we have

\[
\Delta(\mu_1(x),\delta) = \begin{cases} H_0 & \mu_1(x) > \delta \\ H_1 & \mu_1(x) \leq \delta \end{cases} = \begin{cases} H_0 & h(\mu_2(x)) > \delta \\ H_1 & h(\mu_2(x)) \leq \delta \end{cases} = \Delta(\mu_2(x), h^{-1}(\delta)), \tag{35}
\]

which shows the equivalence of the two classifiers, with suitable selected thresholds. Lastly, when \( \beta \) holds, it yields that the classifier with model \( \mu(x) \) has as equivalent decision function \( \Delta(p_0(x), h^{-1}(\delta)) \), which establishes the equivalence with the GLRT-UA.

We are now ready to prove Theorem 3.

**Proof of Theorem 3.** We consider the modified model \( \tilde{\mu}(x) = \mu(x) - b \), which removes the bias term \( b \), and by Lemma 2 yields an equivalent classifier.

Let \( \tilde{x}_\ell, \ell = 1, \ldots, L \) be the distinct vectors of the dataset \( D_0 \), and let us define the matrix

\[
\Phi_0 = [\phi(\tilde{x}_1), \ldots, \phi(\tilde{x}_L)]. \tag{36}
\]

Let us consider the change of variable from \( w \) to \( \tilde{w} = [\tilde{w}_1, \ldots, \tilde{w}_L]^T \), with

\[
\Phi_0^T \tilde{w} = \tilde{w}. \tag{37}
\]

From the orthonormal condition, the system of equations \( \beta \) is uniquely solvable, thus we can optimize \( \tilde{w} \) to minimize the loss function, instead of optimizing \( w \). To write \( \beta \) as a function of \( \tilde{w} \), first we note that from \( \beta \) we have \( \Phi_0 \Phi_0^T = I \) the identity matrix, and also

\[
w^T = w^T \Phi_0 \Phi_0^T \tilde{w} = \sum_{\ell=1}^L \tilde{w}_\ell. \tag{38}
\]

Then, considering an input \( x \), the error model correction term from \( \beta \) becomes

\[
e_n^2 = [b - w^T \phi(x_n)]^2 \tag{39}
\]

and \( \beta \), becomes

\[
\rho_{\text{OCLSSVM}}(D_0, w, b) = \frac{1}{2} w^T w + \frac{1}{2} C \sum_{n=1}^{N_0} [b - w^T \phi(x_n)]^2. \tag{40}
\]

Lastly, from \( \beta \) and \( \beta \), the objective function becomes (in the new variable \( \tilde{w} \))

\[
\rho_{\text{OCLSSVM}}(D_0, \tilde{w}, b) = \frac{1}{2} \sum_{\ell=1}^L \tilde{w}_\ell^2 + \frac{1}{2} C \sum_{n=1}^{N_0} \left[ b - \tilde{w}(x_n) \right]^2, \tag{41}
\]

where \( \ell(n) \) is the index of the unique vector corresponding to \( x_n \), i.e., \( x_n = \tilde{x}_{\ell(n)} \).

For \( N_0 \to \infty \) we have

\[
\lim_{N_0 \to \infty} \rho_{\text{OCLSSVM}}(D_0, \tilde{w}, b) = \frac{1}{2} \sum_{\ell=1}^L \tilde{w}_\ell^2 + \frac{1}{2} C N_0 \sum_{\ell=1}^L p_0(\tilde{x}_\ell)|b - \tilde{w}_\ell|^2, \tag{42}
\]

and it holds

\[
\lim_{N_0 \to \infty} \rho_{\text{OCLSSVM}}(D_0, \tilde{w}, b) = \frac{1}{2} \sum_{\ell=1}^L \tilde{w}_\ell^2 + \frac{1}{2} C N_0 \sum_{\ell=1}^L p_0(\tilde{x}_\ell)|b^2 + \tilde{w}_\ell^2 - 2b\tilde{w}_\ell|, \tag{43}
\]

Next, we maximize over \( \tilde{w} \) by nulling the derivative of the loss function

\[
\frac{\partial \rho_{\text{OCLSSVM}}(D_0, \tilde{w}, b)}{\partial \tilde{w}_\ell} = 0, \tag{44}
\]

which yields

\[
(1 + C N_0 p_0(\tilde{x}_\ell)) \tilde{w}_\ell - C N_0 b p_0(\tilde{x}_\ell) = 0, \tag{45}
\]

and

\[
\tilde{w}_\ell = \frac{C N_0 b p_0(\tilde{x}_\ell)}{1 + C N_0 p_0(\tilde{x}_\ell)}. \tag{46}
\]

Hence, for any bias value \( \tilde{b} \), such that

\[
\frac{\partial \rho_{\text{OCLSSVM}}(D_0, \tilde{w}, b)}{\partial b} \bigg|_{b=\tilde{b}} = 0, \tag{47}
\]
the resulting model is
\[ \bar{\mu}(x) = \frac{CN_0 \bar{b}_0(x)}{1 + CN_0 \bar{b}_0(x)} \] for \( x = \bar{x}_\ell. \) (47)

From (47) we conclude that \( \bar{\mu}(x) \) is a monotone non-negative function of \( p_0(x) \) and by Lemma 2 the resulting classifier is equivalent to the GLRT-UA.

Note that transformation functions of infinite size are typical of SVM, thanks to the kernel trick [26], by which what matters for the model is the kernel \( k(x, y) = \phi^T(x)\phi(y) \) between samples \( x \) and \( y. \)

As transformation function we can for example consider the following mapping, which is appropriate when the vector samples are taken from a discrete set of \( L \) values, thus also during testing only vectors \( \bar{x}_\ell, \ell = 1, \ldots, L, \) may appear.

Defining the \( L \)-size column vector \( \omega(\ell) \) with entries
\[ [\omega(p)]_i = \begin{cases} 0 & i \neq \ell, \\ 1 & i = \ell, \end{cases} \] a feature-space transformation function satisfying (31) is \( \phi(x) = \omega(\ell). \) In practice, this requires finding all unique sample vectors in the dataset \( D_0 \) and assigning them an integer \( \ell \).

However, we should observe that the practical implementation of the hypothesis of Theorem 3 may be difficult. First, the transformation function (45) strictly depends on the dataset \( D_0 \). In fact, the size of vector \( \phi(x) \) obtained from the transformation grows with the size of the dataset.

Moreover, when the sample space \( \mathcal{X} \) is continuous, an infinite number of the target-class sample vectors appearing in the test phase are not present in the dataset \( D_0 \), making the orthonormal condition problematic. A solution to this problem is to consider a (vector) quantized version of \( \mathcal{X} \), for which the dataset \( D_0 \) of quantized samples from the target class will then sufficiently representative and the hypotheses of Theorem 3 will be satisfied. This problem is left as a subject of future research.

VI. NUMERICAL RESULTS

In this section we assess the performance of the proposed one-class classifiers and compare them with both the AE classifier and the GLRT-UA.

A. Datasets

For training, datasets \( D_0 \) and \( D_1^* \) are used. For testing, the dataset \( T = \{T_0, T_1 \} \) is used, where \( T_i \) is the dataset of samples from class \( \mathcal{H}_i \).

Sample vectors have \( M = 4 \) entries and are acquired by a digital system that clips entries of the vector outside of the range \([-14, 14] \), thus any entry \( m \) such that \( |x|_m > 14 \) is saturated at 14, while entries \( |x|_m < -14 \) are saturated at -14. Let \( A_3 = [-14, 14] \times \cdots \times [-14, 14] \) be the domain of the clipped vectors. Therefore, for the artificial dataset \( D_1^* \), we consider vectors with independent entries uniformly generated in the interval \([-14, 14] \).

As model for the sample vectors, we consider two scenarios: the Gaussian Scenario, and the Mixture Scenario.

Gaussian Scenario: \( x \) has a clipped multivariate Gaussian distribution with unitary variance per entry and independent entries, i.e., for \( i = 0 \) (target class) and \( 1 \) (alternative class), entry \( j \) of sample vector \( x \) has PDF
\[
\begin{align*}
p_i(a_j) &= \begin{cases} f_G(a_j), & a_j \in (-14, 14), \\ \delta_D(a_j = 14) f_{\geq 14} f_G(a_j) & a_j = 14, \\ \delta_D(a_j = -14) f_{\leq -14} f_G(a_j) & a_j = -14, \\ 0, & \text{otherwise}, \end{cases}
\end{align*}
\]
where
\[
f_G(a) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(a - \gamma)^2}{2}}.
\]

\( \delta_D(\cdot) \) is Dirac delta function; for the target class (thus for samples of datasets \( D_0 \) and \( T_0 \) the mean is \( \gamma_0 = 0 \cdot 1_4 \), (here \( 1_4 = [1, 1, 1, 1]^T \)), while for the alternative class in the test phase (dataset \( T_1 \)) is \( \gamma_1 = 3 \cdot 1_4 \). Fig. 1 shows the sampling PDF of the first element of sample vectors, from the testing datasets \( T_0 \) and \( T_1 \), and from the artificial dataset \( D_1^* \).

Mixture Scenario: \( x \) is a mixture of multivariate Gaussian distributions with unitary variance, different numbers of components \( \nu_i \), means \( \{\gamma_{i,m}\}, m = 1, \ldots, \nu_i \), and mixing probabilities \( \{q_{i,m}\} \), i.e., entry \( j \) of sample vector \( x \) has PDF for \( i = 0 \) (target class) and \( 1 \) (alternative class), entry \( j \) of sample vector \( x \):
\[
\begin{align*}
p_i(a_j) &= \begin{cases} f_M(a), & a_j \in (-14, 14), \\ \delta_D(a_j = 14) f_{\geq 14} f_M(a_j) & a_j = 14, \\ \delta_D(a_j = -14) f_{\leq -14} f_M(a_j) & a_j = -14, \\ 0, & \text{otherwise}, \end{cases}
\end{align*}
\]
where
\[
f_M(a) = \frac{1}{\sqrt{2\pi}} \sum_{m=1}^{\nu_i} q_{i,m} e^{-\frac{|a - \gamma_{i,m}|^2}{2}}.
\]
and from the artificial dataset $D$ element of sample vectors, from the testing datasets $T$ for the alternative class we have $25000$ performance is assessed) is performed over a test dataset of the AE. For all approaches, the test phase (from which their classifier. We compare them with the GLRT UA and with SVM classifiers, and the performance of the OCLSSVM.

B. Compared Solutions

We assess the performance of the GLRT-UA-based NN and SVM classifiers, and the performance of the OCLSSVM classifier. We compare them with the GLRT-UA and with the AE. For all approaches, the test phase (from which their performance is assessed) is performed over a test dataset of 25000 samples coming from both the target and the alternative classes. We now detail the parameters used for each classifier.

GLRT-UA-Based NN (GLRT-UA-NN) Classifier: We design the NN with 7 layers with 40, 32, 24, 16, 8, 4, and 1 neurons, respectively; all the neurons have sigmoid activation functions. The training lasted for 5 epochs; the one-class training and validation datasets have 60000 and 15000 samples, respectively. The artificial dataset used for training has 60000 samples.

GLRT-UA-Based LS-SVM (GLRT-UA-LS-SVM) Classifier: As kernel function we use the Gaussian radial basis function having kernel function

$$k(x, y) = e^{-\|x-y\|^2}.$$  

Due to the computational cost of the SVM approach, we used a training dataset containing 5000 samples.

One-class least squares SVM (OCLSSVM) Classifier: The transformation function and the training datasets are those used for the GLRT-UA-LS-SVM classifier. Note that this function does not satisfy the hypothesis of Theorem 3 since we are considering sample vectors in a continuous domain. As for the GLRT-UA-LS-SVM, the (one-class) training dataset contained 5000 samples.

Autoencoder (AE) Classifier: According to the results of [25], it is not restrictive to consider a linear AE, with 4 neurons in both input and output layers, and linear activation functions. In the hidden layer we have instead either $K = 1$, 2, or 3 neurons, still with linear activation functions. Weights are initialized randomly. The model has been trained with 5 epochs and the datasets used for the GLRT-UA-NN classifier.

C. ROC Performance

To evaluate the performance of the classifiers we consider the receiver operating characteristic (ROC) curves, showing the MD probability as a function of the FA probability achieved during the test phase.

Gaussian Scenario: Fig. 3 shows the ROC for the various considered solutions in the Gaussian Scenario. Considering that a classifier is more effective when the ROC is more pushed to lower values (south-west part of the graph), yielding lower MD and FA probabilities, we note that the GLRT-UA-based classifiers perform as the GLRT-UA, as expected. This occurs also for the OCLSSVM classifier, although it is not configured as in the hypotheses of Theorem 3. We also note that the GLRT-UA-based classifiers significantly outperform the AE classifier. The AE classifier performance instead increases as $K$ decreases, achieving more compact latent space. However, even with the smallest value, $K = 1$, the AE classifier is much less accurate than the GLRT-UA-based classifiers, while the AE classifier has a much worse performance.

Mixture Scenario: Fig. 4 shows the ROC for the classifiers and the GLRT-UA in the Mixture Scenario. In this case, all classifiers and the GLRT-UA are better performing than in the Gaussian Scenario, due to the more marked differences between the PDFs of the samples of the two classes. Also in this case, we observe that all GLRT-UA-based classifiers have a similar performance and show a ROC very close to that of the GLRT-UA.

VII. Conclusions

We considered the OCC problem and aimed at identifying classifiers that learn to implement the GLRT-UA, based on the availability of only the target dataset. We have identified three solutions, two are NN and SVM models trained as two-class classifiers using an artificially generated dataset, and the third is the OCLSSVM model with a proper transformation function. We have investigated the conditions under which these models converge to the GLRT-UA, then confirmed by
numerical results on Gaussian and Gaussian mixture datasets. We have also proved that the AE one-class classifier does not converge in general to the GLRT-UA. We conclude that in the considered scenarios, the GLRT-UA-based classifiers outperform the AE classifier, achieving lower MD and FA probabilities.

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