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ABSTRACT

Anomaly detection based on one-class classification algorithms is broadly used in many applied domains like image processing (e.g. detection of whether a patient is "cancerous" or "healthy" from mammography image), network intrusion detection, etc. Performance of an anomaly detection algorithm crucially depends on a kernel, used to measure similarity in a feature space. The standard approaches (e.g. cross-validation) for kernel selection, used in two-class classification problems, can not be used directly due to the specific nature of a data (absence of a second, abnormal, class data). In this paper we generalize several kernel selection methods from binary-class case to the case of one-class classification and perform extensive comparison of these approaches using both synthetic and real-world data.

Keywords: anomaly detection, model selection, one-class classification, SVDD, kernel width, empirical risk

1. INTRODUCTION

In a one-class classification problem statement, it is assumed that we mainly use data of one, normal, class to build a decision function that describes characteristics of the data. On the other hand data of the other abnormal class are either not used at all or used to refine the obtained data description. The one-class classification is broadly applied to many real application domains namely image processing, network intrusion detection, user verification in computer systems, machine fault detection, etc. In most of the real-world applications for one-class classification, the number of normal data samples is much larger than that of abnormal data samples or abnormal samples are even not available at all [1]. The reason is that collecting normal data is inexpensive and easy in comparison to collecting abnormal data. For example in machine fault detection applications, a normal data can be collected directly under the normal condition of a machine while collecting an abnormal data requires observation of machines until they break. Since the prevalence of one class, in a one-class classification, the boundary decision primarily comes from the dominant class compared to a binary classification, where the data of both classes are used to construct the boundary decision.

One of the most popular approaches for one-class classification is based on support vector models. These models have a nice inherited property allowing to build simple linear decision boundaries in highly non-linear infinite-dimensional spaces thanks to the kernel trick. The most wide-spreadly used kernels are Gaussian kernels. Although these techniques became extremely popular in recent years, there still exists an open question of the kernel bandwidth selection, which, as in binary classification, is crucial for model performance. Despite similarity to the binary classification problems, the standard approaches for bandwidth selection, like cross-validation, can not be used for the one-class classification models due to specific nature of the data (absence of second, abnormal, class data).

In this paper we concentrate on Support Vectors Data Description (SVDD) [2] which is a one-class classification algorithm from the family of support vector models. The main difference from a standard one-class SVM is that in a linear case SVDD builds a sphere surface around the normal data instead of a linear hyperplane, separating the normal data from the origin (in a feature space).

Several approaches for kernel selection were proposed in the literature. Some of them are intended for binary classification but can be generalized to the one-class problem, some are specially designed for one-class classification problem. For example, in [3] authors proposed an empirical risk for one-class SVM and proved that under certain conditions it converges to the real risk. Another approach [4] is based on an idea that a kernel width should be selected in such a way that a fraction of outliers and support vectors in the final model should be close to their corresponding theoretical estimates, depending on parameters of the SVDD algorithm. In [5] authors try to optimize the decision region directly in order to get neither too sparse nor too dense area. All the mentioned approaches imply building and comparing several models w.r.t. some criterion, while in [6] a direct optimization method for kernel parameters is proposed without explicit model building.

In this paper we propose an original method for SVDD model selection based on empirical risk approximation using oversampling with SMOTE [7] and develop a methodology for SVDD model selection. Finally, we generalize several kernel selection methods from binary-class case to the case of one-class classification and perform extensive comparison of these approaches using both synthetic and real-world data.

2. ANOMALY DETECTION USING SVDD

We consider Support Vector Data Description (SVDD) proposed in [2] for the one-class classification problem. Let us have a dataset $D = \{X_1, \ldots, X_l\}$, $X_i \in \mathbb{R}^n$. Let $\phi_\gamma(\cdot)$ be some mapping to a high-dimensional space depending on scalar parameter $\gamma \in \mathbb{R}_+$. In this space we solve the following optimization problem:

$$\begin{cases} R^2 + \frac{1}{\nu l} \sum_{i=1}^{l} \xi_i \to \min_{R,a} \\ \|\phi_\gamma(X_i) - a\|^2 \leqslant R^2 + \xi_i & , i = 1, \ldots, l, \\ \xi_i \geqslant 0, & i = 1, \ldots, l. \end{cases} \tag{1}$$

Physical meaning of such an optimization problem statement is that we are looking for a minimum volume ball in high-dimensional space defined by $\phi_\gamma(\cdot)$, containing the dataset. Herewith we allow some points to be outside the boundary of the ball and controll their number by ν. The penalty in (1) is equivalent to l_1 penalty that zeros out some of the parameters. In our case it means that several points will belong exactly to the surface of the ball [2]. We can re-write (1) in dual form and find that a decision function, predicting whether a point is an anomaly or not, is defined through the kernel $K_\gamma(X, X') = \langle \phi_\gamma(X), \phi_\gamma(X') \rangle$ and has the form $f_\gamma(X) = \text{sign} \left(\sum_{i=1}^{l} \alpha_i K_\gamma(X, X_i) - \rho \right)$ for some $\alpha_i \geq 0$ and ρ. A typical example of the kernel we are using is $K_\gamma(X, X') = \exp\left(-\|X - X'\|^2 / \gamma\right)$, $\gamma > 0$.

3. MODEL SELECTION TECHNIQUES

In this section we give brief descriptions of several model selection approaches for SVDD, which are based on optimization of some risk functions.

3.1 Support Vectors and Anomalies Fraction Optimization

Complexity of the model is described by the number of support vectors $X_i \in D$ corresponding to $\alpha_i > 0$. In the original paper [2] authors proved that parameter ν in (1) is an upper bound for the fraction of elements in the train data marked as anomaly (outliers) and a lower bound for the fraction of elements used as support vectors. Let us define the risk function as follows

$$R_\gamma^{\text{SV}} = (\nu - f_{\text{SV},\gamma})^2, \tag{2}$$

where $f_{\text{SV},\gamma}$ is a fraction of support vectors in the dataset, defining the current decision function $f_\gamma(X)$. Minimizing R_γ^{SV} we can balance complexity and classification accuracy on the train set.

3.2 Empirical Risk

Another approach would be to reduce the one-class classification to binary classification [3]. It can be proved that the following empirical risk converges to a real risk of this binary classification problem

$$R_\gamma^{\text{empirical}} = \frac{1}{(1-\nu) \cdot l} \sum_{i=1}^{n} [f_\gamma(X_i) = -1] + \frac{1}{\nu} \mathbb{E}_\mu [f_\gamma(X_i) = 1], \tag{3}$$

where $\mathbb{E}_\mu[f(X_i) = 1]$ denotes average error of classification on anomaly elements assuming that they have distribution μ. This value is estimated using Monte Carlo simulation. Generally, for modeling μ it is reasonable to use a least favorable uniform distribution.

3.3 Risk based on Oversampling

In empirical risk (3) the same dataset is used for a model construction and its risk estimation leading to a biased estimates. That is why for the risk assessment we propose to use sampling based on SMOTE [7], an oversampling technique, designed for the imbalanced binary classification. We define the risk as

$$R_\gamma^{\text{SMOTE}} = \frac{1}{(1-\nu) \cdot m} \sum_{i=1}^{m} \left[f_\gamma(\tilde{X}_i) = -1 \right] + \frac{1}{\nu} \mathbb{E}_\mu [f_\gamma(X_i) = 1] \tag{4}$$

New examples $\tilde{X}_i$ of a normal data are generated synthetically based on the training set and the SMOTE algorithm. The first summand in (4) is proportional to the number of synthetic normal elements marked by the classifier as anomalies. The second summand is the same as in (3).

3.4 Kernel Matrix Optimization

Another popular idea is to optimize a kernel matrix directly without building an anomaly detection model. For example, in [6] a simple statistic was proposed:

$$R_\gamma^{\text{kernel}} = \frac{\bar{k}_\gamma}{s_\gamma^2}, \tag{5}$$

where $\bar{k}_\gamma = \frac{\sum_{i=2}^{n} \sum_{j=i}^{n} K_\gamma(X_i, X_j)}{(n-1)(n-2)}$ and $s_\gamma^2 = \frac{\sum_{i=2}^{n} \sum_{j=i}^{n} (\bar{k}_\gamma - K_\gamma(X_i, X_j))^2}{(n-1)(n-2)}$ are a normalized sum of the kernel matrix elements and a normalized variance of the kernel matrix elements correspondingly.

3.5 Kernel Polarization

Another approach for tuning the kernel matrix is a so-called polarization optimization. It was originally proposed for binary classification problems but can be naturally generalized for one class classification problems [3]. In order to calculate the polarization we generate an artificial anomaly data $\{X_{l+1}, \ldots, X_{2l}\}$ from a uniform distribution. All elements of the initial data set are marked as normal data and finally we have a set of elements (X_i, y_i), $i = 1, \ldots, 2l$, where $y_i = 1$ for $i = 1, \ldots, l$ and $y_i = -1$ for $i = l+1, \ldots, 2l$. The polarization risk is calculated as [11]

$$R_\gamma^{\text{polar}} = -\sum_{i,j=1}^{2l} y_i \cdot K_\gamma(X_i, X_j) \cdot y_j. \tag{6}$$

4. NUMERICAL EXPERIMENTS

In this section we describe our settings for the numerical experiments and provide results of kernel selection techniques comparison.

4.1 Validation Error

The real risk of anomaly detection consists of two parts: misclassification of points from a normal distribution as anomalies and misclassification of abnormal data as a normal.

For measuring the quality of a decision function we will use sum of these errors on independent validation data set normalized by the number of elements. Let $\left\{X_1^{\text{normal}}, \cdots, X_s^{\text{normal}}\right\}$ be the set of normal elements in the validation set and $\left\{X_1^{\text{anomaly}}, \cdots, X_m^{\text{anomaly}}\right\}$ be the set of anomaly elements in the validation set. Then the real risk estimate is calculated as follows:

$$R_\gamma^{\text{val}} = \frac{1}{s} \sum_{i=1}^{s} \left[f_\gamma\left(X_i^{\text{normal}}\right) = -1 \right] + \frac{1}{m} \sum_{j=1}^{m} \left[f_\gamma\left(X_j^{\text{anomaly}}\right) = 1 \right]. \tag{7}$$

The validation risk behavior depends on a dimensionality n of a data. A typical behavior is presented in figure 1a. Generally there is a plateau of almost the same validation error values for some range of $\gamma > 0$.

4.2 Behavior of the Risk Functions

In order to understand a typical behavior of the introduced risk functions we estimate R_γ^{val} of the constructed model for different values of γ and compare it to the estimates of the risks. In these experiments we fix the value of ν to 0.1, meaning that we have 10% of anomalies. We generate 100 points of normal data from a mixture of two 5-dimensional normal distributions with means at $[1,1,1,1,1]^T$ and $[-1,-1,-1,-1,-1]^T$, and identity covariance matrices. Also we generate 100 anomalies from the uniform distribution on $[-5,5]^5$. For the validation a huge dataset from the same distributions is drawn.

Empirical risk (see figure 1b) looks very similar to the validation error, ranges of plateaus mostly coincide. Risk based on SMOTE oversampling (see figure 1c) looks even more similar to the real validation error. But in either cases choosing the minimizer of the risk as an optimal value for γ we obtain similar results. In case of support vectors based risk (see figure 1d) the plateau of the risk is much wider than those of the validation error. The kernel risk (see figure 1e) behaves very smoothly with a single minimum as it was shown in [6] but this mimimum is biased with respect to the optimal value of γ. Finally, the polarization risk (see figure 1f) also gives a single minimum and the optimum value belongs to the plateau of the validation error.

4.3 Distribution of Anomalies

We use a uniform distribution of anomalies when calculating the proposed risk functions. It is natural to test how these risk functions depend on the distribution of anomalies. We use a normal distribution with variance, comparable to

(a) Validation error behavior

(b) Empirical risk

(c) SMOTE risk
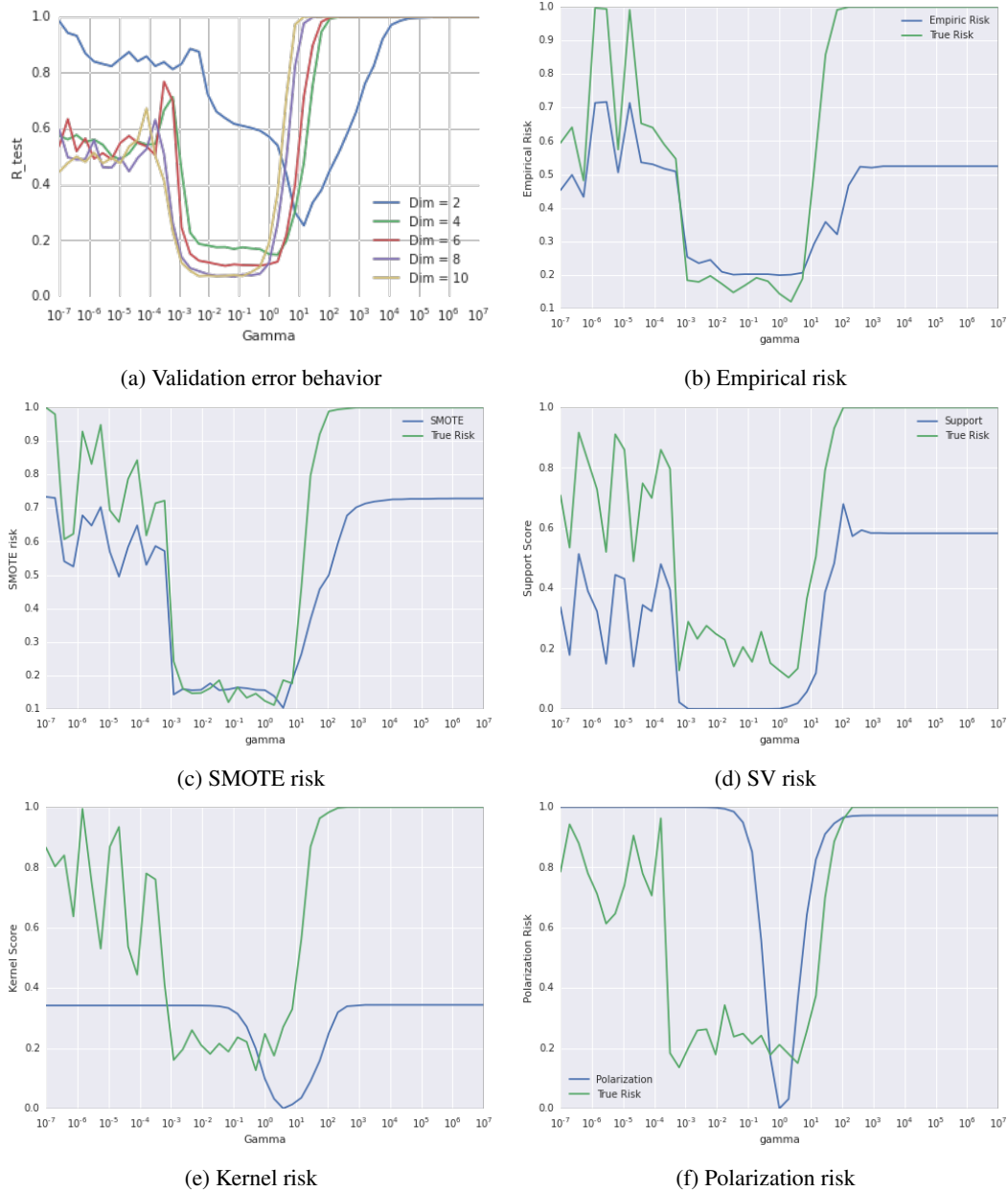
(d) SV risk

(e) Kernel risk

(f) Polarization risk

Figure 1: Dependency of a risk function and a validation error on γ

the range of the normal data, to generate anomalies in the learning data sample. At the same time when estimating risks we use uniformly distributed synthetic anomalies. From figure 2 we see that it is still possible to use uniformly generated synthetic anomalies even if true anomalies are generated from another distribution; and we can select a reasonable γ as the largest value from the plateau of the corresponding risk function.

4.4 Real World Data

Real world data were taken from `http://homepage.tudelft.nl/n9d04/occ/index.html`. These data sets are generated from multi class classification problems like "Iris Dataset", "Sonar", etc. For these problems we considered each class as normal and added anomalies from a uniform distribution to get a one-class classification problem. Borders of the uniform distribution were taken as double borders of the normal class. Number of anomalies were equal to 5%, 10% and 15% of a normal class size. Finally we constructed 96 datasets with smallest value of n equal to 5 and biggest

(a) Empiric risk (b) SMOTE risk

(c) Polarization risk (d) Empiric risk
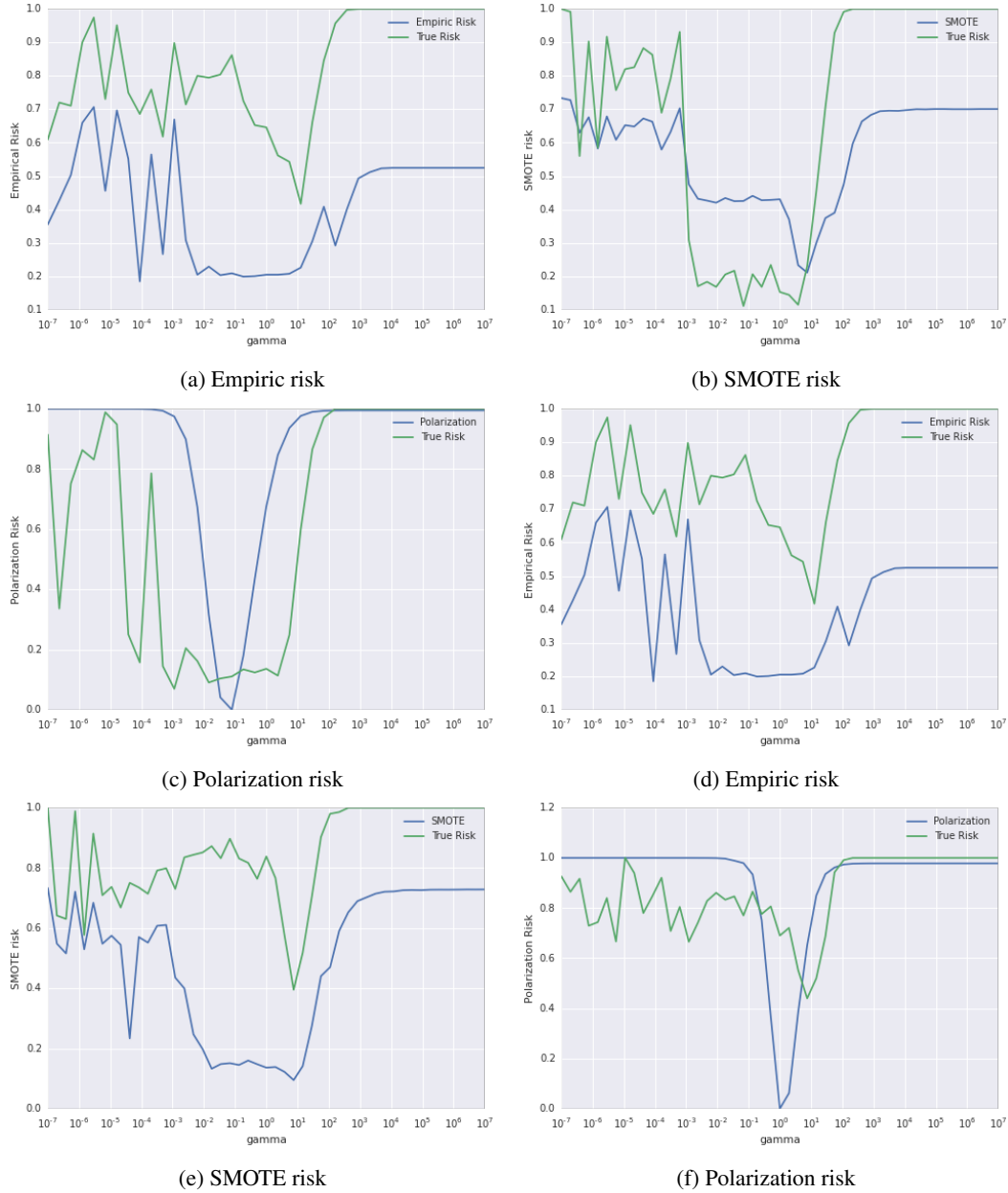
(e) SMOTE risk (f) Polarization risk

Figure 2: Dependency of a risk function and a validation error on γ for a non-uniform anomaly distribution

value of n equal to 1909. For some of the datasets $l \ll n$ (datasets, obtained from "Leukemia" and "Colon" classification problems). For majority of datasets $l \leq 1000$, but also there are several big datasets like those, obtained from "Spam Base" ($l = 4600$) and "Concordia" ($l = 4000$) classification problems. Also there are data sets with a very small l like that obtained from "Leukemia" ($l = 72$) classification problem.

To compare model selection methods on real data we use Dolan-More curves [12] which are built in the following way. Let $\{R_1, \dots, R_K\}$ be the set of considered model selection methods, $\{D_1, \dots, D_M\}$ be the set of tasks (datasets), q_{ti} be the quality of the method i on the dataset t. For each method i we introduce $p_i(\beta)$, a fraction of datasets, on which the method i is worse than the best one not more than β times:

$$p_i(\beta) = \frac{1}{T} \left| \left\{ t : q_{ti} \geq \frac{1}{\beta} \max_i q_{ti} \right\} \right|, \ \beta \geq 1.$$
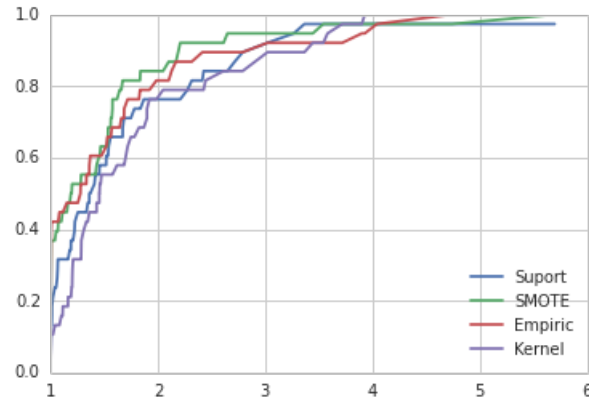
Figure 3: Dolan-More curves for comparison of model selection methods on real data

For example, $p_i(1)$ is a fraction of datasets where the method i is the best. A graph of $p_i(\beta)$ is called Dolan-More curve for the method i. This definition implies that the higher the curve, the better the method. Note that Dolan-More curve for a particular method depends on other methods considered in comparison.

From figure 3 we can see that perfomances of the SMOTE risk and of the Empirical risk are quite similar, but the curve for the SMOTE risk is slightly higher than that for the Empirical risk. The kernel risk and the Support Vectors risk provides worse perfomance.

5. CONCLUSIONS

We considered Support Vectors Data Description as a one-class classification algorithm; generalized several model selection methods from binary classification for SVDD model selection and performed extensive comparison of these approaches using synthetically generated data and real-world data sets.

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