



Two-class support vector data description

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ABSTRACT

Support vector data description (SVDD) is a data description method that can give the target data set a spherically shaped description and be used to outlier detection or classification. In real life the target data set often contains more than one class of objects and each class of objects need to be described and distinguished simultaneously. In this case, traditional SVDD can only give a description for the target data set, regardless of the differences between different target classes in the target data set, or give a description for each class of objects in the target data set. In this paper, an improved support vector data description method named two-class support vector data description (TC-SVDD) is presented. The proposed method can give each class of objects in the target data set a hypersphere-shaped description simultaneously if the target data set contains two classes of objects. The characteristics of the improved support vector data descriptions are discussed. The results of the proposed approach on artificial and actual data show that the proposed method works quite well on the 3-class classification problem with one object class being undersampled severely.

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1. Introduction

In recent years, the problem of data description or one-class classification [1] received a great deal of research. In domain description the task is to give a description of a training set of objects and to detect which (new) objects resemble this training set. This description should cover the class of objects represented by the training set, and ideally should reject all other possible objects in the object space [2].

As a method of data description, the support vector data description (SVDD) proposed by Tax and Duin [2,3] received more attention in recent years. The SVDD was first presented [2] and again with extensions and a more thorough treatment [3]. The boundary function is modeled by a hypersphere, a geometry that can be made less constrained by mapping the data points to a high-dimensional space where the classification is performed. This leads to a methodology known as the kernel trick in statistics and machine learning [4]. Schölkopf et al. [5] proposed a conceptually different approach to one-class classification where a hyperplane was used to separate the target objects from the origin with maximal margin. The solutions were, however, shown to be equivalent to those of the SVDD when radial basis expansions are used. Lee et al. [6] presented an improving

support vector data description using local density degree (D-SVDD); results showed that the D-SVDD had better performance than SVDD and a k-nearest-neighbor data description method. The SVDD was improved by weighing each data point by an estimate of its corresponding density. The density was approximated either by a k-nearest-neighbor or by a Parzen window approach [7]. A boundary method for outlier detection based on support vector domain description was presented [8], which tried to modify the SVDD boundary in order to achieve a tight data description with no need of kernel whitening. With the derivation of the distance between an object and its nearest boundary point in input space, the proposed method could efficiently construct a new decision boundary based on the SVDD boundary. A fuzzy multi-class classifier [9] was presented based on SVDD and improved possibilistic c-means (PCM).

The SVDD has found uses in a wide range of applications. Firstly, SVDD was used for outlier detection to detect uncharacteristic objects from a data set. SVDD was used for anomaly detection in hyperspectral remote sensing imagery [10]. SVDD was also applied to the detection of defects from several datasets of fabric samples with different texture backgrounds [11]. Other applications include pump failure detection [3], face recognition [12,13], speaker recognition [14], image retrieval [15] and medical imaging [16]. Secondly, the SVDD can be used for special classification problems, where one class (outlier class) is severely undersampled, while the other classes are sampled well. We can see that the application of SVDD on outlier detection is essentially

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the same as that on classification problems with one class (outlier class) being severely undersampled. A real example is a machine diagnostics problem [3] in which the current states of a machine are detected. An alarm is raised when the machine shows a problem. Measurements on the normal working conditions of a machine are very cheap and easy to obtain, while the measurements of outliers, which require the destruction of the machine in all possible ways, would be very expensive. However, another similar but more complex machine diagnostics problem is that the current conditions of two different machines are detected only by one computer simultaneously. An alarm is raised when each machine shows a problem and the alarm should also show which machine has a problem. In this case, measurements on the normal working conditions of each of the two machines are very cheap to obtain, while measurements of outliers would be very expensive, which require the destruction of each machine in all possible ways.

The main idea of SVDD is to map the original normal training data both nonlinearly and implicitly into a potentially much higher inner product space or in other words feature space, and to search for a hypersphere with minimal volume containing most of the mapped training data. A new object, which is subjected to the same mapping, is recognized as a target if its image lies inside the hypersphere; otherwise, it is recognized as an outlier. Several key variables such as radius and center of the hypersphere are involved in the search of the hypersphere. The application of SVDD is generally to treat one class of objects as outlying objects, and all other classes of objects as the target set [2,3]. Traditional SVDD can only give a description for the target data set, regardless of the differences of different target classes in the target data set, or for one class of objects in the target data set. However, in real life, the target data set often contains more than one class of objects and each class of objects needs to be described and distinguished simultaneously. For example, in the complex machine diagnostics problem mentioned above, the current conditions of two different machines are examined by one computer synchronously. An alarm is raised when a machine shows a problem and the alarm should show which of the two machines has a problem. In this case, the measurements on the normal working conditions of one machine are regarded as one class of objects in the target data set, while the measurements on the normal working conditions of the other machine are regarded as the other class of objects in the target data set. Because the measurements of outlier class (outliers) would be very expensive, which require the destruction of each machine in all possible ways, we need to give each class of objects in the target data a hypersphere-shaped boundary simultaneously. This way, we can solve the complex machine diagnostics problem.

In this paper, inspired by the idea of SVDD [2,3], we propose an improved support vector data description method. The proposed method can give each class of objects of the target data set a hypersphere-shaped boundary simultaneously, if the target data set contains two classes of objects. Since the proposed method can deal with target training set with two classes of objects, it is called two-class support vector data description (TC-SVDD) compared to the SVDD [2,3]. In this paper, we only consider the case where no negative examples (outliers) are available, the same case of SVDD is called normal data description [3].

The rest of the paper is organized as follows: in Section 2, a brief introduction to SVDD will be presented. The theory of the proposed TC-SVDD will be presented in Section 3. Some characteristics of the proposed method will be discussed in Section 4. Some experiments data are used to show the performance of the proposed method in Section 5. Finally, Section 6 contains some conclusions.

2. Brief introduction to SVDD

The objective of SVDD [2,3] is to find a sphere or domain with minimum volume containing all or most of the data. Let $\{x_i | x_i \in X, i=1, \dots, N\}$ be the given training data set with the data space $X \subset R^d$. Let a and R denote the center and radius of the sphere, respectively. This goal is formulated as a constrained convex optimization problem:

$$\begin{aligned} \min_{R, a, \xi_i} F(R, a, \xi_i) &= R^2 + C \sum_i \xi_i \\ \text{s.t. } \begin{cases} \|x_i - a\|^2 \leq R^2 + \xi_i, & i = 1, \dots, N, \\ \xi_i \geq 0, & i = 1, \dots, N. \end{cases} \end{aligned} \quad (1)$$

where ξ_i is a slack variable that allows the possibility of outliers in the training data set. The parameter C controls the trade-off between the volume and the errors. Constructing the Lagrangian function with Lagrange multipliers α_i, γ_i gives

$$L(R, a, \xi_i, \alpha_i, \gamma_i) = R^2 + C \sum_i \xi_i - \sum_i \alpha_i [R^2 + \xi_i - (x_i - a)^2] - \sum_i \gamma_i \xi_i \quad (2)$$

Setting partial derivatives of R , a and ξ_i to zero gives the constraints

$$\sum_i \alpha_i = 1, \quad a = \sum_i \alpha_i x_i, \quad (3)$$

$$C - \gamma_i - \alpha_i = 0 \Rightarrow 0 \leq \alpha_i \leq C. \quad (4)$$

Substituting (3) into (2) gives the dual problem of (1)

$$\begin{aligned} \max L &= \sum_i \alpha_i (x_i \cdot x_i) - \sum_{i,j} \alpha_i \alpha_j (x_i \cdot x_j) \\ \text{s.t. } \begin{cases} \sum_i \alpha_i = 1, \\ 0 \leq \alpha_i \leq C, \quad i = 1, \dots, N. \end{cases} \end{aligned} \quad (5)$$

where $(x \cdot y)$ is the inner product of x and y .

Solving problem (5) gives a set α_i . A training object x_i and its corresponding α_i satisfy one of the three following conditions [2,3]:

- (i) $\|x_i - a\|^2 < R^2 \Rightarrow \alpha_i = 0$;
- (ii) $\|x_i - a\|^2 = R^2 \Rightarrow 0 < \alpha_i < C$;
- (iii) $\|x_i - a\|^2 > R^2 \Rightarrow \alpha_i = C$.

The objects with the coefficients $\alpha_i > 0$ are called the support vectors. From the above relations we can see only the support vectors are needed in the description of the sphere. The center of the sphere could be calculated by (3). The radius R of the sphere can be obtained by calculating the distance from the center of the sphere to any support vector with $0 < \alpha_i < C$, which provides the sparse representation of the domain description.

To determine whether a test point z is within the sphere, the distance from z to the center of the sphere has to be calculated. A test object z is accepted when this distance is smaller than the radius, i.e.,

$$\|z - a\|^2 = (z \cdot z) - 2 \sum_i \alpha_i (z \cdot x_i) + \sum_{i,j} \alpha_i \alpha_j (x_i \cdot x_j) \leq R^2. \quad (6)$$

The method can be made more flexible [2,3], analogous to [4], i.e., the inner product $(x_i \cdot x_j)$ can be replaced by a new inner product $K(x_i, x_j)$ satisfying Mercer's theorem. An ideal kernel function would map the target data onto a bounded, spherically shaped area in the feature space and outlier objects outside this area. The polynomial kernel and the Gaussian kernel are discussed in [2,3,6].

An example description by SVDD with Gaussian kernel for a 2 dimensional banana shaped data set with two classes of objects

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