Improving support vector data description using local density degree

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Abstract

We propose a new support vector data description (SVDD) incorporating the local density of a training data set by introducing a local density degree for each data point. By using a density-induced distance measure based on the degree, we reformulate a conventional SVDD. Experiments with various real data sets show that the proposed method more accurately describes training data sets than the conventional SVDD in all tested cases.

Keywords: D-SVDD; Support vector data description; One-class classification; Data domain description; Outlier detection

1. Introduction

The purpose of data domain description is to give a compact description of a set of data referred to as target data. It is usually used for outlier detection or a conventional classification problem especially where one of the classes is undersampled [1]. Recently, a support vector data description (SVDD) inspired by support vector machines [2] was invented by Tax and Duin [3]. In a SVDD, the compact description of target data is given as a hypersphere with minimal volume containing most of the data objects in a high-dimensional feature space using some kernel functions [3]. Despite the usefulness of a SVDD [3], the conventional SVDD (C-SVDD) does not take into account the density distribution of a target data set, since, it only considers the small portion of data that lie around the most outer region in a high-dimensional feature space. In many real world problems, however, each target data point may differ in the degree of significance due to its density: the target data in a higher density region are more significant than those in a lower density region in describing a target data set because the data in a higher density region should be included in the compact description than other data. Hence, if all data are treated as equivalent in describing a target data set, without considering such difference in density degree, the solutions are likely to be less optimal.

To address the above problem in the C-SVDD and find a more robust and more reliable description of a target data set, we propose a new SVDD to reflect the different local density of a target data set by introducing the notion of a local density degree for each data point. By using a density-induced distance measure based on the degree, we generalize the C-SVDD. We refer to the proposed method as a density-induced SVDD (D-SVDD).
2. Density-induced support vector data description

2.1. Extraction of local density degree

In this paper, we propose a method to extract a local density degree for each data point from a target data set using a nearest neighborhood approach. Let us calculate a local density degree \( \rho_i \) for a target data point \( \mathbf{x}_i \). By using \( d(\mathbf{x}_i, \mathbf{x}_j^K) \), the distance between \( \mathbf{x}_i \) and \( \mathbf{x}_j^K \) (the \( K \)th nearest neighborhood of \( \mathbf{x}_j \)), and the mean distance of \( K \)th nearest neighborhoods of all target data, \( \text{MEAN}^{K} \), the local density degree \( \rho_i > 0 \) for \( \mathbf{x}_i \) is defined by

\[
\rho_i = \exp \left( \omega \times \frac{\text{MEAN}^K}{d(\mathbf{x}_i, \mathbf{x}_j^K)} \right), \quad i = 1, \ldots, n,
\]

where \( \text{MEAN}^K = \langle 1/n \rangle \sum_{i=1}^n d(\mathbf{x}_i, \mathbf{x}_j^K) \), \( n \) is the number of data in a target class, and \( 0 \leq \omega \leq 1 \) is a weighting factor. Note that this method reports higher local density degree \( \rho_i \) for the data in a higher density region: the data with lower \( \rho_i \) values. Moreover, a bigger \( \omega \) produces higher local density degrees.

To incorporate the density degrees into search of the optimal description in a SVDD, we introduce a new geometric distance called a density-induced distance. Suppose each target data point can be expressed as \((\mathbf{x}_i, \rho_i)\). We define a density-induced distance, \( \delta_i \), between \( \mathbf{x}_i \) and the center of a hypersphere \((\mathbf{a}, R)\) as

\[
\delta_i = \left( \rho_i (\mathbf{x}_i - \mathbf{a}) \cdot (\mathbf{x}_i - \mathbf{a}) \right)^{1/2},
\]

where \( \mathbf{a} \) and \( R \) are the center and the radius of the hypersphere, respectively. Note that \( \delta_i \) increases with increasing \( \rho_i \). Hence, to enclose the data point with increased \( \delta_i \) owing to higher local density degree \( \rho_i \), the radius of a minimum-sized hypersphere should be increased; the data point with higher density degree has stronger influence on the search of the minimum-sized hypersphere.

2.2. Mathematical formulation

We first find a hyperspherical model \((\mathbf{a}, R)\) which gives a closed boundary around target data with no training error with regard to the density-induced distance. By minimizing \( R \), we find the optimal hypersphere which includes all the target data. Then, we can obtain the optimal hypersphere \((\mathbf{a}^*, R^*)\) by minimizing the objective function \( O(\mathbf{a}, R) \):

\[
O = R^2 \quad \text{subject to} \quad \rho_i (\mathbf{x}_i - \mathbf{a}) \cdot (\mathbf{x}_i - \mathbf{a}) \leq R^2, \quad i = 1, \ldots, n.
\]

To allow the possibility of training error, and therefore to make the model more robust, the density-induced distance between each target data \( \mathbf{x}_i \) and the center \( \mathbf{a} \) does not have to be strictly smaller than \( R \), but data points with distance larger than \( R \) should be penalized. We handle this case using a slack variable \( \zeta_i \geq 0 \) which is the distance between the boundary \( \Omega \) and \( \mathbf{x}_i \) outside \( \Omega \). Using the slack variable for each target data point, we change the objective function in Eq. (3) into

\[
O = R^2 + C \sum_{i=1}^n \zeta_i \quad \text{subject to} \quad \rho_i (\mathbf{x}_i - \mathbf{a}) \cdot (\mathbf{x}_i - \mathbf{a}) \leq R^2 + \zeta_i, \quad \zeta_i \geq 0, \quad i = 1, \ldots, n,
\]

where \( C > 0 \) is a control parameter which gives the trade-off between the volume of the description and the training errors. Note that \( \zeta_i \) plays a similar role with the slack variable in the C-SVDD [3], but it has a different meaning. \( \zeta_i \) equals \( \delta_i^2 - R^2 \) for a training error data point, otherwise it is 0. It implies that \( \zeta_i \) also contains the information of local density.

Minimizing Eq. (4) is an optimization problem. Therefore by introducing Lagrange multipliers, we can construct the Lagrangian:

\[
L(\mathbf{R}, \mathbf{a}, \mathbf{\zeta}, \alpha, \beta) = R^2 + C \sum_{i=1}^n \zeta_i - \sum_{i=1}^n \alpha_i \left( R^2 + \zeta_i \right) - \sum_{i=1}^n \beta_i \zeta_i,
\]

where \( \alpha_i \geq 0 \) and \( \beta_i \geq 0 \) are Lagrange multipliers, from which we can derive the following conditions at the solution point:

\[
\sum_{i=1}^n \alpha_i = 1, \quad \mathbf{a} = \frac{1}{T} \sum_{i=1}^n \alpha_i \rho_i \mathbf{x}_i, \quad T = \sum_{i=1}^n \alpha_i \rho_i, \quad \beta_i = C - \alpha_i.
\]

Combining the conditions with Eq. (5), we obtain the dual representation of the optimization problem: maximize \( D(\mathbf{\alpha}) \)

\[
D(\mathbf{\alpha}) = \sum_{i=1}^n \alpha_i \rho_i \mathbf{x}_i \cdot \mathbf{x}_i - \frac{1}{T} \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \rho_i \rho_j \mathbf{x}_i \cdot \mathbf{x}_j
\]

subject to \( \sum_{i=1}^n \alpha_i = 1 \), \( 0 \leq \alpha_i \leq C \), \( T = \sum_{i=1}^n \alpha_i \rho_i \), \( i = 1, \ldots, n \). Note that the dual form for this case has only the Lagrange multiplier \( \alpha_i \); other variables and Lagrange multiplier \( \beta_i \) have disappeared. Furthermore, when \( \rho_i = 1 \), this dual representation is equivalent to the formalism of a C-SVDD [3]. Thus, this proposed method is a general extension of the C-SVDD.

This dual representation is a linear constrained optimization problem; hence we can derive the \( \mathbf{\hat{x}}_g \) that satisfies the Eq. (7). After solving Eq. (7), we can derive the \( \mathbf{a}^* \) and the \( R^* \) of the solution of the problem from Eqs. (6) and (4), respectively. Unlike in the C-SVDD [1], \( \mathbf{a}^* \) is weighted by the local density degree \( \rho_i \). The center of the optimal hypersphere is shifted to a higher density region. Using a
As seen in Eqs. (7) and (8), the dual form of the objective function for the D-SVDD is

\[
I(\mathbf{x}_t) = \left( \mathbf{x}_t \cdot \mathbf{x}_t - \frac{2}{T} \sum_{i=1}^{n} \rho_i \mathbf{z}_i \mathbf{x}_t \cdot \mathbf{x}_i \right) - \frac{1}{T^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \rho_i \rho_j \mathbf{z}_i \mathbf{z}_j \mathbf{x}_i \cdot \mathbf{x}_j \leq R^2^2. \tag{8}
\]

As seen in Eqs. (7) and (8), the dual form of the objective function and the decision function of the D-SVDD are represented entirely in terms of inner products of pairs of target data points. Thus, we can kernelize the D-SVDD for flexible description. The kernelized version of the decision function for the D-SVDD is

\[
f(\mathbf{x}_t) = I(\mathbf{x}_t, \mathbf{x}_t) - \frac{2}{T} \sum_{i=1}^{n} \rho_i \mathbf{z}_i K(\mathbf{x}_t, \mathbf{x}_i) - \frac{1}{T^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \rho_i \rho_j \mathbf{z}_i \mathbf{z}_j K(\mathbf{x}_i, \mathbf{x}_j) \leq R^2^2. \tag{9}
\]

where \(K(\cdot, \cdot)\) is a kernel function [2].

### 3. Experiments and conclusion

To investigate the success of these attempts, we conducted various tests in which three versions of the C-SVDD and three versions of the proposed method were applied to IRIS [4], and LEUKEMIA [5]. Two polynomial kernel functions and a Gaussian kernel function were used for flexible description [2]. The model parameters were found by cross validation to identify optimal solutions of the C-SVDD. The same parameter set with the C-SVDD and \(K = 3\) in Eq. (1) were used for the proposed method. We conducted the same experiments with two versions of a \(k\)-nearest-neighbor data description method [1], \(k\)-NNDD.

The average error rates of prediction accuracies of ten independent runs for the data sets are given in Table 1. The label of a target data class is indicated in the first column; the data in other classes are the candidates of negative data that should not be included in a target data description. For the IRIS data set, the two versions of the \(k\)-NNDD method showed 4.20 and 6.73% average error rates when the label of a target class is 0. For the same data sets, the C-SVDD showed 3.40, 31.33 and 3.47% error rates for each version. The proposed D-SVDD method, however, showed 2.80, 2.93 and 0.42% error rates. That is the D-SVDD improved the C-SVDD in all versions used, and the D-SVDD with a Gaussian kernel function had the best performance. Moreover, when a degree-5 polynomial kernel function was used, the performance of the D-SVDD was not severely deteriorated, which is not the case with the C-SVDD because the results of the C-SVDD with a higher degree of a polynomial kernel are dominantly determined by the data with larger norms [3]. Similar results were obtained for the LEUKEMIA data set. For the LEUKEMIA data set, the D-SVDD method had 6.05% error rate whereas the error rates with the C-SVDD and the \(k\)-NNDD method were respectively 18.68 and 18.03% when a Gaussian kernel function was used or \(k = 3\) was used. From these results, we draw a conclusion that the proposed method showed better prediction accuracies than the C-SVDD for all the data sets used regardless of the type of kernel functions. Moreover, the best performance was obtained when the D-SVDD with a Gaussian kernel function was used.

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Table 1

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<th>Class no.</th>
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References