Abstract

Support Vector Data Description (SVDD) is a machine-learning technique used for single-class classification and outlier detection. SVDD formulation with kernel function provides a flexible boundary around data. The value of kernel function parameters affects the nature of the data boundary. For example, it is observed that with a Gaussian kernel, as the value of kernel bandwidth is lowered, the data boundary changes from spherical to wiggly. The spherical data boundary leads to underfitting, and an extremely wiggly data boundary leads to overfitting. In this paper, we propose empirical criterion to obtain good values of the Gaussian kernel bandwidth parameter. This criterion provides a smooth boundary that captures the essential geometric features of the data.

1. Introduction

Support Vector Data Description (SVDD) is a machine-learning technique used for single-class classification and outlier detection. SVDD is similar to Support Vector Machines and was first introduced by Tax and Duin (Tax & Duin, 2004). It can be used to build a flexible boundary around single-class data. The data boundary is characterized by observations designated as support vectors. SVDD is used in domains where the majority of data belongs to a single class. Several researchers have proposed use of SVDD for multivariate process control (Sukchotrat et al., 2009; Camci & Chinnam, 2008). Other applications of SVDD involve machine condition monitoring (Widodo & Yang, 2007; Ypma et al., 1999) and image classification (Sanchez-Hernandez et al., 2007).

1.1. Mathematical Formulation

Normal Data Description:
The SVDD model for normal data description builds a minimum radius hypersphere around the data.

Primal Form:
Objective Function:

\[
\min R^2 + C \sum_{i=1}^{n} \xi_i,
\]

subject to:

\[
\|x_i - a\|^2 \leq R^2 + \xi_i, \forall i = 1, \ldots, n, \quad (2)
\]

\[
\xi_i \geq 0, \forall i = 1, \ldots n. \quad (3)
\]

where:
\(x_i \in \mathbb{R}^m, i = 1, \ldots, n\) represents the training data, 
\(R : \) radius, represents the decision variable,
\( \xi_i \) : is the slack for each variable,
\( \alpha \) : is the center, a decision variable,
\( C = \frac{1}{\alpha \tau} \) : is the penalty constant that controls the trade-off between the volume and the errors, and,
\( f \) : is the expected outlier fraction.

**Dual Form:**
The dual formulation is obtained using the Lagrange multipliers.

**Objective Function:**

\[
\max \sum_{i=1}^{n} \alpha_i (x_i, x_i) - \sum_{i,j} \alpha_i \alpha_j (x_i, x_j), \tag{4}
\]

subject to:

\[
\sum_{i=1}^{n} \alpha_i = 1, \tag{5}
\]

\[
0 \leq \alpha_i \leq C, \forall i = 1, \ldots, n. \tag{6}
\]

where:
\( \alpha_i \in \mathbb{R} \): are the Lagrange constants,
\( C = \frac{1}{\alpha \tau} \) : is the penalty constant.

**Duality Information:**
Depending upon the position of the observation, the following results hold good:

**Center Position:**

\[
\sum_{i=1}^{n} \alpha_i x_i = a. \tag{7}
\]

**Inside Position:**

\[
\|x_i - a\| < R \rightarrow \alpha_i = 0. \tag{8}
\]

**Boundary Position:**

\[
\|x_i - a\| = R \rightarrow 0 < \alpha_i < C. \tag{9}
\]

**Outside Position:**

\[
\|x_i - a\| > R \rightarrow \alpha_i = C. \tag{10}
\]

The radius of the hypersphere is calculated as follows:

\[
R^2 = (x_k, x_k) - 2 \sum_i \alpha_i (x_i, x_k) + \sum_{i,j} \alpha_i \alpha_j (x_i, x_j). \tag{11}
\]

\( \forall x_k \in SV_{<C} \), where \( SV_{<C} \) is the set of support vectors that have \( \alpha_k < C \).

**Scoring:**
For each observation \( z \) in the scoring data set, the distance \( dist^2(z) \) is calculated as follows:

\[
dist^2(z) = (z, z) - 2 \sum_i \alpha_i (x_i, z) + \sum_i \alpha_i \alpha_j (x_i, x_j). \tag{12}
\]

The scoring dataset points with \( dist^2(z) > R^2 \) are designated as outliers.

The circular data boundary can include a significant amount of space with a very sparse distribution of training observations. Scoring with this model can increase the probability of false positives. Hence, instead of a circular shape, a compact bounded outline around the data is often desired. Such an outline should approximate the shape of the single-class training data. This is possible with the use of kernel functions.

**Flexible Data Description:**
The Support Vector Data Description is made flexible by replacing the inner product \( (x_i, x_j) \) with a suitable kernel function \( K(x_i, x_j) \). The Gaussian kernel function used in this paper is defined as:

\[
K(x_i, x_j) = \exp \left(-\frac{\|x_i - x_j\|^2}{2s^2}\right) \tag{13}
\]

where \( s \): Gaussian bandwidth parameter.

The modified mathematical formulation of SVDD with kernel function is as follows:

**Objective function:**

\[
\max \sum_{i=1}^{n} \alpha_i K(x_i, x_i) - \sum_{i,j} \alpha_i \alpha_j K(x_i, x_j), \tag{14}
\]

Subject to:

\[
\sum_{i=1}^{n} \alpha_i = 1, \tag{15}
\]

\[
0 \leq \alpha_i \leq C, \forall i = 1, \ldots, n. \tag{16}
\]

The results 7 through 10 hold good when the kernel function is used in the mathematical formulation.

The threshold \( R^2 \) is calculated as:

\[
R^2 = K(x_k, x_k) - 2 \sum_i \alpha_i K(x_i, x_k) + \sum_{i,j} \alpha_i \alpha_j K(x_i, x_j) \tag{17}
\]

\( \forall x_k \in SV_{<C} \), where \( SV_{<C} \) is the set of support vectors that have \( \alpha_k < C \).

**Scoring:**
For each observation \( z \) in the scoring dataset, the distance \( dist^2(z) \) is calculated as follows:

\[
dist^2(z) = K(z, z) - 2 \sum_i \alpha_i K(x_i, z) + \sum_i \alpha_i \alpha_j K(x_i, x_j). \tag{18}
\]

The scoring dataset points with \( dist^2(z) > R^2 \) are designated as outliers.
1.2. Importance of Kernel Bandwidth Value

The flexible data description is preferred when the data boundary needs to closely follow the shape of the data. The tightness of the boundary is a function of the number of support vectors. In the case of a Gaussian kernel, it is observed that if the value of outlier fraction $f$ is kept constant, the number of support vectors identified by the SVDD algorithm is a function of the Gaussian bandwidth parameter $s$. At a very low value of $s$, the number of support vectors is very high, approaching the number of observations. As the value of $s$ increases, the number of support vectors reduces. It is also observed that at lower values of $s$, the data boundary is extremely wiggly. As $s$ is increased, the data boundary becomes less wiggly, and it starts to follow shape of the data. At higher values of $s$, the data boundary starts becoming spherical. The selection of an appropriate value of $s$ is tricky and often involves experimenting with several values till a good data boundary is obtained. This paper provides an empirical criterion for selecting a good value of the Gaussian kernel bandwidth parameter. The corresponding data boundary is smooth and captures essential visual features of the data.

The rest of the paper is organized as follows. Section 2 illustrates how data boundary changes with $s$ using two-variable datasets of known geometry. The empirical criterion for selecting a good value of $s$ is introduced and validated. Section 3 provides analysis of real-life data using the proposed method. A review of related work and comparison with existing methods are provided in Section 4. Finally, conclusions and areas for further research are provided in Section 5.

2. Peak Criterion

We experimented with several two-dimensional datasets of known geometry to understand the relationship between a data boundary and the bandwidth parameter. We considered the data boundary to be of good quality if it closely followed the contours of the data shape. We noticed that the objective function value at optimality is a function of the value of the Gaussian bandwidth parameter $s$. More importantly, we observed that values of $s$ that provide a good data boundary. And they are the first critical points of the first derivative of optimal objective function value with respect to $s$ i.e. the points where the second derivative is zero. The criterion of selecting an appropriate value of $s$ based on the value of the second derivative of the optimal objective function value with respect to $s$ is termed the Peak criterion. In this paper, the first and second derivative values are computed using the method of finite differences. We are not making any statement about the presence of an analytical derivative of the optimal objective function value as a function of $s$.

As mentioned in the preceding paragraph, we experimented with several data sets of known geometry. Out of all data sets, we selected the results for banana-shaped, star-shaped, and a dataset with three non-overlapping clusters to present in this paper. The experimental approach and results are first explained in detail with the example of banana-shaped data. It is followed by the results obtained for the star-shaped and three-cluster data.

We created a two-dimensional banana-shaped data with 267 observations. The majority of the observations in this data belong to a single class, with very few outliers (fraction outliers, $f=0.001$). Figure 2(a) provides a scatter plot of the data. For our experimentation, we looked at the plot of number of support vectors against $s$ as shown in figure 1 to decide the range of values of $s$. At low values of $s$, majority of 267 observations are identified as support vectors. As $s$ increased, the number of support vectors generally decreased. For all values of $s$ beyond 5, the number of support vectors remained constant at 3. We trained the data with the SVDD algorithm for different values of $s$ in the range from 0.0001 to 8.0 in the increments of 0.05, keeping $f$ constant at 0.001. This range of values for $s$ ensured that we covered all possible number of support vectors, which can define the data boundary.

At $s = 0.1$, each point in the data was identified as a support vector, representing a very wiggly boundary around the data. As the value of $s$ increased from 0.1 to 0.6, the data boundary was still wiggly, with many “inside” points identified as the support vectors. A very well defined boundary around the data was first observed at $s=0.7$. As $s$ increased from 0.7 to 1.0, the boundary continued to conform to the banana shape, with the number of support vectors dropping from 44 to 32. Beyond $s=1$, as the number of support vectors decreased, the boundary started losing its true banana shape. At higher values of $s$, at and above 4, the support vectors enveloped on the outer parabola of the banana shape. To confirm the shape of the data boundary, we scored each training result on a 200x200 point data grid.

Figure 1. Number of support vectors vs. $s$: banana-shaped data
Scoring results for select values of $s$ are provided in Figure 2.

Figure 3 shows the value of dual objective function (refer to equation 14) and the first derivative of the optimal objective function value with respect to $s$, both plotted against $s$. The optimal value of the objective function is a decreasing function of $s$. As $s$ increases, the first derivative of the optimal objective function value first decreases. It remains relatively flat between $s=0.4$ to $s=0.8$, indicating the first range of values of $s$ which includes critical points of the first derivative. After $s=0.8$, the first derivative starts to increase again.

Figure 4 shows the value of the second derivative of optimal value of the objective function, with respect to $s$ plotted against $s$. At $s=0.20$, the second derivative value is -0.20. As $s$ increases, the value of the second derivative starts increasing. Between $s=0.5$ and 0.85, the second derivative was close to zero for the first time. We observed that the value(s) of $s$, between 0.5 and 0.85, provided a data boundary of good quality. The interval $[0.5, 0.85]$ appears to form a set of critical points. The data boundary using $s=0.7$ is shown in figure 2(c). This data boundary obtained using $s=0.7$ captures the essential geometric properties of the banana-shaped data as compared to any other values of $s$ outside the $[0.5, 0.85]$ interval and this value of $s$ is from the first set of critical points.

To decide if the value of the second derivative is zero, we fitted a penalized B-spline to the second derivative using the TRANSREG procedure available in the SAS software (SAS, 2015). If the 95% confidence interval of the fitted value of second derivative contained zero, we would consider that second derivative value as zero.

We performed similar experimentation using star-shaped data and the data set with three distinct clusters. The three cluster data was obtained from the SAS/STAT User’s guide (SAS, 2015). Figure 5(a) shows the scatter plot of data containing three distinct clusters.

Similar to banana-shaped data, we trained the three-cluster dataset using different values of $s$ from 0.001 to 8 in increments of 0.05. Scoring was performed on a 200x200 data point grid to confirm the shape of the data boundary. Scoring results for select values of $s$ are provided in figure 5.

Figure 6 shows the second derivative of the optimal value of the objective function with respect to $s$ against $s$ for three-cluster data. The results are similar to the banana-shaped data. Between $s=0.95$ and 1.25, the second derivative was close to zero for the first time. We observed that the value(s) of $s$ between 0.95 and 1.25 provided a data boundary of good quality. The interval $[0.95, 1.25]$ appears to form a set of critical points.

Figure 2. Data boundary for banana-shaped data. Fig (b) thru (d) show results of scoring on a 200x200 data grid. Light gray color indicates outside points, dark gray color indicates inside points and black color indicates support vectors.
Kernel bandwidth selection for SVDD

Figure 3. Objective function value and first difference for banana-shaped data

Figure 4. Penalized B-spline fit for second derivative: star-shaped data

to form a set of critical points. The data boundary using $s=1.1$ is shown in Figure 5(c). This data boundary obtained using $s=1.1$ captures the essential geometric properties of the three-cluster data as compared to any other values of $s$ outside the [0.9, 1.25] interval and this value of $s$ is the first set of critical points.

Next, we conducted our experiments with the star-shaped data. Figure 7(a) shows the corresponding scatter plot. The star-shaped dataset was trained using different values of $s$ from 0.001 to 8 in the increments of 0.05. Scoring was performed on a 200x200 data point grid to confirm the shape of data boundary. Scoring results for select values of $s$ are provided in Figure 7.

Figure 8 shows the second derivative of optimal value of objective function with respect to $s$ against $s$ for the star-shaped data. At $s=0.9$, the second derivative was close to zero for the first time. A data boundary of good quality was observed at $s=0.9$, as shown in figure 7 (b). The point $s=0.9$ is a critical point. The data boundary obtained using $s=0.9$ captures the essential geometric properties of the star-shaped data as compared to any other values of $s$ and this value of $s$ is from the first critical point.

Figure 5. Data boundary for three-cluster data. Fig (b) thru (d) show results of scoring on a 200x200 data grid. Light gray color indicates outside points, dark gray color indicates inside points and black color indicates support vectors.
We tried our analysis on data sets with diverse geometrical shapes. For all data sets, the fact that a good quality data boundary can be obtained using value of $s$ from the first set of critical points, provides the empirical basis for our method.

3. Case Study: Analysis of Shuttle Data

Section 2 provided values of $s$ using the Peak criterion for different two-dimensional data sets. For such data sets a good value of $s$ can be visually judged. Next, we wanted to test Peak criterion with high dimensional datasets, where visual feedback about a good value of $s$ is not possible. We also compared if values of $s$ obtained using Peak criterion are consistent with values of $s$ obtained using an unrelated criterion, such as the $F_1$-measure. In this section we provide results of our experiments with higher dimensional Statlog (shuttle) dataset (Lichman, 2013). The data consists of nine numeric attributes and one class attribute. Out of 58,000 total observations, 80% of the observations belong to class one. A random sample of 2000 observations belonging to class one, was selected for training. Scoring was performed to determine if the model could accurately classify an observation as belonging to class one. The SVDD model was trained and subsequently scored for values of $s$ ranging from 1 to 100 in increments of 1. For each value of $s$ the model performance was quantified using the $F_1$-measure (Zhuang & Dai, 2006).

The $F_1$-measure is defined as follows:

$$F_1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}},$$

(19)

where:

$$\text{Precision} = \frac{\text{true positives}}{\text{true positives} + \text{false positives}},$$

(20)

$$\text{Recall} = \frac{\text{true positives}}{\text{true positives} + \text{false negatives}}.$$  

(21)

Figure 7. Data boundary for star-shaped data. Fig (b) thru (d) show results of scoring on a 200x200 data grid. Light gray color indicates outside points, dark gray color indicates inside points and black color indicates support vectors.
We chose the $F_1$-measure because it is a composite measure that takes into account both the Precision and the Recall. Models with higher values of $F_1$-measure provide a better fit. The $F_1$-measure can be used independently to choose a good value of $s$.

The plot of the $F_1$-measure against a value of $s$ is shown in Figure 9. A maximum value of $F_1$-measure is obtained at $s=17$. Also, the value of $F_1$-measure is very close to the maximum value around $s=17$. Figure 10 shows the plot of the second derivative of optimal value of objective function with respect to $s$ plotted against $s$ for the shuttle data. The values of $s$ between 13 and 20, where the second derivative is nearly zero represents the first set of critical points. The fact that value of $s=17$ obtained using the $F_1$-measure belongs to the set $[13,20]$, obtained by the Peak criterion, provides the empirical evidence that Peak criterion works successfully with higher dimensional data.

4. Related Work

In support vector machines, cross-validation is a widely used technique for selecting the Gaussian bandwidth parameter (Hastie et al., 2009). Cross-validation requires training data that belongs to multiple classes. Hence, unless a good sample for normal class and outlier class is available, cross-validation is not a feasible technique for selecting Gaussian bandwidth parameter value in SVDD. The Peak criterion is an unsupervised method that works on single class data. In this section, performance of the Peak criterion is compared against unsupervised methods for selecting Gaussian bandwidth parameter value published in the literature.

**Method of Coefficient of Variation (CV) (Evangelista et al., 2007):**

Selects a value of $s$ that maximizes the coefficient of variation of the kernel matrix.

$$CV = \frac{\text{Var}}{\text{Mean} + \epsilon}$$

where:

- $\text{Var}$ and $\text{Mean}$ are variance and mean of the non-diagonal entries of the kernel matrix,
- $\epsilon$ is a small value to protect against division by zero or round-off error. In our CV method computations, we set the value of $\epsilon$ to 0.000001.

**Method of Maximum Distance (MD) (Khazai et al., 2011):**

Obtains a value of $s$ based on maximum distance between any pair of points in the training data.

$$s = \frac{d_{\text{max}}}{\sqrt{-\ln(\delta)}}$$

where:

- $d_{\text{max}} = \max\|x_i - x_j\|^2$: maximum distance between any two pairs of points,
- $\delta = \frac{1}{n(1-f) + 1}$,
- $n$ : Number of observation in training data,
- $f$ : the expected outlier fraction. In our MD method computations, we set the value of $f$ to 0.001
Method of Distance to the Farthest Neighbor (DFN) (Xiao et al., 2014):

Uses distances of the training data points to their farthest neighbors and distances to their nearest neighbors. The optimal value of $s$ is obtained by maximizing the following objective function:

$$f_0(s) = \frac{2}{n} \sum_{i=1}^{n} \max_{j \neq i} k(x_i, x_j) - \frac{2}{n} \sum_{i=1}^{n} \min_j k(x_i, x_j).$$

(24)

where:

- $n$: number of observations in training data,
- $k(x_i, x_j)$: kernel distance between observations $i$ and $j$,

We calculated the values of $s$ for the banana-shaped, three-cluster, and star-shaped data using the CV, MD and DFN method. Table 1 summarizes these results and also provides the value of $s$ obtained using the Peak criteria.

The scoring results using values of $s$ recommended by above methods are illustrated in Figure 11, Figure 12 and Figure 13. For all three datasets, when compared against existing methods, the Peak criterion clearly provides a data boundary of best quality. The method of Coefficient of Variation also provides a data boundary of fairly good quality.

| Data      | CV   | MD   | DFN  | Peak         |
|-----------|------|------|------|--------------|
| Banana    | 0.5  | 46   | 2.4  | 0.5 to 0.85  |
| Three-cluster | 0.2  | 77   | 2.55 | 0.95 to 1.25 |
| Star      | 0.5  | 35   | 1.7  | 0.9          |

Table 1. Comparison of $s$ value

5. Conclusions

A criterion for selecting the value of Gaussian kernel bandwidth parameter $s$ is proposed in this paper. Good quality data boundary that closely follows data shape can be obtained at values of $s$ where the second derivative of optimal dual objective function value with respect to $s$ first reaches zero. For certain data sets, the method provides a range of values where this criterion holds good. Any value of $s$ within this range provides a good data boundary. Starting with a very low value of $s$, the search for a good value of $s$ can be abandoned once the second derivative of the optimal objective function reaches zero. As outlined in Section 4, the proposed method provides better results compared to existing methods. The criterion also provides good results when used for high dimensional data.
Kernel bandwidth selection for SVDD

(a) Original data

(b) CV

(c) MD

(d) DFN

(e) Peak

Figure 13. Star-shaped data

References

Camci, Fatih and Chinnam, Ratna Babu. General support vector representation machine for one-class classification of non-stationary classes. *Pattern Recognition*, 41 (10):3021–3034, 2008.

Evangelista, Paul F, Embrechts, Mark J, and Szymanski, Boleslaw K. Some properties of the gaussian kernel for one class learning. In *Artificial Neural Networks–ICANN 2007*, pp. 269–278. Springer, 2007.

Hastie, Trevor, Tibshirani, Robert, and Friedman, Jerome. *Unsupervised learning*. Springer, 2009.

Khazai, Safa, Homayouni, Saeid, Safari, Abdolreza, and Mojaradi, Barat. Anomaly detection in hyperspectral images based on an adaptive support vector method. *Geoscience and Remote Sensing Letters, IEEE*, 8(4):646–650, 2011.

Lichman, M. UCI machine learning repository, 2013. URL http://archive.ics.uci.edu/ml.

Sanchez-Hernandez, Carolina, Boyd, Doreen S, and Foody, Giles M. One-class classification for mapping a specific land-cover class: Svd classification of fenland. *Geoscience and Remote Sensing, IEEE Transactions on*, 45 (4):1061–1073, 2007.

SAS/STAT 14.1 user’s guide. SAS Institute Inc, 2015.

Sukchotrat, Thuntee, Kim, Seoung Bum, and Tsung, Fugee. One-class classification-based control charts for multivariate process monitoring. *IIE transactions*, 42(2): 107–120, 2009.

Tax, David MJ and Duin, Robert PW. Support vector data description. *Machine learning*, 54(1):45–66, 2004.

Widodo, Achmad and Yang, Bo-Suk. Support vector machine in machine condition monitoring and fault diagnosis. *Mechanical Systems and Signal Processing*, 21(6): 2560–2574, 2007.

Xiao, Yingchao, Wang, Huangang, Zhang, Lin, and Xu, Wenli. Two methods of selecting gaussian kernel parameters for one-class svm and their application to fault detection. *Knowledge-Based Systems*, 59:75–84, 2014.

Ypma, Alexander, Tax, David MJ, and Duin, Robert PW. Robust machine fault detection with independent component analysis and support vector data description. In *Neural Networks for Signal Processing IX, 1999. Proceedings of the 1999 IEEE Signal Processing Society Workshop.*, pp. 67–76. IEEE, 1999.

Zhuang, Ling and Dai, Honghua. Parameter optimization of kernel-based one-class classifier on imbalance learning. *Journal of Computers*, 1(7):32–40, 2006.