Anomaly Classification with the Anti-Profile Support Vector Machine

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Abstract

We introduce the anti-profile Support Vector Machine (apSVM) as a novel algorithm to address the anomaly classification problem, an extension of anomaly detection where the goal is to distinguish data samples from a number of anomalous and heterogeneous classes based on their pattern of deviation from a normal stable class. We show that under heterogeneity assumptions defined here that the apSVM can be solved as the dual of a standard SVM with an indirect kernel that measures similarity of anomalous samples through similarity to the stable normal class. We characterize this indirect kernel as the inner product in a Reproducing Kernel Hilbert Space between representers that are projected to the subspace spanned by the representers of the normal samples. We show by simulation and application to cancer genomics datasets that the anti-profile SVM produces classifiers that are more accurate and stable than the standard SVM in the anomaly classification setting.

1 Introduction

The task of anomaly, or outlier, detection [12, 8, 1] is to identify data samples that deviate significantly from a class for which training samples are available. We explore anomaly classification as an extension to this setting, where the goal is to distinguish data samples from a number of anomalous and heterogeneous classes based on their pattern of deviation from a normal stable class. Specifically, presented with samples from a normal class, along with samples from 2 or more anomalous classes, we want to train a classifier to distinguish samples from the anomalous classes. Since the anomalous classes are heterogeneous using deviation from the normal class as the basis of classification instead of building a classifier for the anomalous classes that ignores samples from the normal class may lead to classifiers and results that are more stable and reproducible.

The motivation for exploring this learning setting is from recent results in cancer genomics [3]. In particular, it was shown that hyper-variability in certain genomic measurements (DNA methylation and gene expression) in specific regions is a stable cancer mark across many tumor types. Furthermore, this hyper-variability increases during stages of cancer progression. This led us to the question
of how to distinguish samples from different stages in the presence of hyper-variability. In essence, how to distinguish samples from different anomalous classes (given by cancer progression stage) based on deviation from a well-defined normal class (measurements from non-cancerous samples).

We introduce the anti-profile Support Vector Machine (apSVM) as a novel algorithm suitable for the anomaly classification task. It is based on the idea of only using the stable normal class to define basis functions over which the classifier is defined. We show that the dual of the apSVM optimization problem is the same as the dual of the standard SVM with a modified kernel function. We then show that this modified kernel function has general properties that ensure better stability than the standard SVM in the anomaly classification task.

The paper is organized as follows: we first present the anomaly classification setting in detail; we next describe the Anti-Profile Support Vector Machine (apSVM), and show that the dual of the optimization problem defined by it is equivalent to the dual of the standard SVM with a specific kernel modification; we next show that this kernel modification leads directly to a theoretical statement of the stability of the apSVM compared to the standard SVM in the anomaly classification setting; we next show simulation results describing the performance and stability of the apSVM; and finally, we present results from cancer genomics showing the benefit of approaching classification problems in this area from the anomaly classification point of view.

## 2 The anomaly classification problem

We present the anomaly classification problem in the binary case, with two anomalous classes. Assume we are given training samples in $\mathbb{R}^p$ from three classes: $m$ datapoints from normal class $Z$, and $n$ training datapoints as pairs $\langle x_1, y_1 \rangle, \ldots, \langle x_n, y_n \rangle$ with labels $y_i \in \{-1, 1\}$ indicating membership of $x_i$ in one of two anomalous classes $A^-$ and $A^+$. Furthermore, we assume that the anomalous classes are heterogeneous with respect to normal class $Z$. Figure 1a illustrates this learning setting for DNA methylation data [3] (see [5] for details on this aspect of cancer epigenetics). It is a two-dimensional embedding (using PCA) of DNA methylation data for normal colon tissues along with benign growths (adenomas) and cancerous growths (tumor). Variability in these specific measurements increases from normal to adenoma to tumor. We would like to build stable and robust classifiers that distinguish benign growths from tumors.
Next we seek to formalize the heterogeneity assumption of the anomaly classification problem. Intuitively, the heterogeneity assumption we make is that given random samples of the same size from the normal class and from the anomalous classes, in expectation, the sample covariance of the anomalous samples is always larger than the covariance of the normal samples. We state our assumption in the case of Reproducing Kernel Hilbert Spaces (RKHS) since we will use this machinery throughout the paper [10, 14]. Recall that in a Bayesian interpretation of this setting, the kernel function associated with a RKHS serves as the covariance of a Gaussian point process.

**Definition 1** (Heterogeneity Assumption). Let $\mathcal{H}$ be a Reproducing Kernel Hilbert Space with associated kernel function $k$. Let $K^m_\mathcal{Y}$ and $K^m_\mathcal{A}$ be the kernel matrices resulting from evaluating the kernel function for a sample of size $m$ of points in the normal and anomalous classes respectively. The heterogeneity assumption is that for every integer $m$, there exists $\epsilon \in \mathbb{R}$, where $0 < \epsilon < 1$ such that $\mathbf{E} \det K^m_\mathcal{Y} / \det K^m_\mathcal{A} < \epsilon$.

Figures 1b and c show that the heterogeneity assumption is satisfied in the DNA methylation data for both linear and radial basis function kernels. Each figure shows the magnitude of the eigenvalues of the resulting kernel matrices. The magnitude of the eigenvalues in both cases is larger for the anomalous classes.

The heterogeneity assumption gives us a hint to construct classifiers that deal with the heterogeneity of the anomalous classes. In Section 3.3, we show that heterogeneity has an impact on robustness and stability of classifiers built from training sets of the anomalous classes. Our goal is to use samples from the stable normal class to create classifiers that are robust. We describe the anti-profile SVM as an extension to Support Vector Machines that accomplishes this goal.

3 The anti-profile SVM

Support Vector Machines (SVMs) are one of the primary machine learning tools used for classification. SVMs operate by learning the maximum-margin separator between two groups of data provided at training time. Any new observation provided to the SVM is classified by determining which side of the separator the new observation lies in. An important advantage of SVMs is that by applying the kernel trick, it is possible to find a hyperplane in a higher dimensional space where the two given classes are linearly separable, even when they are not linearly separable in their original feature spaces, and by virtue of the kernel trick this computation can be performed at no significant cost. While primarily designed for binary classification, SVMs have been extended for many other problems, such as multi-class classification and function estimation.

3.1 The SVM as weighted voting of basis functions

Here we review SVMs from a function approximation perspective [14]: consider a set of $n$ observations, each observation being drawn from $X \times Y$, where $X \in \mathbb{R}^p$, and $Y \in \{-1, 1\}$. Here $p$ is the number of features in each observation, or the dimensionality of the feature space. Thus each observation consists of a pair $(x_i, y_i)$, $x_i \in \mathbb{R}^p$ and $y_i \in \{-1, 1\}$, for $i = 1..n$; here $y_i$ indicates which of the two classes the observation belongs to. If we introduce a new observation $x'$ which needs to be classified, then the classification problem amounts to comparing $x'$ to the existing set of points and combining the comparisons to make a decision.

To make the comparisons between observations, we make use of a similarity function. Let $k(x_i, x_j)$ be a positive-definite similarity function which compares two points $x_i, x_j \in \mathbb{R}^p$. Weighing the similarity of the new observation to each existing observation, the difference of the sum of weighted similarities for the two groups will provide the necessary classification: $g(x) = d + \sum_{i=1}^{n} c_i k(x, x_i)$. Here $c_i \geq 0 \ \forall i$ is the weight associated with each point, and $d$ is a bias term. Classification is then based on the sign of the expansion: $f(x) = \text{sgn} [g(x)]$.

Usually in SVMs function $k$ is further assumed to have the reproducing property in a Reproducing Kernel Hilbert Space $\mathcal{H}$ associated with $k$: $(f,k(\cdot,\cdot))_\mathcal{H} = f(x)$ for all $f \in \mathcal{H}$, and in particular $(k(x,\cdot),k(y,\cdot))_\mathcal{H} = k(x,y)$. In this case, the basis functions in the classifier correspond to representatives $k(x, \cdot)$. In the standard SVM, the representatives of all training points are potentially used as basis functions in the classifier, but effectively only a small number of representatives are used as basis functions, namely the Support Vectors. However, for a given problem, we may choose a different
set of points for the derivation of the set of basis functions; the basis functions determine how the
similarities are measured for a new point.

3.2 The Anti-Profile SVM optimization problem

The core idea in the anti-profile SVM (apSVM) is to make use of this characterization of the Support
Vector Machine as a linear expansion of basis functions defined by representers of training samples.
In order to address the heterogeneity assumption underlying the anomaly classification problem we
define basis functions only using samples from the stable normal class.

Formally, we restrict the set of functions available to define the subspace of \( \mathcal{H} \) spanned by the
representers of samples \( z_1, \ldots, z_m \) from normal class \( Z \): \( f(x) = d + \sum_{i=1}^{m} c_i k(z_i, x) \). To estimate
coefficients \( c_i \) in the basis expansion we apply the usual regularized risk functional based on hinge loss

\[
R_{\text{reg}}(f) = \frac{1}{n} \sum_{j=1}^{n} (1 - y_j f(x_j))_+ + \frac{\lambda}{2} \|h\|_H^2,
\]

where \((\cdot)_+ = \max(0, \cdot)\), \( f(x) \) is defined as \( f(x) = d + h(x) \), and \( \lambda > 0 \) is a regularization
parameter. By the reproducing kernel property, we have in this case that \( \|h\|_H^2 = c^T K_n c \) where \( K_n \)
is the kernel matrix defined on the \( m \) normal samples.

The minimizer of the empirical risk functional is given by the solution of a quadratic optimization
problem, similar to the standard SVM, but with two kernel matrices used: \( K_n \), defined in the pre-
vious paragraph, and \( K_s \), which contains the evaluation of kernel function \( k \) between anomalous
samples \( x_1, \ldots, x_n \) and normal samples \( z_1, \ldots, z_m \):

\[
\begin{align*}
\min_{d,c,\xi} & \quad e^T \xi + \frac{n\lambda}{2} c^T K_n c \\
\text{s.t.} & \quad Y(K_s c + de) + \xi \geq e, \xi \geq 0
\end{align*}
\]

Here we use slack variables \( \xi = (\xi_1, \xi_2, \ldots, \xi_n)' \), denote the unit vector of size \( n \) as \( e \), and define
matrix \( Y' \) as the diagonal matrix such that \( Y_{ii} = y_i \).

3.3 Solving the apSVM optimization problem

The Lagrangian of problem 1 is given by

\[
L(c, d, \xi, \alpha, \beta) = e^T \xi + \frac{n\lambda}{2} c^T K_n c - \alpha^T [Y(K_s c + de) + \xi - e] - \beta^T \xi
\]

where \( \alpha_{n \times 1} = (\alpha_1, \ldots, \alpha_n)' \) and \( \beta_{n \times 1} = (\beta_1, \ldots, \beta_n)' \) are the Lagrangian multipliers. Minimizing
with respect to \( z, c \) and \( d \), we find that the Wolfe dual of problem 1 is

\[
\begin{align*}
\max_{\alpha} & \quad e^T \alpha - \frac{1}{2n\lambda} \alpha^T Y \tilde{K} Y \alpha \\
\text{s.t.} & \quad 0 \leq \alpha \leq e, e^T Y \alpha = 0
\end{align*}
\]

where \( \tilde{K} = K_s K_n^{-1} K_s^T \). Here we assume \( K_n^{-1} \) represents a pseudo-inverse in the case where \( K_n \)
is not positive definite.

For a standard SVM, the objective of the Wolfe dual is \( e^T \alpha - \frac{1}{2n\lambda} \alpha^T Y K Y \alpha \), with \( K \) the kernel ma-
trix the training datapoints. Thus the dual problem of the apSVM has the same form as the standard
SVM dual problem with the exception that kernel matrix \( K \) is replaced by induced kernel matrix \( \tilde{K} \)
in the apSVM. Kernel matrix \( \tilde{K} \) essentially represents an indirect kernel between anomalous sam-
pies induced by the set of basis functions determined by the samples from the normal class. Since the
essential form of the SVM solution is unchanged by the modification, this provides the addi-
tional advantage that the modified SVM can be solved by the same tools that solve a regular SVM,
but with a different kernel matrix provided. For our particular problem domain, we use the indirect kernel to represent deviation from the profile of normal samples, and thus refer to this classifier as the anti-profile SVM.

### 3.4 Characterizing the indirect kernel

We saw above that the apSVM can be solved as a standard SVM with induced kernel $\tilde{K} = K_n K_n^{-1} K_n^T$. In this section we characterize this indirect kernel, and state a general result that elucidates how the apSVM can produce classifiers that are more robust and reproducible than a standard SVM in this setting.

**Proposition 1.** Let $P_Z$ be the linear operator that projects representers $k(x, .) \in \mathcal{H}$ to the space spanned by the representers of the $m$ normal samples of the anomaly classification problem. Induced kernel $k$ satisfies $k(x, y) = k(P_Zk(x, .), P_Zk(y, .))$.

**Proof.** Projection $P_Zk(x, .)$ is defined as $P_Zk(x, .) = \sum_{i=1}^{m} \hat{\beta}_i k(z_i, .)$ where

\[
\begin{align*}
\hat{\beta} &= \arg \min_{\beta} \frac{1}{2} \|k(x, .) - \sum_i^m \beta k(z_i, .)\|^2_{\mathcal{H}} \\
&= \arg \min_{\beta} \frac{1}{2} \langle k(x, .) - \sum_i^m \beta k(z_i, .), k(x, .) - \sum_i^m \beta k(z_i, .) \rangle_{\mathcal{H}} \\
&= \arg \min_{\beta} \frac{1}{2} \left( \sum_{i,j} \langle k(z_i, .), k(z_j, .) \rangle_{\mathcal{H}} - \sum_i \langle k(x, .), k(z_i, .) \rangle_{\mathcal{H}} \right) \\
&= \arg \min_{\beta} \frac{1}{2} \left( \beta^T K_n \beta - k_{zx} \beta \right),
\end{align*}
\]

where $k_{zx}$ is the vector with element $i$ equal to $k(z_i, x)$. From (3) we get $\hat{\beta} = K_n^{-1} k_{zx}$. Therefore $(P_Zk(x, .), P_Zk(y, .))_{\mathcal{H}} = k_{zx}^T K_n^{-1} k_{zy} = k(x, y)$. $\square$

This proposition states that the indirect kernel is the inner product in Reproducing Kernel Hilbert Space $\mathcal{H}$ between the representers of anomalous samples projected to the space spanned by the representers of normal samples. By the heterogeneity assumption of Definition 1, the space spanned by any subset of anomalous samples will be smaller after the projection. In particular, the smallest sphere enclosing the projected representers will be smaller, and from results such as the Vapnik-Chapelle support vector span rule [13], classifiers built from this projection will be more robust and stable.

### 4 Simulation Study

We first present simulation results that show that the apSVM obtains better accuracy in the anomaly classification setting while providing stable and robust classifiers. We generated samples from three normal distributions as follows: if $A^+$ and $A^-$ are the anomalous classes that we need to distinguish, and $Z$ is the normal class, then for a given feature we draw datapoints from distributions $Z = \mathcal{N}(0, \sigma_Z^2)$, $A^- = \mathcal{N}(0, \sigma_A^-)$ and $A^+ = \mathcal{N}(0, \sigma_A^+)$. To simulate our problem setting, we set $\sigma_Z^2 < \sigma_A^- < \sigma_A^+$.

Results have been obtained from tests written on R (version 2.14) with R packages kernlab (version 0.9-14) [7] and symath (version 0.952). The symath tool provides a fitting for the entire path of the SVM solution to a model at little additional computational cost [4]. Using the resulting fit, the SVM classifications for any given cost parameter can be obtained. For our experiments, the testing set accuracy was computed for each value of cost along the regularization path, and the best accuracy possible was obtained; ties were broken by considering the option with the least number of support vectors used. Note that a small ridge parameter (1e-10) was used in the symath method to avoid singularities in computations.
Figure 2: (A) Accuracy results in simulated anomaly classification data. The anti-profile SVM achieves better accuracy than the standard SVM. (B) Stability results in simulated data. The anti-profile SVM uses a smaller proportion of training points as support vectors. SVMs that use fewer support vectors are more robust and stable.

Each training set contained 20 samples from each of $A^-$ and $A^+$ classes, while each testing set contained 5 samples from each class; 20 samples from class $Z$ were used for the anti-profile SVM. For a given number of features, each test was run 10 times and the mean accuracy computed. To estimate the hyperparameter for the radial basis kernel, the inverse of the mean distance between 5 normal and 5 anomalous samples (chosen randomly) was used.

Figure 2a shows the accuracy of a standard SVM and the apSVM using an RBF kernel for simulated data with $\sigma_Z = 1$, $\sigma_{A^-} = 2$, $\sigma_{A^+} = 4$. With a radial basis kernel, the anti-profile SVM was able to achieve better classification than the regular SVM.

We characterize the stability of a classifier using the proportion of training samples that are selected as support vectors. Classifiers that use a small proportion of points as support vectors are more robust and stable to stochasticity in the sampling process. The more support vectors used by an SVM, the more likely it is that the classification boundary will change with any changes in the training data. Hence a boundary that is defined by only a few support vectors will result in a more robust, reliable SVM. Figure 2b shows that in the simulation study the apSVM used fewer support vectors than the standard SVM while obtaining better accuracy.

5 Application to cancer genomics

The motivation for this work is from recent studies of epigenetic mechanisms of cancer. Epigenetics is the study of mechanisms by which the expression level of a gene (i.e. the degree to which a gene can exert its influence) can be modified without any change in the underlying DNA sequence. Recent results show that certain changes in DNA methylation are closely associated with the occurrence of multiple cancer types. In particular, the existence of highly-variable DNA-methylated regions in cancer as compared to normals (i.e. healthy tissue) has been shown. Furthermore, these highly-variable regions are associated with tissue differentiation, and are present across multiple cancer types. Another important observation made there is that adenomas, which are benign tumors, show intermediate levels of hyper-variability in the same DNA-methylated regions as compared to cancer and normals.

This presents an interesting machine learning problem: distinguishing between cancer and adenoma based on the hyper-variability of their methylation levels with respect to normal samples? A successful tool that can classify between the two groups can have far-reaching benefits in the area of personalized medicine and diagnostics. Since the two classes are essentially differentiated by the degree of variability they exhibit with respect to normals, for our purpose we can abstract the problem to the setting we present here as anomaly classification.
5.1 Methylation data results

We study the performance of the apSVM in a dataset of DNA methylation measurements obtained for colon tissue from 25 healthy samples, 19 adenoma samples, and 16 cancer samples, for 384 specific positions in the human genome \cite{3}. As mentioned previously, the cancer samples exhibit higher variance than healthy samples, with adenoma samples showing an intermediate level of variability (Figure 1). We used the same classification methods mentioned in the previous section, but with multiple runs, for each run randomly choosing 80% of tumor samples for training and the remaining for testing. Figure 3 shows the results obtained using a radial basis kernel. While the indirect kernel performs either at the same level or marginally better than the regular kernel, then anti-profile SVM uses much less support vectors than the standard SVM, thus providing a much more robust classifier.

5.2 Expression data results

We further applied our method to gene expression data obtained with a clinical experiment on adrenocortical cancer \cite{2}. The data contains expression levels for 54675 probesets, for 10 healthy samples, 22 adenoma samples, and 32 cancer samples. The data shows the same pattern with regard to hyper-variability as the methylation data. Using the same methods as before, the results obtained using a linear kernel are shown in Figure 4. For feature selection, the features were ranked according to \( \log \frac{\text{var(Carcinoma)}}{\text{var(Adenoma)}} \) and for a given number \( n \) as the number of features to be used, \( n \) features with the highest variance ratio were selected. While both the standard SVM and the apSVM provided almost perfect classification, there is a significant difference in the number of support vectors used, with the indirect kernel requiring much fewer support vectors and hence providing a more stable classifier.

6 Discussion

We have introduced the anti-profile Support Vector Machine as a novel algorithm to address the anomaly classification problem. We have shown that under the assumption that the classes we are trying to distinguish with a classifier are heterogeneous with respect to a third stable class, we can define a Support Vector Machine based on an indirect kernel using the stable class. We have shown that the dual of the apSVM optimization problem is equivalent to that of the standard SVM with the addition of an indirect kernel that measures similarity of anomalous samples through similarity to the stable normal class. Furthermore, we have characterized this indirect kernel as the inner product in a Reproducing Kernel Hilbert Space between representers that are projected to the subspace spanned by the representers of the normal samples. This led to the result that the apSVM will learn classifiers that are more robust and stable than a standard SVM in this learning setting. We have shown by simulation and application to cancer genomics datasets that the anti-profile SVM does in fact produce classifiers that are more accurate and stable than the standard SVM in this setting.
Figure 4: Classification results for gene expression in cancer [2]. Similar to Figure 3, the accuracy of both the standard and anti-profile SVM is similar (in this case almost perfect testset accuracy is achieved by both classifiers). However, the anti-profile SVM again uses fewer support vectors, leading to classifiers that are more robust and stable.

While the motivation and examples provided here are based on cancer genomics we expect that the anomaly classification setting is applicable to other areas. In particular, we have started looking at the area of statistical debugging as a suitable application [16].

The characterization of the indirect kernel through projection to the normal subspace also suggests other possible classifiers suitable to this task. For instance, by defining a margin based on the projection distance directly. Furthermore, connections to kernel methods for quantile estimation [11] will be interesting to explore.

Another direction of interesting research would be to further solidify the stability characterization we provide in Section 3.4. For instance, by exploring the relationship to other leave-one-out bounds [9, 6, 15, 5], and the span rule for kernel quantile estimation [10].

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