Abnormal Subspace Sparse PCA for Anomaly Detection and Interpretation

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ABSTRACT
The main shortage of principle component analysis (PCA) based anomaly detection models is their interpretability. In this paper, our goal is to propose an interpretable PCA-based model for anomaly detection and interpretation. The propose ASPCA model constructs principal components with sparse and orthogonal loading vectors to represent the abnormal subspace, and uses them to interpret detected anomalies. Our experiments on a synthetic dataset and two real world datasets showed that the proposed ASPCA models achieved comparable detection accuracies as the PCA model, and can provide interpretations for individual anomalies.

Keywords
Anomaly detection, PCA, Anomaly interpretation, sparsity, optimization

1. INTRODUCTION
Principal Component Analysis (PCA) is one of the best-known statistical analysis techniques for detecting anomalies and has been applied to many kinds of data, such as network intrusion detection, failure detection in production systems, and so on [4] [21] [16] [11]. In these domains, pinpointing the sources of detected anomalies is also very important for real applications such as diagnosing failures and recovering systems/networks. Hence, for each detected anomaly, an ideal model should also be able to interpret the reasons of its detection, which we refer to as the problem of anomaly interpretation.

Traditional PCA-based anomaly detection models are not suitable for anomaly interpretation [22] [17], as they judge whether a data instance is an anomaly or not based on the length of its projection on the abnormal subspace spanned by the less significant principal components, and there is no direct mapping between PCA’s dimensionality-reduced subspace and the original feature space. Existing approaches [22] added a separated interpretation step to solve this problem by using techniques such as decision trees. However, such indirect interpretation often failed to reveal the true causes of the anomalies detected by PCA-based methods [17]. Another recent work [11] proposed the joint sparse PCA (JSPCA) model to identify a low-dimensional approximation of the abnormal subspace, so that all anomalies can be localized onto a small subset of original feature variables. However, for individual anomaly interpretation, especially anomalies of different types, we need a more accurate and direct way of interpretation.

This paper aims to design an interpretable PCA-based anomaly detection model. Our key observation is that if we manage to construct principal components (PCs) with sparse and orthogonal loading vectors to represent the abnormal subspace, a detected anomaly can be interpreted by identifying the set of such PCs on which the anomaly has large projection values. We propose interpretable Abnormal subspace sparse PCA (ASPCA) models for anomaly detection and interpretation in this paper, and make the following two contributions.

First, we formulate two objective functions for ASPCA: one extracts the most significant sparse orthogonal PCs first, and the other extracts the least significant sparse orthogonal PCs first, which prioritizes the sparsity of the abnormal subspace. To the best of our knowledge, the proposed ASPCA models are the first PCA-based models that are suitable for individual anomaly detection and interpretation. Second, we propose an optimization method for ASPCA models with a semidefinite programming (SDP) relaxation step and a global sparsity optimization step. Our experiments on a synthetic dataset and two real world datasets showed that the proposed ASPCA models achieved comparable detection accuracies as the PCA model, and can provide interpretations for individual anomalies.

The rest of this paper is organized as follows. Section 2 introduces the proposed ASPCA models. Section 3 describes the optimization methods for ASPCA models. Section 4 presents a comprehensive experimental evaluation. Section 5 discusses the related work. Finally, Section 6 provides some concluding remarks.

2. RELATED WORK
PCA is mostly known as a dimension reduction tool [12], but it is also widely used as an anomaly detection method.
3. PCA FOR ANOMALY DETECTION AND INTERPRETATION

3.1 Notations

Bold uppercase letters such as $X$ denote a matrix and bold lowercase letters such as $x$ denote a column vector. Greek letters such as $\lambda, \mu$ are coefficients. $||X||_F$ is the Frobenius norm of $X$, and $||X||_{1,1}$ is the $L_{1,1}$ norm of $X$ as $||X||_{1,1} = 1|X|_1^T$. A dataset is represented as an $n \times p$ data matrix $D$, where each row vector corresponds to a $p$-dimensional data instance, and each column vector corresponds to a feature variable. $A = D^T D$ is $D$’s covariance matrix. $Tr(A)$ represents the trace of matrix $A$. Card($A$) denotes the cardinality (number of non-zero elements) of matrix $A$. $I$ is the identity matrix. $S^p$ is the set of all symmetric semidefinite matrices in $\mathbb{R}^{p \times p}$.

3.2 PCA for Anomaly Detection

Principal Component Analysis (PCA) is a dimensionality-reduction technique that captures the highest variance of a multi-dimensional dataset in a lower dimensional subspace defined by a set of orthogonal eigenvectors. Given a $p$-dimensional dataset, a detection model can be constructed by forming a “normal subspace” (defined by the first $k$ principal components returned by PCA) and an “abnormal subspace” (the remaining subspace by removing the normal subspace). Since the normal subspace captures the highest variance of the dataset, PCA-based detection methods assume that this $k$-subspace corresponds to the normal trends of the dataset, and all normal data tends to have almost zero length projection on the abnormal subspace. Therefore, given a $p$-dimensional data, the model can detect whether it is an anomaly or not based on whether it is primarily expressed by the normal or abnormal subspace.

More formally, let $V_1 = (v_1, \ldots, v_k)$ be the normal subspace defined by the first $k$ principal components with $v_1, \ldots, v_k$ being the orthogonal loading vectors, and $V_2 = (v_{k+1}, \ldots, v_p)$ be the abnormal subspace defined by the remaining $p-k$ principal components with $v_{k+1}, \ldots, v_p$ being the orthogonal loading vectors of these PCs. Given a $p$-dimensional data $y$, its residual $\hat{y}$ is defined as:

$$\hat{y} = y - V_1 V_1^T y.$$  

The squared length of $\hat{y}$, called the squared prediction error (SPE), is the metric to indicate whether $y$ is an anomaly or not. The larger SPE is, the more likely $y$ is an anomaly.

3.3 Anomaly Interpretation

When the SPE score of a given instance $y$ is over a predefined threshold, $y$ is considered as an anomaly. It is then important to understand where the abnormality of $y$ comes from, i.e., what anomalous feature behaviors of $y$ are more responsible for distinguishing $y$ from normal data. We call this problem as Anomaly Interpretation. The anomaly interpretation for PCA is difficult, as there is no direct mapping between PCA’s dimensionality-reduced subspace and the original feature space for anomaly detection. In other words, the length of $\hat{y}$ can be used to detect anomaly, whereas interpreting $\hat{y}$ directly is meaningless.

Given the normal subspace $V_1$ and abnormal subspace $V_2$, we can rewrite $\hat{y}$ as follows:

$$\hat{y} = y - V_1 V_1^T y = V_2 V_2^T y.$$  

To design an interpretable PCA-based anomaly detection model, we have the following proposition.

**Proposition 3.1.** Given $V_2 = (v_{k+1}, \ldots, v_p)$, where $v_{k+1}, \ldots, v_p$ are orthogonal loading vectors, SPE can be expressed by

$$SPE = \hat{y}^T \hat{y} = \sum_{i=k+1}^p (v_i^T y)^2.$$  

**Proof.**

$$SPE = \hat{y}^T \hat{y} = y^T V_2 V_2^T V_2 y = (y^T V_2)(V_2^T V_2)(V_2^T y) = (V_2^T y)^T (V_2^T y) = \sum_{i=k+1}^p (v_i^T y)^2.$$  

In other words, SPE is equal to the square sum of $y$’s scalar projection on each abnormal PCs, so that we can identify the set of PCs that are responsible for the abnormality indicated by high projection values. Unfortunately, these PCs
are still difficult to interpret, since each abnormal PC is complicated as it is a linear combination of all feature variables. To make them interpretable, we have to make these abnormal PCs sparse, i.e., each represented by a few feature variables. Hence, our key observation is that if we manage to extract PCs with sparse and orthogonal loading vectors to represent abnormal subspace, these loading vectors can be used to detect and interpret anomalies. The orthogonality guarantees that Eqn. 4 holds, so that the abnormality can be translated to high projection values on a set of abnormal PCs, while the sparsity guarantees that these abnormal PCs are interpretable. We call the above method as the Abnormal Subspace Sparse PCA (ASPCA) method. Now we use an example to illustrate this idea.

We synthesized a dataset with 500 normal records and 15 anomalies (first 100 normal records are shown in Figure 1a). Each data record has 7 features named from A to G, and the normal records were generated with four patterns, A ≈ B, D ≈ C + A, F ≈ 0, and G ≈ 0. The anomalies were generated as three categories by breaking the first three patterns, respectively. The loading matrix of PCs obtained by PCA is shown in Figure 1b, where the last four PCs can be used to detect anomalies but difficult to interpret. Now, if we can make the loading vectors of last four PCs sparse and orthogonal as shown in Figure 1c, they can be used to detect and interpret anomalies simultaneously. Now, the interpretation of a detected anomaly can be conducted in two steps. First, we can identify the set of projections that contribute the most for a high SPE score according to Eqn. 4. Then, we can interpret these projections one by one, by identifying which original feature variables are responsible for each projection, and how each projection triggers a high SPE score.

Figure 1: Synthetic data and loading matrices obtained by PCA and ASPCA

Recently, Jiang et al. [11] proposed a joint sparse PCA (JSPCA) model to achieve a sparse representation of the abnormal subspace too. The main idea was to identify a low-dimensional approximation of the abnormal subspace using a subset of feature variables, where all abnormal PCs are represented by the same subset of feature variables as shown in Figure 2. Although JSPCA can identify the set of features that distinguish the anomalies, it has two limitations that fail to meet our goals. First, the features identified by JSPCA are optimized for all anomalies as a whole. In particular, if anomalies are of different types, which is a common case for domains such as network intrusion detection or system failure detection, they should be interpreted by different sets of features inherently. As an unsupervised method, JSPCA cannot assume that anomalies in the dataset are of the same type, and cannot handle them well if they indeed are of different types. Second, JSPCA can only identify the important features for anomaly detection, but no direct interpretation as why anomalies are detected.

3.4 Abnormal Subspace Sparse PCA

Now we need to formulate the objective function of the Abnormal Subspace Sparse PCA (ASPCA) problem. The recently studied sparse PCA framework [5] adds a sparsity constraint on the principal components (PCs). However, we cannot use this framework directly to solve our problem. The main reason is that the sparse PCA framework usually does not enforce orthogonality on the resultant sparse PCs. Consequently, the resultant sparse PCs cannot be used to define the normal and abnormal subspaces, as the abnormal PCs are not the orthogonal complement of the normal PCs.

By enforcing orthogonality, sparse PCA can be used to solve our ASPCA problem, which we denote as forward ASPCA (shorted as ASPCA-F). Given a covariance matrix A and a sparsity constraint constant k, for each i = 1, ..., p, ASPCA-F tries to solve:

$$\arg \max_{v_i} v_i^T A v_i,$$

$$s.t. v_i^T v_i = 1, v_i^T v_j = 0 \forall 1 \leq j < i, \text{Card}(v_i) \leq k.$$  (5)

The last d loading vectors obtained by solving Eqn. 5 are used for detecting and interpreting anomalies.

One of the drawbacks of the ASPCA-F framework is that the last abnormal PCs tend to have poor sparsity. To solve this problem, we propose a Backward ASPCA framework (shorted as ASPCA-B) that extracts the least significant orthogonal PCs first, which prioritizes the optimization of the sparsity of the abnormal subspace. To see how it works, we first show that the process of standard PCA can be reversed, so that eigen vectors with smaller eigen values are extracted first by the following proposition.

![Figure 2: Loading matrix obtained by JSPCA](image-url)
Proposition 3.2. Given a covariance matrix $A = D^T D$, if we have already extracted the eigenvectors $v_{k+1}, v_{k+2}, ..., v_n$ with the $n-k-1$ smallest eigen values, and remaining eigenvectors are $v_1, v_2, ..., v_k$ with eigen values $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_k$ of $A$, the solution of Eqn. (6) is the eigenvector with the eigen value $\lambda_i$.

$$\begin{align*}
\text{argmin}_{v} & \quad v^T A v \\
\text{s.t.} & \quad v^T v = 1, \quad v^T v_i = 0 \quad \forall k < i \leq n
\end{align*}$$

Proof. We project $v$ on $(v_1, ..., v_n)$, $v = \sum_{i=1}^{n} \alpha_i v_i = \sum_{i=1}^{k} \alpha_i v_i$, where $\alpha_i = v^T v_i$. As $v^T v_j = 0, i \neq j$, we have $v^T v = \sum_{i=1}^{k} \alpha_i^2 = 1$. Then,

$$v^T A v = (\sum_{i=1}^{k} \alpha_i v_i) (\sum_{i=1}^{k} \alpha_i A v_i) = (\sum_{i=1}^{k} \alpha_i \lambda_i v_i) (\sum_{i=1}^{k} \alpha_i \lambda_i v_i)$$

$$= \sum_{i=1}^{k} \alpha_i^2 \lambda_i v_i + \sum_{i=1}^{k} \sum_{j=1, j \neq i}^{k} \alpha_i \alpha_j \lambda_i \lambda_j v_i v_j$$

$$= \sum_{i=1}^{k} \alpha_i^2 \lambda_i$$

As $\lambda_1 \geq \lambda_k, i \leq k$, we know $v^T A v = \sum_{i=1}^{k} \alpha_i^2 \lambda_i \geq \sum_{i=1}^{k} \alpha_i^2 \lambda_k = \lambda_k$. And we know $\min_{\alpha} v^T A v \leq v^T A v_k = \lambda_k$, so $\min_{\alpha} v^T A v = \lambda_k$.

With the optimum $\hat{v} = \sum_{i=1}^{k} \alpha_i v_i$, we have:

$$\lambda_k - \sum_{i=1}^{k} \alpha_i^2 \lambda_i = \sum_{i=1}^{k} \alpha_i^2 (\lambda_k - \lambda_i) = 0$$

$$\lambda_k - \lambda_i \leq 0, i < k$$

So, we know that $\alpha_i \neq 0$ only if $\lambda_i = \lambda_k$. Hence, $\hat{v}$ is a linear combination of the eigenvectors with eigen value $\lambda_k$, and $\hat{v}$ must be an eigenvector with eigen value $\lambda_k$ too.

Obviously, the proposition also holds for $k = n$. Together we see that using Eqn. (6) eigenvectors can be calculated in an increasing order of eigen values. Now, we add a sparsity constraint to Eqn. (6) and form the objective function for our ASPCA-B framework as follows.

Given a covariance matrix $A$ and a sparsity constraint constant $k$, for each $i = 1, ..., d$, our ASPCA-B framework tries to solve:

$$\begin{align*}
\text{argmin}_{\alpha} & \quad \alpha^T A \alpha_i \\
\text{s.t.} & \quad \alpha^T v_i = 1, \quad \alpha^T v_j = 0 \quad \forall 1 \leq j < i, Card(v_i) \leq k
\end{align*}$$

When we extract $d$ loading vectors $v_1, ..., v_d$ to span a subspace $S_h$, we make sure that the orthogonal complement of $S_h$ has major variance for describing the normal patterns in the dataset, so that $S_h$ is the abnormal subspace and the resultant $d$ sparse principal components can be used to detect and interpret anomalies.

### 4. METHODOLOGY

We derive a solution for Eqn. (7) following the semidefinite programming (SDP) relaxation framework proposed by [5].

We then modify it to solve Eqn. (7). Finally, we further optimize the sparsity of all the obtained abnormal components with the constraint of spanning the same subspace using the alternating minimization scheme inspired by [23].

**Solving ASPCA-F with SDP Relaxation.**

We first transform Eqn. (5) without the orthogonality constraint $v_i^T v_i = 0, \forall 1 \leq j < i$ to Eqn. (8) through a SDP relaxation.

$$\begin{align*}
\text{argmax}_{X_i} & \quad Tr(A X_i) \\
\text{s.t.} & \quad X_i \succeq 0, \quad \text{rank}(X_i) = 1, \quad Tr(X_i) = 1, \quad Card(X_i) < k^2
\end{align*}$$

where $X_i$ is a positive semi-definite matrix with the constraint $\text{rank}(X_i) = 1$, which can be uniquely decomposed as $X_i = v_i v_i^T$. With $X_i = v_i v_i^T$, $\text{Tr}(X_i) = 1$ is equivalent to $v_i^T v_i = 1$, $\text{Card}(X_i) \leq k^2$ is equivalent to $\text{Card}(v_i) \leq k$, and we have $v_i^T A v_i = \text{Tr}(A v_i v_i^T) = \text{Tr}(A X_i)$.

Now let $V_i = (v_1, v_2, ..., v_n)$ and $R_i = V_i V_i^T$, the orthogonality constraint $v_i^T v_j = 0, \forall 1 \leq j < i$ is equivalent to $\|V_i^T v_1\|^2 = 0$ and $\|V_i^T v_{k+1}\|^2 = v_i^T v_{k+1} V_i^T v_{k+1} = \text{Tr}(R_{k+1} X_i) = 0$. Similarly as in [5], we relax $\text{Card}(X_i) < k^2$ to $\|X_i\|_{1,1} < k$ and move it to the objective function with a coefficient $\lambda$. Finally, the non-convex constraint $\text{rank}(X_i) = 1$ is dropped, and we have an objective function that can be solved by semidefinite programming (SDP) as in Eqn. (9).

$$\begin{align*}
\text{argmax}_{X_i \in \mathbb{S}^p} & \quad Tr(A X_i) - \lambda \|X_i\|_{1,1} \\
\text{s.t.} & \quad X_i \succeq 0, \quad Tr(X_i) = 1, \quad Tr(R_i X_i) = 0
\end{align*}$$

As $\text{rank}(X_i)$ might not be 1, so we use the dominant eigenvector of $X_i$ as the approximate solution for $v_i$.

**Solving ASPCA-B with SDP Relaxation.**

To solve Eqn. (5) following the same steps above, we can get Eqn. (10) which is still a convex programming problem and can be solved by semidefinite programming (SDP).

$$\begin{align*}
\text{argmin}_{X_i \in \mathbb{S}^p} & \quad Tr(A X_i) + \lambda \|X_i\|_{1,1} \\
\text{s.t.} & \quad X_i \succeq 0, \quad Tr(X_i) = 1, \quad Tr(R_i X_i) = 0
\end{align*}$$

**Global Sparsity Optimization.**

Let $V = (v_1, ..., v_d)$ be the set of sparse loading vectors extracted by solving Eqn. (7) or Eqn. (10) which is also a set of basis vectors spanning the abnormal subspace. Notice that for any set of basis vectors $e_1, ..., e_d$ spanning the same subspace, we have

$$\text{SPE} = \sum_{i=1}^{d} (v_i e_i)^2 = \sum_{i=1}^{d} (e_i^T e_i)^2$$

Hence, we can employ a global sparsity optimization step to make the basis vectors of the same abnormal subspace sparser. To this end, we form the following optimization problem on an orthogonal transformation matrix $X$,

$$\begin{align*}
\text{argmin}_{X} & \quad \|V X\|_{1,1} \\
\text{s.t.} & \quad X^T X = I
\end{align*}$$
Let \( \mathbf{C} = \mathbf{VX} \), we transform this problem to the following regression problem,

\[
\min_{\mathbf{X}, \mathbf{C}} \|\mathbf{V} - \mathbf{C} \mathbf{X}^T\|_F + \mu \|\mathbf{C}\|_{1,1}
\]

\[\text{s.t. } \mathbf{X}^T \mathbf{X} = \mathbf{I}\]  \( (13) \)

Eqn. \( (13) \) can be solved by using the alternating minimization scheme as in [22], with initial \( \mathbf{X} \) being an identity matrix. Initially, we set \( \mu = \|\mathbf{V}\|_F/\|\mathbf{VX}\|_{1,1} \) to emphasize more on the sparsity objective, and gradually degrade \( \mu \) to a small value to ensure \( \mathbf{C} \) spanning the same subspace as \( \mathbf{V} \) through the last iterations.

Adding the global sparsity optimization step to ASPCA-F and ASPCA-B, we have two new models ASPCA-FG and ASPCA-BG, respectively. Algorithms 1 and 2 summarize the entire optimization process, where \( \mathbf{A} \) is the covariance matrix of the input dataset, \( d \) is the number of sparse principal components extracted from the abnormal subspace, \( \text{max} \_ \text{iter} \) is the number of iterations for the global sparsity optimization, and the output loading matrix \( \mathbf{V} \) contains \( d \) orthogonal and sparse loading vectors for detecting and interpreting anomalies.

**Algorithm 1** Forward Abnormal Subspace Sparse PCA with Global Optimization (ASPCA-FG)

**Input:** \( \mathbf{A}, d, \lambda, \) and \( \text{max} \_ \text{iter} \)

**Output:** \( \mathbf{V} \)

1: for \( i = 1 \) to \( p \) do
2: \( \mathbf{V}_{i-1} \leftarrow (v_1, v_2, ..., v_{i-1}) \);
3: \( \mathbf{R}_{i-1} \leftarrow \mathbf{V}_{i-1} \mathbf{V}_{i-1}^T \);
4: Optimize \( v_i \) with given \( \mathbf{A}, \mathbf{R}_{i-1} \) according to Eqn. \( (9) \) using SDP;
5: end for
6: \( \mathbf{V} \leftarrow (v_{p-d+1}, ..., v_p) \);
7: Optimize \( \mathbf{X}, \mathbf{C} \) with given \( \mathbf{V}, \text{max} \_ \text{iter} \) according to Eqn. \( (13) \) using the alternating minimization scheme;
8: \( \mathbf{V} \leftarrow \mathbf{C} \mathbf{X} \);
9: return \( \mathbf{V} \);

**Algorithm 2** Backward Abnormal Subspace Sparse PCA with Global Optimization (ASPCA-BG)

**Input:** \( \mathbf{A}, d, \lambda, \) and \( \text{max} \_ \text{iter} \)

**Output:** \( \mathbf{V} \)

1: for \( i = 1 \) to \( d \) do
2: \( \mathbf{V}_{i-1} \leftarrow (v_1, v_2, ..., v_{i-1}) \);
3: \( \mathbf{R}_{i-1} \leftarrow \mathbf{V}_{i-1} \mathbf{V}_{i-1}^T \);
4: Optimize \( v_i \) with given \( \mathbf{A}, \mathbf{R}_{i-1} \) according to Eqn. \( (10) \) using SDP;
5: end for
6: \( \mathbf{V} \leftarrow (v_1, v_2, ..., v_d) \);
7: Optimize \( \mathbf{X}, \mathbf{C} \) with given \( \mathbf{V}, \text{max} \_ \text{iter} \) according to Eqn. \( (13) \) using the alternating minimization scheme;
8: \( \mathbf{V} \leftarrow \mathbf{C} \mathbf{X} \);
9: return \( \mathbf{V} \);

## 5. EXPERIMENT

### 5.1 Datasets

Our proposed ASPCA models were evaluated on the synthetic data introduced in Section 2, a medical dataset Breast-Cancer, and a network intrusion detection dataset KDD99.

- Breast Cancer Wisconsin (Diagnostic) Data Set [1] provides features to distinguish malignant and benign tumors. The features describe characteristics of the cell nuclei present in a digitized image of a fine needle aspirate (FNA) of a breast mass. As there are plenty cells for a breast mass, the features are three important statistics (mean, standard error, and worst value) on 10 features for each cell: radius, texture, perimeter, area, smoothness, compactness, concavity, concave points, symmetry and fractal dimension. There are 357 benign records, and we kept the first 10 malignant records to transform the classification task to an anomaly detection task, same as the other works [11, 13] did. All 30 real-valued features were deducted by the mean values and linearly scaled to \([-1,1]\).

- KDD 99 Intrusion Dataset [2] is a widely used data for anomaly and intrusion detection. Each instance is a connection record classified as normal or one of 22 classes of attacks. Attacks fall into four main groups: DoS, Remote-to-local, User-to-root, and Probe. We chose all normal and part of the abnormal records in 10% KDD99 datasets as shown in Table 1 as picking the first 500 records on smurf,neptune, back, teardrop, satan, ipsweep, and portsw eep and all records on other attacking types. The number of records for each type are shown in brackets in Table 1 as picking the first 500 records on smurf,neptune, back, teardrop, satan, ipsweep, and portsw eep and all records on other attacking types. The number of records for each type are shown in brackets in Table 1 too. We followed a similar preprocessing procedure as in [11]. There are 41 features including seven categorical features which were mapped into distinct positive integers from 0 to \( m - 1 \) (\( m \) is the number of states for the categorical feature). For example, 0 to 2 in protocol_type stands for TCP, UDP, and ICMP. Logarithmic scaling was applied on duration, src_bytes, and dst_bytes, and all features were deducted by the mean values and linearly scaled to \([-1,1]\).

### 5.2 Methodology

We compared our proposed ASPCA models with the standard PCA model for detection and sparsity performance, and with two state-of-the-art analytical models on PCA results: the JSPCA model [11] and a decision tree model used in [22] for interpretation performance. For the decision tree model, we formed the training set with all predicted normal records and anomalies returned by our ASPCA model as negative and positive samples, respectively. Then the decision trees were trained using the CART model from MATLAB and trimmed manually for the best interpretation.

The parameters used in our model were listed in Table 2 and discussed in Section 5.3. The number of PCs used in PCA equals the total number of features minus the number of abnormal PCs for all datasets. The results of JSPCA on the synthetic data were obtained by choosing the best performed parameters, and we directly reported their results on KDD99 in [11]. Note that, our ASPCA models make no assumptions on the anomalies in the dataset, and we built one model on the entire KDD99 dataset with anomalies from all different categories, whereas JSPCA built four models on KDD99, each including anomalies for a single major attacking category [11].

Finally, we implemented all methods with MATLAB and...
CVX, and performed all experiments on a laptop computer with 16 GB memory and a Intel(R) Core(TM) i7-4870HQ 2.50GHz CPU.

5.3 Experimental Results

5.3.1 Detection Evaluation

We first compared the various ASPCA models with the standard PCA model on the anomaly detection performance. Because all models can obtain a perfect ROC curve for the Synthetic data, we only show the ROC curves on Breast-Cancer and KDD99 in Figure 3a and Figure 3b, respectively. Note that, since ASPCA-F and ASPCA-FG use the same abnormal subspace to detect anomalies, their ROC curves are identical which are labeled as ASPCA-F(G). Similarly, the ROC curves of ASPCA-B and ASPCA-BG are labeled as ASPCA-B(G). From Figure 3a and Figure 3b, we can see that our proposed ASPCA-F(G) and ASPCA-B(G) models performed similarly or even better than PCA on anomaly detection for both datasets.

5.3.2 Sparsity Evaluation

The next set of experiments were designed to compare the sparsity of the loading matrix generated by various ASPCA models and we used the result of PCA as our baseline. We used three metrics to evaluate the sparsity of the loading matrix of the abnormal PCs, namely, \(||V||_{1,1}, Card_{0.1}\), (number of entries with absolute values bigger than 0.1), and \(Card_{0.01}\), (number of entries with absolute values bigger than 0.01), and showed the results in Table 3. We can see that all ASPCA models improved the sparsity of the loading matrix greatly over the baseline. For all datasets, the ASPCA-B model achieved better sparsity performance than the ASPCA-F model. The global optimization step improved \(||V||_{1,1}\) values for both models on Breast-Cancer and KDD99. However, in terms of cardinality, ASPCA-FG performed worse than ASPCA-F on Breast-Cancer. The global optimization step achieved the largest sparsity improvement on KDD99, as it has more abnormal PCs than the other two datasets leaving more room for the global optimization. Overall, the ASPCA-BG model achieved the best sparsity performance.

The loading matrices returned by PCA and ASPCA-B (the other three ASPCA models have very similar results) on the Synthetic data are shown in Figure 4. We can see that all ASPCA models leave some loading vectors with poor sparsity towards the end, which should be avoided as they are part of abnormal subspace. On the contrary, ASPCA-B leaves the loading vectors not so sparse towards the beginning, which need no interpretation as they belong to the normal subspace.

5.3.3 Interpretation Evaluation

Now we evaluate the interpretation performance of the ASPCA-BG model, as it has the best sparsity performance. Since we want to see how true anomalies are interpreted by our model, we selected a threshold value on SPE to ensure most of the true anomalies are detected. We show the threshold values, false positive rates (FPR), and true positive rates (TPR) for all three datasets in Table 4. We can see that all ASPCA models leave some loading vectors with poor sparsity towards the end, which should be avoided as they are part of abnormal subspace. On the contrary, ASPCA-B leaves the loading vectors not so sparse towards the beginning, which need no interpretation as they belong to the normal subspace.
we can successfully detect and interpret anomalies as well. Similar to the ones in Table 5. Using these abnormal PCs, we tell the source of each individual anomaly. Unlike JSPCA, the rules indicated by the abnormal PCs.

**Figure 4:** Loading matrix of PCs of Breast-Cancer (Top) and KDD99 (Bottom) obtained by PCA, ASPCA-F, ASPCA-B, ASPCA-FG, and ASPCA-BG from left to right.

![Loading Matrix](image)

**Table 4:** SPE Threshold

| Dataset  | SPE Threshold | TPR | FPR |
|----------|---------------|-----|-----|
| Synthetic | 0.25          | 1   | 0   |
| Breast-Cancer | 0.1003      | 1   | 0.0476 |
| KDD99    | 0.5075        | 0.8610 | 0.0659 |

**Table 5:** Components on Synthetic Data

| Index | Components                                                                 |
|-------|---------------------------------------------------------------------------|
| 1     | $0.3099A + 0.3122B + 0.6478C - 0.6430D$                                    |
| 2     | $0.7095A - 0.7047B$                                                      |
| 3     | $1F$                                                                     |
| 4     | $1G$                                                                     |

**Figure 5:** Heatmap of projection values of anomalies on abnormal PCs for Synthetic Data

The projection values of 15 anomalies on these PCs are shown in Table 5 and Figure 5, respectively. As shown in Table 5, the first three PCs correspond to the rules of $D \approx C + A$, $A \approx B$, and $F \approx 0$, respectively. The anomalies breaking these rules indeed have large projection values on the corresponding PCs. Thus, our ASPCA-BG model can not only identify the set of features that are responsible for an anomaly, but also tell the cause of the anomaly, i.e., breaking the rules indicated by the abnormal PCs.

JSPCA also successfully identified the relevant features $(A, B, D, F)$ as suggested in Figure 4. However, it cannot tell the source of each individual anomaly. Unlike JSPCA, our ASPCA models make no assumptions on whether there are anomalies present in the dataset for model training. Keeping only normal data from the Synthetic dataset, the ASPCA-BG model found four abnormal PCs with loading vectors $(0.31, 0.31, 0.64, 0.64, 0, 0, 0, 0)\top$, $(-0.71, 0.71, 0, 0, 0, 0)\top$, $(0, 0, 0, 0, 0, 0, 1)\top$, and $(0, 0, 0, 0, 0, 0, 1)\top$, which are very similar to the ones in Table 5. Using these abnormal PCs, we can successfully detect and interpret anomalies as well.

**Figure 6:** Decision tree on Synthetic Data

| Node | Features | Value |
|------|----------|-------|
| 1    | $0.3099A$ |       |
| 2    | $0.3122B$ |       |
| 3    | $0.6478C$ |       |
| 4    | $0.6430D$ |       |
| 5    | $0.7095A$ |       |
| 6    | $0.7047B$ |       |
| 7    | $1F$      |       |
| 8    | $1G$      |       |
| 9    | $-0.2172$ |       |
| 10   | $1.377$   |       |
| 11   | $2.197$   |       |
| 12   | $3.064$   |       |
| 13   | $3.06464$ |       |

The decision tree was shown in Figure 6 where on each node we showed the feature and its value used to partition the data, the number of true positives detected by ASPCA-BG in red, the number of false positives in yellow, and the number of normal data detected by ASPCA-BG in green. We can see that the decision tree model needs several rules to describe a group of anomalies which could be easily described by a clear linear combination and a threshold. In Figure 6, only the third type of anomalies, which has a large absolute value on F, is easy for the decision tree model to interpret.

**Breast-Cancer:** The projection values of 10 anomalies on the abnormal PCs obtained by ASPCA-BG for Breast-Cancer are shown in Figure 4. We can see that the malignant records have two patterns: the first four records have large projection values on the 2nd, 3rd, and 4th PCs, the rest records have large projection values on the first PC and moderate projection values on the 6th PC. We show these
The loading matrix of the abnormal PCs obtained by JSPCA on Breast-Cancer is shown in Figure 8. The relevant features are area\_se, concavity\_mean, area\_worst, fractal\_dimension\_se, perimeter\_worst, and compactness\_worst. As we can see, JSPCA cannot tell the different causes of individual anomalies. The decision tree obtained on Breast-Cancer is shown in Figure 9. Our ASPCA-BG model detected 10 true positives, 18 false positives, and 339 true negatives (shown on the root node in red, yellow, and green, respectively) with the chosen SPE threshold. The tree used concavity\_mean to separate positive and negative samples. However, the attribute concavity\_mean is orthogonal to the abnormal subspace obtained by our ASPCA-BG model, which means it is not the feature based on which our ASPCA-BG model detects anomalies. Hence, using decision trees to interpret results of a subspace-based model, such as ours, may lead to misleading interpretations.

KDD99: With the given SPE threshold, our ASPCA-BG model detected 4397 true positives on KDD99. Although our model is intended to analyze individual anomalies, we can also summarize interpretations of similar anomalies to make our discussion easier. We used a simple way to generate signatures on whether an anomaly has low or high projection values on the set of abnormal PCs. Then anomalies were grouped according to their signatures, so that the components in the signature of each group is common for most of the anomalies in the group.

In Table 7, we listed some major signatures found by the above method. Actually, for most of the cases, we can associate each signature group with an anomaly type quite well. The two numbers listed for each anomaly type are the number of detected anomalies by our model and the number of total anomalies of this type, respectively. The two numbers listed for each signature group are the number of the anomalies of this type and the total number of anomalies in the group, respectively. Some anomaly types only have one main corresponding signature groups, whereas we identified three main signature groups for warezclient\[R2L\]. For the ith PC, iL and iH represent low and high projection values on it, respectively. Finally, the components appeared in these signatures are shown in Table 8.
From Table 8 we can see that the signatures for different anomaly types varied a lot, from which we often can find the components that are consistent with the nature of each anomaly type. For example, smurf[DoS] attacks are also known as popular form of DoS packet floods, which turn out to have high src_count and count values (i.e., 16H and 8H). Teardrop[DoS] attacks try to break the host by sending mangled IP fragments, which led to high wrong_fragment values (i.e., 18H). We can see similar trends for Probe attacks too. For example, ipsweep[Probe] attacks sweep different hosts (IPs) to find cracks for hacking (i.e., 19H), whereas portsweep[Probe] attacks try to visit different service (i.e., 6H) and short connection duration (i.e., 7L). Buffer overflow[U2R] attackers try to gain the root authority on the host, and 24H indicates that the user has logged into the server with root shell. Warezclient[R2L] attackers try to download files in forbidden directories from the FTP servers.

The results obtained by JSPCA are shown in Table 8. The selected features by JSPCA are more general and similar for all categories. Some of the important features for specific attacks are missing too, for instance, root_shell for User-2-Root[U2R] attacks and hot and is_guest_login for R2L attacks as mentioned in [18].

We show the decision tree obtained on KDD99 in Figure 10. The features captured by the decision tree are consistent with the components discovered by our ASPCA-BG model to a large extent. For example, low same_srv_rate was chosen to detect neptune and satan DoS attackers, which is the same as using 2L in our model to detect the same attacks. Similarly, high protocol_type values (i.e., using ICMP protocol) was chosen to detect ipsweep and smurf attackers (detected by 1H in our model). Low dst_host_srv_count with high hot values is an important character of warezclient and guest-passed attacks (identical to 5H and 20H in our model). An interesting observation on the decision tree in Figure 10 is that a node on the tree will stop splitting as soon as the samples in the node are mostly positive or negative ones. For example, the left child node of the root in Figure 10 stopped splitting with anomalies from different attack types, in which case, our model can provide more information on the differences of the these attack types.

5.4 Parameter Selection

Our ASPCA models has two parameters to select: the number of abnormal PCs and the coefficient λ on sparsity. We know that PCA-based anomaly detection methods are sensitive to the number of PCs [17]. We plotted the detection accuracy (in terms of Area Under ROC Curve (AUC)) with different number of abnormal PCs on Breast-Cancer (with λ = 5) and KDD99 (λ = 100) in Figure 11. We selected 20 normal PCs (i.e., 10 abnormal PCs) for Breast-Cancer data and 6 normal PCs (i.e., 35 abnormal PCs), for KDD99 data, to achieve the highest AUC values for our baseline method PCA, to make the comparisons on detection accuracy fair.

The coefficient λ is a trade-off between the sparsity and the additional variance on components. With less additional variance, the variances on the whole detection space for various ASPCA models are closer to the one of PCA. We showed the variance, sparsity (valued by ||V||_1) and AUC values obtained by varying the value of λ on KDD99 and Breast-Cancer in Table 10 for ASPCA-FG and ASPCA-BG. We can see that our models are not very sensitive to λ in terms of AUC, and we selected λ = 5 for Breast-Cancer, λ = 100 for KDD99 for moderate sparsity and variance. The trends are similar for ASPCA-F and ASPCA-B, which were omitted due to space constraints. We selected the same λ values for ASPCA-F and ASPCA-B, as in ASPCA-FG and ASPCA-BG, respectively.

Table 8: Components on KDD99

| Index | Components                                      |
|-------|------------------------------------------------|
| 1     | 0.8996 protocol_type + 0.3658 logged_in        |
| 2     | 0.9494 same_srv_rate                            |
| 3     | 0.9585 dst_bytes                               |
| 4     | -0.0002 if_same_srv_rate - 0.2222 logged_in    |
| 5     | 0.1722 dst_host_same_srv_rate - 0.6286 dst_host_srv_count |
| 6     | 0.9466 dst_host_diff_srv_rate                   |
| 7     | 0.9114 duration                                |
| 8     | 0.9995 count                                   |
| 9     | 0.9716 flag                                    |
| 10    | 0.9984 dst_host_error_rate                     |
| 11    | 0.9981 src_error_rate                          |
| 12    | 0.9981 error_rate                              |
| 13    | 0.9985 dst_host_error_rate                     |
| 14    | 0.9997 is_guest_login                          |
| 15    | 0.9994 src_count                               |
| 16    | 0.9996 wrong_fragment                          |
| 17    | 0.9970 dst_host_same_srv_rate - dst_host_srv_count |
| 18    | 0.9999 hot                                     |
| 19    | 1.0 root_shell                                 |

Figure 10: Decision tree on KDD99

Figure 11: Selection on the number of normal PCs
6. CONCLUSIONS AND FUTURE WORK

Traditional PCA-based anomaly detection models are not suitable for anomaly interpretation, limiting its usage in the domains where interpretation is essential. In this paper, we found that the sparsity and orthogonality of the loading vectors are the keys to anomaly interpretation, and proposed an interpretable PCA-based anomaly detection model, the ASPCA model. We designed forward and backward ASPCA models and evaluated them on two real world datasets. Our model achieved similar or even better anomaly detection performance as the traditional PCA model, and provided meaningful interpretation for individual anomalies. Our future works will focus on three directions: 1) how to improve efficiency on high dimensional datasets; 2) how to extend our model to robust PCA for better detection performance; 3) how to extend our model to kernel PCA.

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