

Detecting Outliers Using Modified Recursive PCA Algorithm For Dynamic Streaming Data

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Abstract

Outlier analysis has been widely studied and has produced many methods. However, there is still rare a method to detect outliers for dynamically streaming batch data (online learning). In the present research, a novel online algorithm to detect outliers in such dataset is proposed. Data points are proceeded by applying a modified recursive PCA to predict sequentially parameters of the model; eigenvalues and eigenvectors of the statistical detection model are recursively updated using approximate values by perturbation methods. More specifically, the recursive eigenstructure is obtained from the derivation of the covariance matrix using the first-order perturbation technique. The Mahalanobis distance is then used as an outlier score. Our algorithm performances are evaluated using some metrics, namely accuration, precision, recall, F1-score, AUC-PR, and the execution time. Results show that the proposed online outlier detection is computationally efficient in time and the algorithm's performance effectiveness is comparable to that of the offline outlier detection algorithm via classical PCA.

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1 Introduction

An outlier is an observation that deviates so much from other observations that it raises the suspicion that it is produced by a different mechanism [15]. In detecting outliers, there are two outlier detection techniques, supervised outlier detection based on classification or regression and unsupervised outlier detection based on clustering. In the digital era, the introduction of a technology system is very important since we have entered an era, namely the era of big data. Big data is data on a large scale in terms of volume, intensity, and complexity that exceeds the capacity of standard analytical tools [27]. Emerson et al. [11] proposed that a data set will be considered large if it exceeds 20% of the RAM on a given machine and very large if it exceeds 50%, in which case even the simplest calculations will consume all the remaining RAM. Consequently, it would be time consuming to process the data using traditional methods. It is better to construct an appropriate algorithm so that the data can be managed properly and efficiently.

Online learning, also known as incremental learning, is a machine learning method that builds a learnable model for effective classification in real-time detection [18]. While, offline learning is a traditional machine learning technique that requires large computational time and time to process all data. The model uses only the previously provided data (a set of historical data). It will then require manually updating the model on more recent emerging data and apply the resulting model whenever the normal system behavior changes. The online algorithm could use all available information without storing or revisiting individual data points [8, 23]. Other previous studies developed several techniques in identifying outliers or anomalies. Bosman et al.^[5] identified anomalies in sensor systems with parameter estimation using the recursive least square (RLS) method, Zangeneh-Nejad et al. [31] studied anomalies with the DIA (Detection, Identification, and Adaptation) algorithm after estimating parameters using the RLS method. Later, Schifano et al. [25] and Wang et al. [29] detected outliers with standardized predictive residuals and to test for outliers in the n-th data where after estimating the parameters with the Bayesian framework method. Hoeltgebaum et al. [17] identified anomalies using The Hall-Buckley Eggleson (HBE) method after estimating parameters using the LASSO method. Then, Ippel et al. [19] estimated the parameters recursively with



stochastic gradient descent. And Majdoubi et al. [22] recursively estimated the parameters based on the recursive least squares method. Thuy et al. [28] provided a method consisting a deep neural network and heuristic algorithms combined with LR to boost the accuracy of attack detections in an intrusion detection system (IDS). Fieri and Suhartono [12] studied two types of soft voting models, namely machine learning-based and deep learning-based to detect offensive language a Twitter dataset and to improve the performance of the soft voting classifier method.

According to Jolliffe [20], Principal Component Analysis (PCA), is one of the oldest and most wellknown multivariate analysis techniques. This PCA method is applied primarily to reduce the dimensions of the dataset by projecting each data point into the first few principal components to obtain data of less dimension while retaining as much as possible of the variation present in the dataset [3, 2]. The Mahalanobis distance is equal to the Euclidean distance between data point and in such a transformed (axisrotated) dataset after dividing each of transformed coordinate values by the standard deviation of that direction. Thus, PCA can also be used to calculate the Mahalanobis distance [1].

In this research, we propose a novel online outlier detection algorithm to identify outliers with Mahalanobis distance using modified recursive PCA where outliers are identified as soon as a new data record appears in dataset. To be explicit, recusive eigenstructures are calculated from the covariance matrix using the first-order perturbation technique. For outlier detection score the Mahalanobis distance is applied. We then evaluate the effectiveness and efficiency of the algorithm performance evaluation using some metrics, i.e. accuration, precision, recall, F1-score, AUC-PR, and the execution time. We apply this online outlier detection algorithm on synthetic dataset.

The remainder of the paper is organized as follows: Section 2 gives recursive formulas for the sample mean and covariance matrix. It also presents approximate perturbation methods for recursive PCA, our proposed online detection algorithm, and algorithm performance evaluation using some metrics. In Section 3, we apply online and offline algorithm approaches to synthetic dataset and discuss the Mahalanobis score, and performance analysis for both approaches. Conclusions are written in Section 4.

2 Materials and Methods

In this section, we build an online outlier detection algorithm consisting of the online parameter estimation formula via modified recursive PCA and identifying the outliers in each new data arrive using the Mahalanobis distance as the outlier score.

2.1 Parameter Estimation via Modified Recursive PCA

We first derive a recursive mean formula. Given vector data $\pmb{x}_1, \pmb{x}_2, ..., \pmb{x}_{n+1} \in \Re^p$. A recursive mean formula is calculated as

$$\boldsymbol{\mu}_{n+1} = \frac{1}{n+1} \sum_{i=1}^{n+1} \boldsymbol{x}_i$$

= $\frac{1}{n+1} \sum_{i=1}^n \boldsymbol{x}_i + \frac{1}{n+1} \boldsymbol{x}_{n+1}$
= $\frac{n}{n+1} \boldsymbol{\mu}_n + \frac{1}{n+1} \boldsymbol{x}_{n+1}.$ (1)

For the covariance matrix, a recursive formula is given by the following

$$C_{n+1} = \frac{1}{n+1} \sum_{i=1}^{n+1} (\boldsymbol{x}_i - \boldsymbol{\mu}_{n+1}) (\boldsymbol{x}_i - \boldsymbol{\mu}_{n+1})^T$$

$$= \frac{1}{n+1} \sum_{i=1}^{n+1} \boldsymbol{x}_i \boldsymbol{x}_i^T - \boldsymbol{\mu}_{n+1} \boldsymbol{\mu}_{n+1}^T$$

$$= \frac{n}{n+1} (\frac{1}{n} \sum_{i=1}^n \boldsymbol{x}_i \boldsymbol{x}_i^T - \boldsymbol{\mu}_n \boldsymbol{\mu}_n^T)$$

$$+ \frac{n}{(n+1)^2} (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n) (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n)^T$$

$$= \frac{n}{n+1} C_n + \frac{n}{(n+1)^2} (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n) (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n)^T$$

$$= C_n + \frac{1}{n+1} [\frac{n}{n+1} (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n) (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n)^T - C_n].$$
(2)

In Eq. (2) we have substituted $\boldsymbol{\mu}_{n+1}$ by Eq. (1). Let \boldsymbol{C}_n be the covariance matrix at step *n*-th whose size is $p \times p$. Assume that at (n + 1)-th, \boldsymbol{C}_n changes slightly by matrix \boldsymbol{B} . This can be written as

$$\boldsymbol{C}_{n+1} = \boldsymbol{C}_n + \varepsilon \boldsymbol{B},\tag{3}$$

with small parameter $\varepsilon = \frac{1}{n+1}$. In other words, C_n is perturbed by **B**. Now, an eigen equation for C_{n+1} is given by

$$\boldsymbol{C}_{n+1}\boldsymbol{v}_{n+1} = \lambda_{n+1}\boldsymbol{v}_{n+1} \Rightarrow (\boldsymbol{C}_n + \varepsilon \boldsymbol{B})\boldsymbol{v}_{n+1} = \lambda_{n+1}\boldsymbol{v}_{n+1},$$
(4)

where $(\lambda_{n+1}, \boldsymbol{v}_{n+1})$ is the eigenpair of \boldsymbol{C}_{n+1} . Assuming that there are p distinct eigenvalues. We denote the *j*-th eigenpair of \boldsymbol{C}_n by $(\lambda_{j,n}, \boldsymbol{v}_{j,n})$ with j = 1, 2, 3, ..., p. The first order asymptotic approximation for $(\lambda_{j,n+1}, \boldsymbol{v}_{j,n+1})$ can be written as

$$\lambda_{j,n+1}(\varepsilon) \approx \lambda_{j,n} + \varepsilon \lambda_{1j,n},\tag{5}$$

$$\boldsymbol{v}_{j,n+1}(\varepsilon) \approx \boldsymbol{v}_{j,n} + \varepsilon \boldsymbol{v}_{1j,n}, \tag{6}$$

with

$$\lambda_{1j,n} = \frac{\langle \boldsymbol{B}\boldsymbol{v}_{j,n}, \boldsymbol{v}_{j,n} \rangle}{\langle \boldsymbol{v}_{j,n}, \boldsymbol{v}_{j,n} \rangle}$$
(7)

1

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$$\boldsymbol{v}_{1j,n} = \sum_{k\neq j}^{p} \frac{\langle \boldsymbol{v}_{k,n}, \boldsymbol{B}\boldsymbol{v}_{j,n} \rangle}{(\lambda_{j,n} - \lambda_{k,n})} \boldsymbol{v}_{k,n} + \beta \boldsymbol{v}_{j,n}, \qquad (8)$$

where β is an arbitrary constant and $\boldsymbol{v}_{j,n}$ is an orthonormal vector. Detailed derivation of Eq. (7) and (8) can be found in [16].

We now apply Eq. (4) to Eq. (2) with $\boldsymbol{B} = \frac{n}{n+1} (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n) (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n)^T - \boldsymbol{C}_n$ and $\varepsilon = \frac{1}{n+1}$. The recursive eigenvalue and eigenvector estimation formula can now be obtained respectively as

$$\lambda_{j,n+1} \approx \lambda_{j,n} + \frac{1}{n+1} (\frac{n}{n+1} \phi_{j,n}^2 - \lambda_{j,n}), \quad (9) \quad \mathbf{10}$$

$$\boldsymbol{v}_{j,n+1} \approx \boldsymbol{v}_{j,n} + \frac{1}{(n+1)} \left(\sum_{k \neq j} \frac{\frac{n}{n+1} \phi_{k,n} \phi_{j,n}}{\lambda_{j,n} - \lambda_{k,n}} \boldsymbol{v}_{k,n} + \beta \boldsymbol{v}_{j,n} \right),$$
(10)
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where $\phi_{j,n} = (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n)^T \boldsymbol{v}_{j,n}, \phi_{k,n} = \boldsymbol{v}_{k,n}^T (\boldsymbol{x}_{n+1} - \boldsymbol{\mu}_n),$ and β is an arbitrary constant.

Outlier Detection Method 2.2

The Mahalanobis distance measures the number of standard deviations that an observation is from the mean of a distribution, introduced by Prasanta Chandra Mahalanobis in 1930 [21]. Then the Mahalanobis distance as the outlier score of a data point \boldsymbol{x} can be defined by

$$score(\boldsymbol{x}) = \sum_{j=1}^{p} \frac{|(\boldsymbol{x} - \boldsymbol{\mu}) \cdot \boldsymbol{v}_j|^2}{\lambda_j}$$
(11)

where $\boldsymbol{\mu}$ is the centroid of the data, λ is the eigenvalue, and \boldsymbol{v} is the eigenvector. For our problem at hand the eigenstructure is given by Eq. (9) and (10). An outlier has to satisfy the following condition

$$score(\boldsymbol{x}) > \sqrt{\chi^2_{d,1-\alpha}}$$
 (12)

where $\chi^2_{d,1-\alpha}$ is chi-square distribution with degrees of freedom d and $(1-\alpha)\%$ the significance level (For more information concerning Eq. (12), see Aggarwal [1])

The Proposed Online Outlier Detection Algo-2.3 rithm

Algorithm 1 describes the procedure of detecting outliers using the Mahalanobis distance via modified recursive PCA. We describe how these parameters are updated and how outliers are identified with every step of new data.

2.4 **Performance Evaluation**

In the field of machine learning and computing, evaluating performance of a classification algorithm is very important [24, 14]. In binary classification, the input

Algorithm 1: Mini-batch Outlier Detection Algorithm via Modified Recursive PCA.

Input: a data matrix
$$X \in \Re^{n \times p}$$

1 Initialization:
2 $\mu_n \leftarrow \frac{1}{n} \sum_{i=1}^n x_i$
3 $C_n \leftarrow \frac{1}{n} \sum_{i=1}^n (x_i - \mu_n) (x_i - \mu_n)^T$
4 $\lambda_{j,n}$ and $v_{j,n}$ of C_n with $j = 1, 2, 3, ..., p$
5 for $n + 1$ to final do
6 $\phi_{j,n} \leftarrow (x_{n+1} - \mu_n)^T v_{j,n}$
7 $\lambda_{j,n+1} \leftarrow \lambda_{j,n} + \frac{1}{n+1} (\frac{n}{n+1} \phi_{j,n}^2 + -\lambda_{j,n})$
8 $\phi_{k,n} \leftarrow (x_{n+1} - \mu_n)^T v_{k,n}$
9 $v_{j,n+1} \leftarrow v_{j,n} + \frac{1}{(n+1)} \sum_{k \neq j} \frac{\frac{n}{n+1} \phi_{k,n} \phi_{j,n}}{\lambda_{j,n} - \lambda_{k,n}} v_{k,n}$
10 $v_{j,n+1} \leftarrow \frac{v_{j,n+1}}{||v_{j,n+1}||}$
11 $\mu_{n+1} \leftarrow \frac{n}{n+1} \mu_n + \frac{1}{n+1} x_{n+1}$
12 $score(x_{n+1}) \leftarrow \sum_{j=1}^p \frac{|(x_{n+1} - \mu_{k+1}) \cdot v_{j,n+1}|^2}{\lambda_{j,n+1}}$
13 if $score(x_{n+1}) > \sqrt{\chi_{d,1-\alpha}^2}$ then
14 | outlier detected
15 | record outlier with label 1
16 | else
17 | | record inlier with label 1
18 | end if
19 | end if
20 end for
Output: binary classification

data is grouped into one of two classes. In measuring the performance of an algorithm that is often used in machine learning, especially the classification model, it creates a confusion matrix [4]. This research performs a binary classification, so the results of the confusion matrix are two classes. The confusion matrix aims to compare the classification results of an algorithm with the truth classification results [13, 9]. The representation of the confusion matrix is a matrix table with four combinations of predicted values and the actual value where the table can be seen in Table 1.

We define the following loss function $I: Y \times Y \to$ $\{TP, TN, FP, FN\}$. Let $y \in \{i_0, i_1\}$ be the prediction where $i_0 =$ inlier and $i_1 =$ outlier. The mapping of the I function as follows [7]

- If $y = i_1$ and $\hat{y} = i_1$, then $I(y, \hat{y}) = TP$;
- If $y = i_0$ and $\hat{y} = i_0$, then $I(y, \hat{y}) = TN$;
- If $y = i_0$ and $\hat{y} = i_1$, then $I(y, \hat{y}) = FP$;
- If $y = i_1$ and $\hat{y} = i_0$, then $I(y, \hat{y}) = FN$.

Next, when the prediction result is a real number, a threshold value of t is needed to distinguish positive and negative classes [10].

Furthermore, we use the results of the confusion matrix table to evaluate the performance of the machine learning algorithm for making predictions, namely by calculating the values of accuracy, precision, recall/sensitivity, F1-score. To add a measure to evaluate



Table 1: Confusion Matrix.

		Predicted values			
		Positive	Negative		
Actual Values	Positive	TP	FN		
	Negative	FP	TN		

the performance of the algorithm, we also use AUC-PR that stands for area under the precision-recall curve [32, 30]. The range of AUC-PR values is between 0 and 1. Generally, the higher the AUC-PR score, the better a classifier performs for the given task. Next, we also calculate the execution time of the algorithm to evaluate the efficiency of the algorithm.

3 Results and Discussion

Our experiments are performed on several synthetic datasets. Our synthetic datasets have same number of data points that are created with the scikit-learn module "make_classification" algorithm [26, 6]. We generate synthetic datasets to simulate a two-class classification problem with 1000 samples (100 samples of the train set and 900 samples of the test set) with different number of features (p = 2, 3, 5, 10) randomly drawn following a standard Normal distribution, i.e $\mathcal{N}(0,1)$ and one binary dependent variable $y \in Y = \{0, 1\}$ being the class of the data points, the distribution of the two classes defined by Y is imbalanced, i.e. the proportion of observations for which y = 0 was 99% and y = 1was 1% with no redundant variables in the dataset. In the following subsections, we compare the Mahalanobis distance results as outlier scores and evaluate the algorithm performance via modified recursive PCA (online algorithm) and classical PCA (offline algorithm) with respect to ground-truth outlier information. In simulating each test data point in the offline outlier detection algorithm, all training data and previous test data are still used.

3.1 Mahalanobis Distance Analysis as Outlier Score

In this section, we show plots of the Mahalanobis score difference on the y-axis obtained from the results of the online and offline algorithm against the test dataset on the x-axis. The scores were obtained from the results of subtracting the Mahalanobis score using the modified recursive PCA method with the classical PCA method.

All plots display the difference in Mahalanobis scores converging to zero for some features although there is a slight spread across some test points. In particular, at 2, 3, and 5 features (Fig. 1 to 3) that the difference in Mahalanobis score values is close to zero. Meanwhile, the 10 features in Fig. 4 show that the Mahalanobis score is slightly different from zero, but still converges around zero.

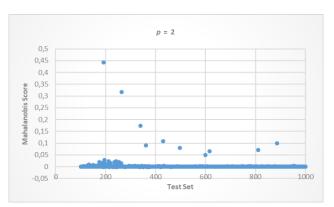


Figure 1: Mahalanobis Score Difference for 2 Features.

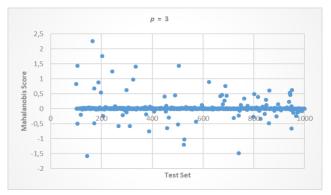


Figure 2: Mahalanobis Score Difference for 3 Features.

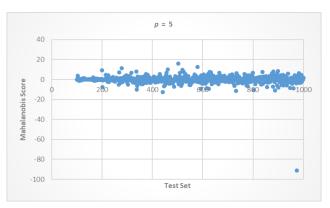


Figure 3: Mahalanobis Score Difference for 5 Features.

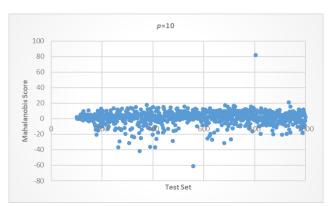


Figure 4: Mahalanobis Score Difference for 10 Features.



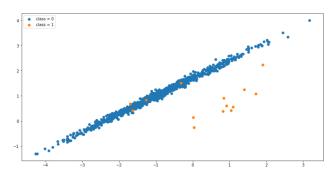


Figure 5: Plot Test Data with Two Features on Ground-Truth.

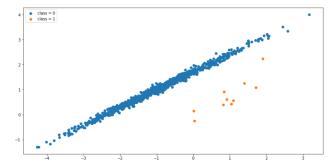


Figure 6: Plot Test Data with Two Features on Offline Algorithm Prediction Values.

3.2 Performance Analysis of Online and Offline Algorithm

In this section, we show the representation of outlier detection results on test data with two features using online and offline algorithms compared to groundtruth. The outliers are shown in yellow color and the inliers are shown in blue color. The ground-truth of the test set used is shown in Fig 5 and the predicted results of the two algorithms on the test data are shown in Fig. 6 and 7. The number of outliers on the groundtruth data is 14 as shown in Table 2. Meanwhile, the number of outliers predicted by the two algorithms is 10 as shown in Table 2. For more details about the outlier detection results with two features, it can be seen in Table 2.

And in this section, we also show the confusion matrix of the results of the online and offline outlier detec-

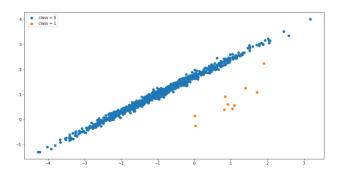


Figure 7: Plot Test Data with Two Features on Online Algorithm Prediction Values.

tion algorithms respect to ground-truth of all test data (Table 3 to 6). The results of the confusion matrix of the two algorithms are exactly the same for 2 and 3 features where both algorithms correctly predict a total of 10 outliers and correctly predict a total of 886 inliers. While the results of the confusion matrix are different for 5 and 10 features. For the 5 features, the offline algorithm correctly predicts a total of 9 outliers and correctly predicts a total of 887 inliers, while the online algorithm correctly predicts a total of 10 outliers and correctly predicts a total of 886 inliers. For 10 features, the offline algorithm correctly predicts a total of 9 outliers and correctly predicts a total of 886 inliers, while the online algorithm correctly predicts a total of 7 outliers and correctly predicts a total of 886 inliers.

Table 7 represents the comparison of the performance results of the online and offline outlier detection algorithms on the given test data. The accuracy and precision values of the two algorithms are very satisfying since the values are more than 0.90, then the accuracy of the two algorithms is exactly the same, only the precision differs slightly on 5 features where the offline algorithm's precision is slightly better. The recall and F1-score of the two algorithms are good enough where the values are in the range [0.50, 0.83], there are only differences in 5 and 10 features where the recall and F1-score of the online algorithm are comparable to the offline algorithm. The AUC-PR of both algorithms is also satisfactory since the value more than 0.75, there are only differences in 5 and 10 features where the offline algorithm's AUC-PR is slightly better. Then the execution time of the online algorithm is always faster than the offline algorithm for each feature. Overall, it can be seen that the effectiveness of the two algorithms decreases slightly as the features increase, the effectiveness of the online algorithm is comparable to the offline algorithm, and the efficiency of the online algorithm is the most outperforming.

4 Conclusions and Remarks

A way to construct an online algorithm to identify outliers for data streams was discussed in this paper. This research applied a recursive schema strategy that predicts the iterative model to update the parameters in the model when new data appears and detects outliers. In other words, an iterative schema plays an important role for data streams. We constructed an online algorithm to identify outliers with Mahalanobis distance using modified recursive PCA. In conclusion, this work showed that in terms of effectiveness the performance of the online algorithm is comparable to that of the offline algorithm and in terms of efficiency the performance of the online algorithm outperforms the offline algorithm.

We remark here that our proposed algorithm is still limited, it is quite appropriate only for the incoming data whose changes are not too large since we apply the perturbation method in our algorithm. Other things,



	Table 2. The Results of Outliers Detection.						
2 Features	Ground-Truth Outlier	Predicted Values					
	(n th test data)		(Online Algorithm)				
	92th						
	$114 \mathrm{th}$	-	-				
	$164 \mathrm{th}$						
	238th	\checkmark	\checkmark				
	$260 \mathrm{th}$						
	326th	-	-				
	$330 \mathrm{th}$	\checkmark	\checkmark				
	$397 \mathrm{th}$						
	498th						
	516th						
	$644 \mathrm{th}$	-	-				
	$710 \mathrm{th}$						
	723th	-	-				
	785th	\checkmark	\checkmark				
Total Outliers	14	10	10				

Table 3: Confusion Matrices Results of The Test Set for 2 Features.

		p = 2			
		Offline Algorithm		Online Algorithm	
		Predicted Values		Predicted Values	
		Positive (1) Negative (0)		Positive (1)	Negative (0)
Actual Values	Positive (1)	10	4	10	4
	Negative (0)	0	886	0	886

Table 4: Confusion Matrices Results of The Test Set for 3 Features.

		p = 3			
		Offline Algorithm		Online Algorithm	
		Predicted Values		Predicted Values	
		Positive (1) Negative (0)		Positive (1)	Negative (0)
Actual Values	Positive (1)	10	4	10	4
	Negative (0)	0	886	0	886

Table 5: Confusion Matrices Results of The Test Set for 5 Features.

		p = 5			
		Offline Algorithm		Online Algorithm	
		Predicted Values		Predicted Values	
		Positive (1) Negative (0)		Positive (1)	Negative (0)
Actual Values	Positive (1)	9	4	10	3
	Negative (0)	0	887	1	886

Table 6: Confusion Matrices Results of The Test Set for 10 Features.

		p = 10			
		Offline Algorithm		Online Algorithm	
		Predicted Values		Predicted Values	
		Positive (1) Negative (0)		Positive (1)	Negative (0)
Actual Values	Positive (1)	9	5	7	7
	Negative (0)	0	886	0	886



The number of Features (p) :		2	3	5	10
Accuracy	Offline Algorithm	1.000	1.000	1.000	0.990
(100%)	Online Algorithm	1.000	1.000	1.000	0.990
Precision	Offline Algorithm	1.000	1.000	1.000	1.000
1 Tecision	Online Algorithm	1.000	1.000	0.910	1.000
Recall -	Offline Algorithm	0.710	0.710	0.690	0.640
	Online Algorithm	0.710	0.710	0.770	0.500
F1-score	Offline Algorithm	0.830	0.830	0.820	0.780
	Online Algorithm	0.830	0.830	0.830	0.670
AUC-PR -	Offline Algorithm	0.859	0.859	0.848	0.824
	Online Algorithm	0.859	0.859	0.841	0.754
Time	Offline Algorithm	0.461	0.480	1.082	1.574
(second)	Online Algorithm	0.300	0.414	0.726	1.286

the present algorithm only applies for the data streams arriving one by one. Therefore, for the future work, an outlier detection algorithm involving the incoming data with mini-batch size issue can be extended.

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