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Quantile Regression and Machine Learning based Hybrid Approach for Outlier Detection in Multivariate Time Series Data

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Abstract - *Univariate and Multivariate techniques can be used to discover outliers in multivariate time data. Univariate approaches are difficult to use because they require prior adjustments. On the other hand, multivariate approaches do not necessitate any prior adjustments and find outliers straight from the original data. The dimensionality reduction concept is used by most multivariate approaches to find outliers or anomalies in the data. The most common technique for dimensionality reduction is Principal Component Analysis (PCA). It is widely used in literature surveys to discover outliers and anomalies. However, it has several disadvantages, including being less interpretable, requiring feature scaling before usage, and losing data. This research proposes a new algorithm that uses a hybrid approach of Quantile Regression and Machine Learning to find outliers in multivariate time series data. The algorithm is compared with well-known techniques PCA and Ordinary least square regression(OLSR). The experimental results revealed that the proposed algorithm is simple, effective, and retain all information while detecting outliers.*

Keywords - *Outlier, Anomaly, Univariate, Multivariate, Quantile Regression, Principal Component Analysis(PCA), Ordinary least square regression(OLSR).*

1. Introduction

An outlier in time series data is a data point that does not follow the overall collective trend, seasonal or cyclic pattern. It is noticeably different from the rest of the data [1, 2, 3]. The study of outliers in time series data investigates unusual patterns throughout time [4] [5]. Detection and correction of outliers are essential to improve the quality of the data [6]. Outlier detection techniques in time series data depend on several aspects such as Input Type, the Outlier Type, the nature of the method, etc. Based on the input data, time series can be categorized as Univariate and multivariate.

Definition 1.1 Univariate time series: Time series X = {x1,x2,…xt}t ϵ T that consists of scalar observations recorded sequentially overtime increment t ϵ T⊆ Z^+

Definition 1.2 Multivariate time series: Time series X = {x1,x2,…xt}t ϵ T that consists of an ordered set of n-dimensional vectors and each of which is recorded at specific time t ϵ T⊆ Z^+ and consists of n observations Xt= {X1t, X2t,….Xnt}.

The simplest analysis is univariate data analysis, which involves only one variable. Multivariate data is defined as data that has three or more variables. Multivariate analysis is essential for any application since it necessitates assessing a large number of dependent variables. In multivariate analysis, outliers can be classified as point, subsequence, or complete time series outliers.

1.1. Multivariate Time Series

Multivariate outliers in Multivariate time series can be detected using Univariate and Multivariate Methods. Univariate approaches can be used to analyze each variable in a multivariate time series without considering any possible interdependencies, leading to loss of information. To solve this challenge while also taking advantage of the fact that univariate detection techniques are well developed, some researchers apply a preprocessing method to multivariate time series to identify a new collection of uncorrelated variables on which univariate techniques can be used. These strategies are based on techniques for reducing dimensionality. For multivariate time series data analysis, several studies have demonstrated dimensionality reduction techniques based on univariate methodology [7] [8] [9] [10] [11]. Table-1 describes the details of the research, based on dimensionality reduction, using the univariate method for multivariate time series data.

Table 1. Univariate Methods for Multivariate time series based on dimensionality reduction

Research Paper	Methodologies used	Characteristics
Streaming Pattern Discovery in Multiple Time-Series [7]	• Principal Component Analysis(PCA) • Posterior univariate point outlier detection • Autoregressive Prediction Model	• Non-Iterative • Temporality • Considers Event of Interest • Detects Outliers
Outlier Detection in Multivariate Time Series by Projection Pursuit [8]	Projection Procedures	• Iterative Algorithm • Temporality • Considers unwanted data • Detect Outliers
Outliers detection in multivariate time series by independent component analysis [9]	Independent Component Analysis(ICA)	• Non-Iterative • Considers Event of Interest • Detect Outliers
Detecting heat events in dairy cows using accelerometers and unsupervised learning [10]	• K-means clustering • Change Detection	• Non-Iterative • Temporality • Considers Event of Interest • Detects Outliers and Events both
An outlier detection algorithm based on cross-correlation analysis for time series dataset [11]	• Cross-correlation analysis • Multilevel Otsu's method	• Iterative Algorithm • Temporality • Considers Event of Interest • Detect Outliers

All of the techniques mentioned above detect outliers; however, they are all dependent on univariate methodologies, and the process is complicated as they need previous transformations. On the contrary, multivariate methodologies do not require previous transformations and detect outliers directly based on original inputs. Model-based, Dissimilarity-based, and Histogram-based multivariate analyses are the three main types. For outlier detection, several studies have been conducted in all three areas. Table 2 summarizes the research conclusions of a multivariate time series study utilizing multivariate methodologies.

Table 2. Summarizes the conclusions of the research multivariate time series study utilizing multivariate methodologies

Research Paper	Methodologies used	Characteristics
Anomaly Detection Using Autoencoders with Nonlinear Dimensionality Reduction [12]	Autoencoders with nonlinear dimensionality reduction Estimation based model	• It is non-incremental • It is best suited for Anomaly detection
Adaptive Streaming Anomaly Analysis [13]	Nonparametric Bayesian method AOTS Prediction based model	• Temporality parameter used • Incremental in Nature • Best suited for Anomaly Detection
Outlier detection for multidimensional time series using deep neural networks [14]	Autoencoders for dimensionality reduction Convolutional neural networks and long-short term memory neural networks Estimation based model	• Temporality parameter used • Best suited for outliers
A Deep Learning Approach for Unsupervised Anomaly Detection in Time Series [15]	Deep convolutional neural network Novel deep learning-based anomaly detection approach (DeepAnT) Prediction based model	• Temporality parameter used • Best suited for Anomaly and outliers.
Robust Anomaly Detection for Multivariate Time Series through Stochastic Recurrent Neural Network [16]	OmniAnomaly, a stochastic recurrent neural network Estimation based model	• Temporality parameter used • Best suited for Anomaly

1.2 Limitations of existing studies

According to a literature review, the majority of univariate and multivariate techniques for multivariate time series employ the dimensionality reduction idea to detect outliers or Anomaly for the data. The majority of the work has been focused on anomaly detection. Outlier detection research has a lot of potentials.

Definition 1.2.1 Anomaly Detection: It identifies patterns in data that do not follow expected patterns.

Definition 1.2.2 Outlier Detection**:** It is the process of enhancing the model's accuracy by dealing with uncommon data occurrences.

PCA is a powerful technique for dimensionality reduction, anomaly identification, and outlier discovery used by numerous academics. However, it has various drawbacks, like being less interpretable, requiring feature scaling before PCA can be used, and losing information. The autoencoder technique is a PCA alternative that has been widely used in the literature to find anomalies and outliers. Autoencoder is more effective than PCA at reconstructing the original data set when k is small. However, autoencoder requires more computation than PCA. The existing techniques used in literation are complex in implementation and lose the information to a certain extent.

The section-2 of the paper will deal with some popular outlier detection strategies in time series. The section-3 will depict the proposed hybrid algorithm of QR with a machine learning approach. The section-4 depicts the experimental setup and dataset. The section-5 will discuss the results and analysis based on experimentation. Finally, the paper will end with conclusions.

2. Popular Outlier Detection Strategies in Time Series

Outlier handling is vital for time series data as it identifies data that significantly differs from the trends of the other values. Outlier treatment is essential as it influences the prediction of future values. Outlier detection in time series can be achieved by several means. As per the literature survey, a few popular techniques are Visualization Techniques, Proximity Based Techniques, Parametric Models, SVM based Models, and Statistical Models. Data needs to be analyzed based on univariate, bivariate, and multivariate dimensions.

Histograms and Box Plot are valuable visualization techniques for univariate analysis. A bar chart is best suited for bi-variate analysis. A-Line Chart is apropos for multivariate analysis. Visualization techniques can detect and present outliers systematically. However, they do not provide information that how much it is significant.

Proximity-based techniques are valuable for bivariate and multivariate analysis. These techniques are based on a distance metric. Euclidian distance is used as a measurement in these techniques.

$$ED(x,c) = \sqrt{\sum(xi - ci)^2} \quad \text{--------(1)}$$

Where xi= i^{th} observation, ci= centroids
Proximity-based techniques are simple and effective. However, runtime complexity is proportionate to the size of the data, so not suitable for a large volume of data.

Parametric models for outlier detection overcome the limitations of Proximity techniques of runtime complexity. However, in these techniques, parameters need to be estimated, so they are not useful for all problems. We cannot use these models for generic purposes. They are applicable for only specific applications.

Support Vector Machine(SVM) is a prevalent machine learning technique. The technique derives a unique separating hyperplane that separates two classes so it can be extended for the outlier detection as well. SVM is suitable for a number of scenarios:

Scenario1: For linearly separable data
Let's say that our function of decision boundary is :

$$f(x) = \pm(A^T x + b) \quad \text{----------(2)}$$

Where f(x) = +1 means all x above the boundary and -1 indicates all x below the boundary.
Certain space exists between the decision boundary and the nearest data point of either class. Rescaling is needed to bifurcate the data above and below the class. After rescaling, we have three equations:

$$A^T x + b = 1 \quad \text{---------(3)}$$

$$A^T x + b = 0 \quad \text{-------- (4)}$$

$$A^T x + b = -1 \quad \text{---------(5)}$$

SVM considers maximal margin to delineate classes. The quadratic programming problem to deal with this situation is expressed in equation (6)

$$Minimum_{A,b}\ (A^T.A)/2 \quad \text{----------(6)}$$

Where subject to yi $(A^T x + b) \geq 1\ (\forall\ data\ points\ xi)$

In this way, SVM clearly defines the boundary for linearly separable data.

Scenario2: For the data not perfectly linearly separable

SVM is also best suited for where data is not perfectly linearly separable. SVM adds a slack variable in equation (6) to achieve this situation.

$$Minimum_{A,b,\epsilon}(A^T.A)/2 \ + \ C\sum_i \epsilon i \qquad \text{--------(7)}$$

Where subject to yi $(A^T x + b) \geq 1 - \epsilon i \ and \ \epsilon i \geq 0 \ (\forall \ data \ points \ xi)$

Scenario3: For nonlinear data

SVM applies the easy formula to deal with nonlinearity in data. If we substitute xi with Øi then it provides higher-dimension mapping. The higher dimension may not be linearly separable in the original space. The equation (7) remains; only all xi are replaced with Øi.

Where subject to yi $(A^T Ø(\text{xi}) + b) \geq 1 - \epsilon i \ and \ \epsilon i \geq 0 \ (\forall \ data \ points \ xi)$

Statistical Models are widely used for outlier detection and are easy to implement. They use a simple technique like probability to detect outliers. The z-score technique is most prominent in this context. It uses mean and standard deviation to detect outliers.

$$Z - Score = (xi - \overline{x}) \ / \ S.D \qquad \text{-----(8)}$$

Where $\overline{x}$ = mean and S.D= Standard deviation

Xi ~ N (μ,σ^2) means she follows a normal distribution.

If the value of the Z-score exceeds a particular threshold value, then it is considered an outlier. The main limitation of this is it is not good for outlier labeling for small data sets. Another limitation is that standard deviation follows central tendency, affecting the extreme value of a single or few observations.

Quantile regression is an emerging statistical technique for a number of applications. It is best suited for outlier detection based on different quantiles. It does not require normalized data. It allows the analyst to eliminate assumptions and identify important variables' determinants. The equation is depicted in equation (9).

$$Q(yi) = \beta 0(r) + \beta 1(r)xi1 + \cdots + \beta m(r)xim \qquad \text{----------(9)}$$

Where m= number of regressor variables.

r = r^{th} quantile

xi=independent variables

yi= dependent variable

3. Proposed Hybrid Algorithm of QR With Machine Learning

Quantile Regression (QR) [17] [18]is a complement to the widely utilized Ordinary Least Squares regression(OLSR) analysis technique [19] [20]. Quantile Regression solves a variety of issues of OLSR. Heteroscedasticity is a common problem for OLSR. OLSR is susceptible to severe outliers, which can dramatically distort the results. Quantile regression is a useful tool for dealing with outliers in a data set. However, it is not capable of offering a more comprehensive answer for the linear and nonlinear interaction between random variables in time series data. The Support Vector Machine (SVM) [21] [22] [23 [24] [25]]is a versatile machine learning technology that has a number of advantages that make it ideal for time series analysis. The few relevant advantages in context to time series are:

- When we don't know what to do with the data, SVMs come in handy.
- SVM's actual strength is the kernel technique. We can solve any complex problem with the right kernel function.
- It handles high-dimensional data reasonably well.
- Models based on support vector machines (SVMs) have been generalized.

The proposed hybrid algorithm is a fusion of Quantile Regression(QR) and Support Vector Machine(SVM) depicted in Table-3.

Table. 3 Steps of Proposed Hybrid Algorithm

Step 1: Extract features F= { f1,f2,f3,…fm} from dataset D= { t1,t2,t3,…..tn}
Step 2: Decide the response variable onto which hybrid algorithm be fitted
Step 3: Select the Gaussian Kernel of SVM $K_f(p,q) = e^{-(\lVert p-q \rVert 2)/2\sigma 2}$
Step 4: Decide the quantile that shall be estimated F_Y(y) = P (Y <= y). The T^{th} quantile is given by $QY(T) = F_Y^{-1}$ = infinite{ y : F_Y(y) >= T} Where T϶ (0,1)
Step 5: Select the tuning parameters associated with the kernel, such as degree, scale, offset, order, sigma

4. Experimental Setup and Dataset

The R programming language was chosen for the investigation for various reasons. It is an open-source software project that may be freely downloaded together with its documentation from the CRAN website. It's amazing for visualization and has many more features than other programs. It provides excellent packages for quantile regression and supports vector machine implementation. A number of packages have been installed for experimentation.

 # Installing Packages
install.packages("quantreg") // For Quantile Regression
install.packages("ggplot2") // For Visualization
install.packages("e1071") // For Support Vector Machine

 # Loading the packages
library(quantreg)
library(ggplot2)
library(e1071)

California Health and Human Services(CHHS) dataset is used for experimentation (https://data.chhs.ca.gov/dataset/covid-19-time-series-metrics-by-county-and-state/resource/046cdd2b-31e5-4d34-9ed3-b48cdbc4be7a). The dataset comprises of statewide COVID-19 cases death tests. The table-4 describes the sample of this dataset.

Table. 4 Sample of Dataset

Fields																
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**	**17**
5/17/2020	Alameda	County	1685886	50	2867	1	94	304	43462	40	2562	62	2389	0	83	1244
5/18/2020	Alameda	County	1685886	95	2962	1	95	2542	46004	157	2719	53	2442	1	84	1122
5/19/2020	Alameda	County	1685886	73	3035	0	95	2349	48353	137	2856	51	2493	4	88	841
5/20/2020	Alameda	County	1685886	75	3110	0	95	2209	50562	115	2971	61	2554	1	89	994
5/21/2020	Alameda	County	1685886	73	3183	1	96	2292	52854	98	3069	52	2606	0	89	1207
5/22/2020	Alameda	County	1685886	65	3248	1	97	2239	55093	83	3152	116	2722	2	91	1380
5/23/2020	Alameda	County	1685886	54	3302	1	98	1099	56192	46	3198	61	2783	0	91	1857
5/24/2020	Alameda	County	1685886	41	3343	1	99	655	56847	27	3225	47	2830	1	92	1576
5/25/2020	Alameda	County	1685886	73	3416	1	100	633	57480	29	3254	70	2900	0	92	1841

Where Fieldnames:

1-Date	2-Area	3-Area_Type	4-Population
5-Cases	6-Cumulative_cases	7-Deaths	8-Cumulative_deaths
9-Total_cases	10-Cumulative_total_cases	11-Positive_tests	12-Cumulative_positive_tests
13-Reported_cases	14-Cumulative_reported_cases	15-Reported_deaths	16-Cumulative_reported_deaths
17-Reported Tests			

5. Results and Analysis

There are 17 features in the dataset presented in the previous section. Because several values in the dataset contain NA values, the data were first preprocessed. Feature extraction was performed after preprocessing. To extract features, the correlation values with cumulative death were employed. Figure 1 depicts the relationship between numerical fields and cumulative death. According to the graph, cumulative positive tests, cumulative reported deaths, cumulative reported cases, cumulative total cases, population, and reported tests fields are all substantially linked with cumulative deaths.

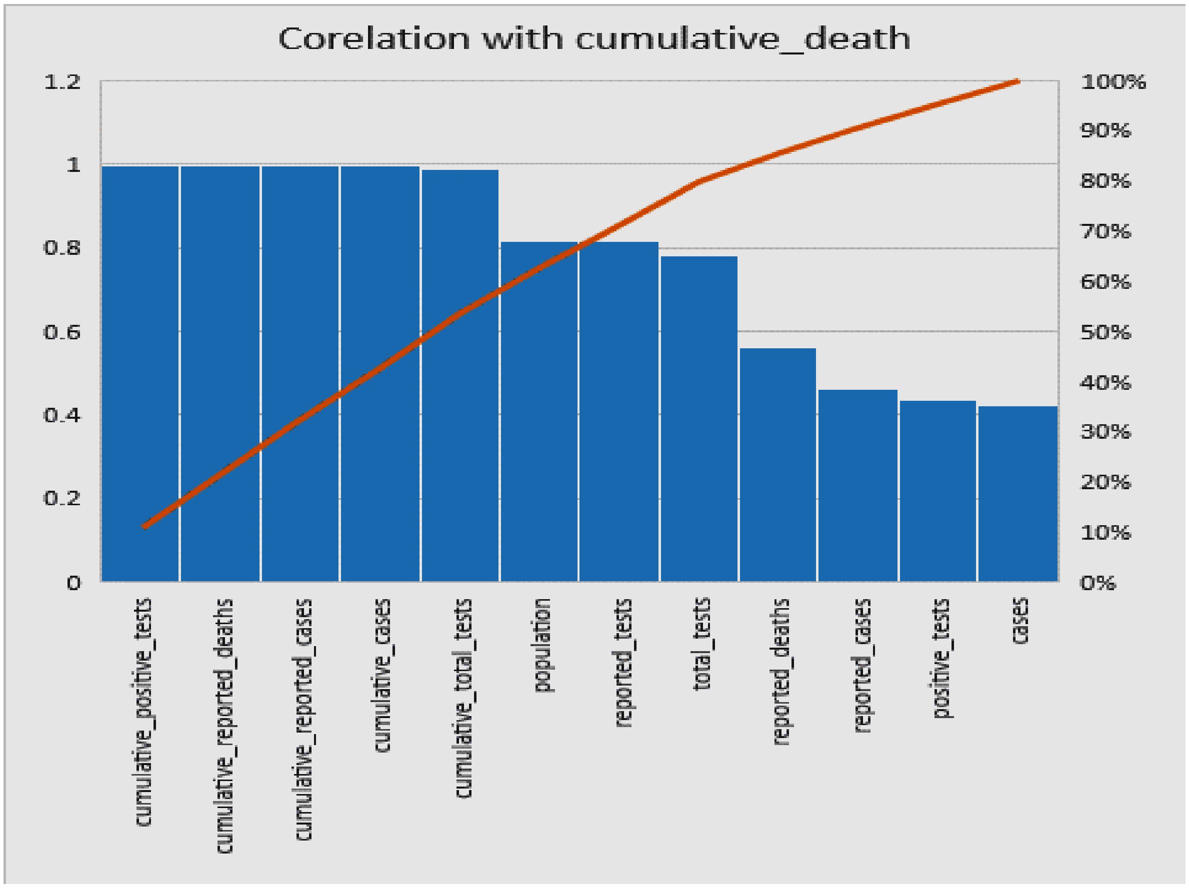

Fig. 1 Correlation of numerical fields with cumulative_death

The famous OLSR model is employed on the data, and its result is depicted in Table-5.

Table. 5 OLSR Model results on a dataset

Min	-227.41
1Q	-16.31
Median	-1.93
3Q	10.09
Max	1031.83
Intercept	7.869e-01
cumulative_positive_tests	1.926e-02
cumulative_reported_deaths	4.787e-01
cumulative_reported_cases	8.373e-03
cumulative_cases	-1.926e-02
cumulative_total_tests	-2.148e-04
population	6.382e-05
reported_tests	2.558e-04

The results demonstrated that the OLSR model only analyses standard quantiles, such as 25%, 50%, and 75%, and that the outcomes are only dependent on central tendency values. It lacks a system for detecting and dealing with outliers or anomalies in the data.

PCA is a single-value decomposition approach that uses eigenvalues and eigenvectors. It's best used to reduce dimensionality. It is commonly utilized in the literature for anomaly and outlier detection. PCA is employed in the dataset, and the result generated is depicted in Table-6.

Table 6. Principal Components of the dataset

	Comp.1	**Comp.2**	**Comp.3**	**Comp.4**	**Comp.5**	**Comp.6**	**Comp.7**
Standard deviation	7.479735e+06	2.457450e+06	9.155847e+04	1.257349e+04	7.516143e+03	3.961634e+03	3.054724e+02
Proportion of Variance	9.024476e-01	9.741343e-02	1.352218e-04	2.550122e-06	9.112543e-07	2.531619e-07	1.505198e-09
Cumulative Proportion	9.024476e-01	9.998611e-01	9.999963e-01	9.999988e-01	9.999997e-01	1.000000e+00	1.000000e+00

PCA significantly decreased the dataset's dimensionality and yielded seven main components. Because the dominance of each of the seven major components is not equal, we can exclude several components to get the final results. However, deciding which elements to maintain for the final transformation is difficult. If we simply use a few components, we will lose a lot of information.

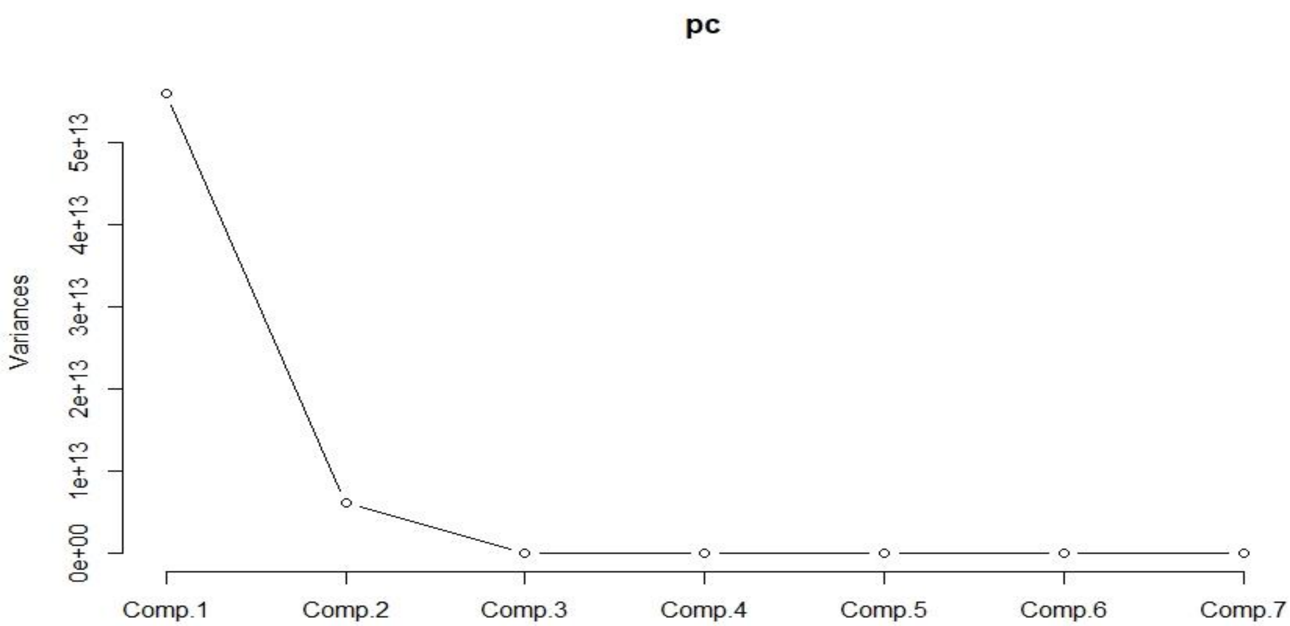

Fig. 2 Line Chart of Principal Components based on dominance

Although component 1 is the most important, selecting multiple other components is tough because they are all in the same line. The PCA did a great job with outliers. However, the method is complicated and results in data loss.

The proposed approach estimates all independent variables (in our example, seven) with different quantiles ranging from 0.1 to 1.0. According to the proposed technique, Table-7 shows estimates of independent variables based on multiple sample quantiles.

Table. 7 Estimates of Independent Variables based on Sample Quantiles

Estimates/ Quantiles	0.05	0.35	0.65	0.95
Intercept	-6.054404e+00	-1.930684e+00	1.435439e-01	4.914375e+01
population	9.596568e-06	2.626092e-05	4.594839e-05	6.677757e-05
cumulative_cases	1.792883e-03	-2.511338e-03	-9.953949e-03	-5.019871e-03
cumulative_total_tests	-8.949740e-05	-1.469825e-04	-1.720447e-04	-1.799076e-04
cumulative_positive_tests	6.537746e-03	9.277995e-03	1.379150e-02	1.270507e-02
cumulative_reported_cases	-7.193738e-03	-1.911073e-03	3.281780e-03	4.440884e-04
cumulative_reported_deaths	9.276051e-01	7.523044e-01	5.906452e-01	5.707302e-01
reported_tests	1.166131e-03	1.504124e-03	2.428976e-03	-1.979883e-04

The suggested approach can calculate independent variable estimates for any quantile. It's simple to spot outliers and deal with them efficiently. In terms of the suggested technique and Ordinary least square regression, Figure-3 illustrates several independent variables' values and confidence intervals (OLSR).

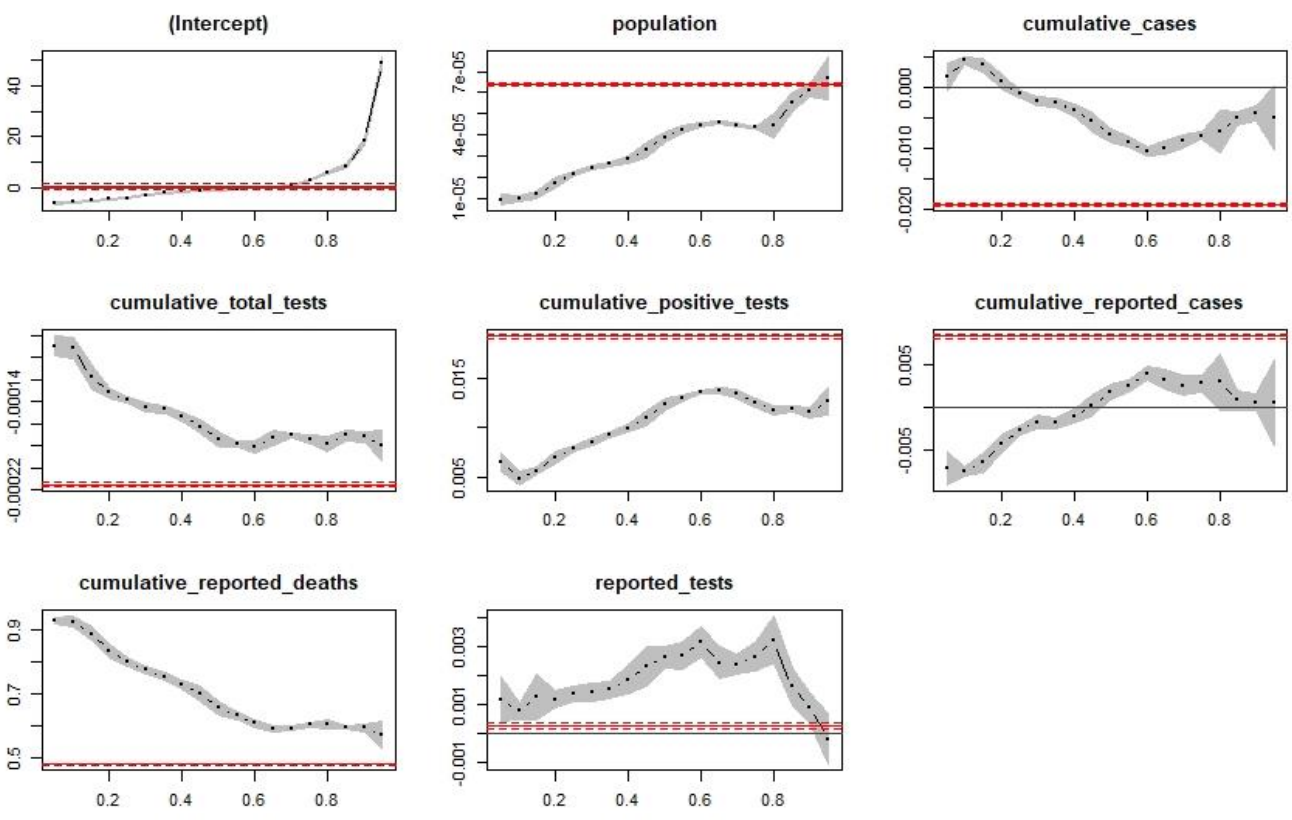

Fig. 3 Values and Confidence Intervals of Proposed Technique VS OLSR

The magnitude of Ordinary least square regression(OLSR) is represented by three red lines (one solid line in the middle and two dotted lines surrounding it). The values are shown by the main solid line, while the confidence interval is represented by the dotted lines surrounding it. The OLSR magnitude is flat and only considers a few quantiles. The insides of the curves with brown and dots are the outcome of the suggested algorithm. The outcome revealed that the magnitude of values in the dataset is made up of the values of all quantiles. When all values are taken into account, the outcome can be terrible. The suggested technique creates independent variable estimates for any quantile, which aids in determining which values are critical for analyzing the problem at hand.

6. Conclusion

Using Quantile Regression and Machine Learning approaches, the research presented a hybrid algorithm for detecting outliers in multivariate time series data. Outlier identification approaches for multivariate time series data currently available have a number of drawbacks. The most notable drawbacks are the complexity of the problem and the loss of data. The suggested technique is based on the well-known quantile regression and machine learning concepts and is constructed with simple stages. The technique is tested using the California Department of Health and Human Services (CHHS) dataset. The dataset contains 27081 observations and 17 variables after preprocessing. Seven high-correlation variables are chosen for the model development based on their correlation with the dependent variable. The well-known OLSR model is used on the data, and the results show that the OLSR model simply looks at conventional quantiles like 25%, 50%, and 75% and that the outcomes are only based on central tendency values. It doesn't have a system to detect and deal with outliers or anomalies in the data. The Principal Component Analysis (PCA) model was used on the same data set, and the findings revealed that PCA did a good job with outliers. However, the procedure is difficult and results in data loss. The proposed approach was tested on the data set, yielding estimates for all independent variables with quantiles ranging from 0.1 to 1.0. Based on the results of the suggested algorithm's testing, it has been determined that:

- The suggested approach can calculate independent variable estimates for any quantile.
- It's simple to spot outliers and deal with them efficiently.
- It does not result in loss of information.
- It helps determine which values are critical for the analysis of the problem at hand.
- It is easy to implement and efficient for outlier detection.

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