



Outlier and Leverage Point Detection Procedures in Nonlinear Regression Models

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ABSTRACT

A major problem that statisticians have been confronted with, while dealing with regression analysis, is presence of outliers in data and a suitable method to detect it. Therefore, the detection of outliers and influential points is an important step of the regression analysis. Even though, some methods of detections have been provided in literature but to the best of our knowledge, the areas on nonlinear regression and detection comparison with respect to the strength and proportion of outliers have not been exploited. Therefore, in this study, the performance of methods of detecting outlier were compared at different proportion and strength of outliers, and sample sizes. Simulation study was conducted to investigate the performance of Dixon, Chi-square and Grub's test in the detection of outliers at different proportion of outliers in first, second or both independent variables. Data were generated based on multiple nonlinear regression model with only two independent variables. Certain proportion (10%, 20, and 30%) of outliers were injected into first, second, and both independent variables at different sample sizes of 10, 30 and 100 to represent small, moderate and large sample sizes respectively. The normal distribution was assumed for the simulation while outliers were from uniform distribution. It was concluded that Deffits (DDi) has the highest probability to detect the actual number of the outliers injected over the sample size from the smallest to the highest followed by Cook's Distance (CDi).

Keywords: Outliers detection, Simulation, Nonlinear regression, High leverage points

INTRODUCTION

In regression analysis, an outlier is an observation which is large or different in magnitude compared to other observations in the data set (Stephen and Senthamarai, 2017). The detection of outliers and influential points is an important step of the regression analysis. Outlier detection methods have been used to detect and remove anomalous values from regression analysis is a statistical technique for analyzing and modelling the relationship between dependent variable and one or more independent variables. This technique uses the mathematical equation to establish the relationship between variables. It is a predictive modelling technique used for forecasting and to find casual effect relationship between the variables. The applications of regression analysis were found in almost every field including physical sciences, chemical sciences, engineering, economics, finance, pharmacology, life and biological sciences, social sciences, and other fields of study. In simple linear regression model, only one independent variable (x) is used to predict a

single dependent variable (y). The scatter diagram is used to diagrammatically display the relationship between independent variable and dependent variable (Montgomery *et al.*, 2015).

A major problem that statisticians have been confronted with, while dealing with regression analysis, is presence of outliers in data and a suitable method to detect it. Therefore, the detection of outliers and influential points is an important step of the regression analysis. Even though, some methods of detections have been provided in literature (see for instance, Liu, Shah, and Jiang, 2004; Stephen and Senthamarai, 2017) but to the best of the researchers' knowledge, the areas on nonlinear regression and detection comparison with respect to the strength and proportion of outliers

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have not been exploited. Therefore, in this study, the performance of three methods of detecting outlier will be compared at different proportion and strength of outliers, and sample sizes in nonlinear regression, so as to determine the best method (s) of detecting outliers for the particular number and strength of outliers.

There are numerous outlier’s detection methods explained by different authors. Most of these authors try to establish algorithms to detect outliers that are based on distance. Some of these approaches to detect outliers in regression model are cluster analysis-based method, distances methods and the statistically approaches, Azeez et al., (2016) proposed five approaches of outlier detection in regression model are considered and the results are used to know which of them perform best. Manenti, and Buzzi-Ferraris (2009) discussed the problem of outlier’s detection in nonlinear regression problems. They concluded that when several outliers are identified, nonlinear regression model is probably inadequate to completely describe the overall experimental field. Michael (2016) conducted a study on identifying outliers for nonlinear regression. The study compared six methods of outliers’ detections developed that combined with three estimation techniques.

Riazoshamshabshah, Midi and Ghilagaber (2018) worked on outlier detection method in Non-linear Regression. Six detection methods were developed that combined with three estimation techniques. The study shows that Cook distance is capable of identifying the correct outliers.

METHODOLOGY

In this study, there are numbers of method of detecting outliers in non-multiple regressions may be classified in to two groups, namely, graphical and analytical methods. However, three different methods of detecting outliers will be considered in this study, these are Cook’s Square Distance (CDi), Deffits Distance (DDi) and Mahalanobis Distance (MDi). These three methods are considered because they are analytical. This study will be based on Simulation to investigate the performance of the methods of detecting outliers in nonlinear regression at different proportion of outliers in first, second or both independent variables.

The methods that will be considered are analytical methods which have their procedures as follows:

Table 1: Outlier Detection Methods.

S/No	Methods	Formula	Cut-off Value
1	Cook’s Distance (CDi)	$CD_i^2 = \left(\frac{e_i^2}{p}\right)\left(\frac{h_{ii}}{1-h_{ii}}\right)$	$CD_i^2 > 0.5$ and that case where $CD_i^2 > 1$ considers any i^{th} observation with values exceeding one (1) is as an outlier. $2\sqrt{p/n}$
2	Deffits Distance (DDi)	$DDi = \frac{\frac{1}{2}e_i}{(\sigma_i(1-h_{ii}))}$	p =Number of independent variable n = sample size of the data. <i>for $n = 10, p = 2. /DEFFIT/ > 0.8944$</i> <i>for $n = 30, p = 2. /DEFFIT/ > 0.5164$</i> <i>for $n = 100, p = 2. /DEFFIT/ > 0.2828$</i>
3	Mahalanobis Distance (MDi)	$MD^2 = (x_i - \bar{x})S^{-1}(x_i - \bar{x})' = (n-1)\left[h_{ii} - \frac{1}{n}\right]$	If $MD^2 > X_{p-1,0.99}^2$ where $X_{p-1,0.99}^2$ is 99th percentile of a chi-square distribution with $p-1$ degrees of freedom then there is an outlier.

Cook’s Square Distance

Cook’s square distance (CDi) of unit i is a measure base on the square of the maximum distance between the OLS estimate on all n points $\hat{\beta}$ and the estimate obtained when the i^{th} point, say $\hat{\beta}_i$. Cook and Weisberg suggest

examining cases with $CD_i^2 > 0.5$ and that case where $CD_i^2 > 1$ should always be studied Cook and Weisberg 1989. This distance measure can be expressed in a general form

$$CD_i^2 = \frac{(\hat{\beta}_i - \beta)'(X'X)(\hat{\beta}_i - \beta)}{p\hat{\sigma}} \quad (1)$$

$i = 1, 2, \dots, n$. However, substitute CD_i^2 statistic may also be rewritten as

$$CD_i^2 = \left(\frac{e_i^2}{p}\right) \left(\frac{h_{ii}}{1-h_{ii}}\right) \quad (2)$$

all of which are related to the full data.

For this research work Cooks square distance ($CD_i^2 > 1$) considers any i th observation with values exceeding one (1) is as an outlier.

Deffits Distance (DDi)

Deffits is a diagnostic meant to show how influential a point is in a statistical regression. Its measure how much the predicted for i would change if the i th case is being excluded from the analysis. For each observation i computed

$(\hat{y}_i - y_{i(i)})$ or $(h_{ii}e_i) / (1 - h_{ii})$ which tells how much the predicted value \hat{y}_i , at the design point x_i would be affected if the i th case were deleted. The standardized version of Deffits is

$$\text{Deffit} = \frac{\frac{1}{2}(h_{ii}^2 e_i)}{(\sigma_i(1-h_{ii}))} \quad (3)$$

σ_i is the standard error estimated with out the point i

h_{ii} is the leverag for the point

$i = 1, 2, \dots, n$. Belsley et al., (1980) suggested that any observation for which

$$/DEFFIT/ > 2\sqrt{p/n} \quad (4)$$

warrants attention for outliers.

p = Number of independent variable n = sample size of the data

for $n = 10, p = 2$. $/DEFFIT/ > 0.8944$

for $n = 30, p = 2$. $/DEFFIT/ > 0.5164$

for $n = 100, p = 2$. $/DEFFIT/ > 0.2828$

Mahalanobis Distance (MDi)

This measures the leverage by means of MD_i (Mahalanobis distance), where

$$MD^2 = (x_i - \bar{x})s^{-1}(x_i - \bar{x})' = (n - 1)[h_{ii} - \frac{1}{n}] \quad (5)$$

$i = 1, 2, 3 \dots n$ Where

$$\bar{x} = \sum x_i / n \text{ and } \sigma^2 = \frac{1}{n-1} \sum (x_i - \bar{x})' (x_i - \bar{x}) \quad (6)$$

If $MD^2 > X_{p-1,0.99}^2$ where $X_{p-1,0.99}^2$ is 99th percentile of a chi-square distribution with $p - 1$ degrees of freedom then there is an outlier.

Source of Data

All data used for this study were simulated, because it might be difficult to get secondary data that contain required number of outliers. Simulation technique is a dependable tool in situations where statistical or mathematical experiment is either too complex or too costly. According to Kapoor (2001), simulation is the process of designing a model of real system by conducting experiments with this model for purpose of understanding the behavior of the operation of the system.

Method of Simulation and Analysis

A set of replication of data sets are generated from the multiple nonlinear regression model with two independent variables stated as follows

$$y_i = \beta_0 + \exp[\beta_1 x_{1i} + \beta_2 x_{2i}] + e_i, \quad \dots 7$$

Where all regression coefficients β_i were fixed to be $\beta_i = 1, i = 0, 1, 2$ and the errors are assumed to be independent. The independent variables were independently simulated from standard normal $N(0,1)$ the outlier were injected to the sample from uniform distributed $U(5,10)$ the data sets are generated with two regressor ($p=2$) and the sample sizes considered are small, moderate and large samples with $n=10, 30,$ and 100 respectively. The outliers are introduced to the simulated data at three different levels of 10%, 20% and 30% for each set of simulated data.

The following procedures were taken for the simulation and analysis:

1. X1 and X2 were simulated from $N(0,1)$ using R Statistical software
2. Ten (10%), twenty (20%) and thirty (30%) percent of outliers were introduced respectively from $U(5, 10)$ into each sample of data generated for X1 and X2 from normal distribution. The simulation was repeated 1000 times.
3. The data simulated were analyzed and the following were examined:

- i. The number of times the outliers were detected.
 - ii. The number of times each test statistics correctly identifies actual percentage number of Outliers introduce were.
 - iii. The probability of times outliers at a higher level.
 - iv. The probability of time outliers at a lower level.
4. The codes for simulations are given below.
 Compute sample size of 10 with 10% outlier on X1, X2 and (X1 & X2) for equation 2, 3 and equation 5 respectively
- 5. From R statistical software, each statistic is computed for each sample and replicates.
 - 6. We make comparison of detection of outliers by counting the number of times that each statistic at a higher level and at a lower level accurately and identifies outliers.

The variation in comparison of three outlier detection methods will provide an indication of the sensitivity of the methods. Thus, the best method(s) were recommended for various sample size.

Table 2: The code of simulation for the comparison for the three method

Sample Size	Outlier Percentage
10	10%
	20%
	30%
30	10%
	20%
	30%
100	10%
	20%
	30%

Computational Procedure

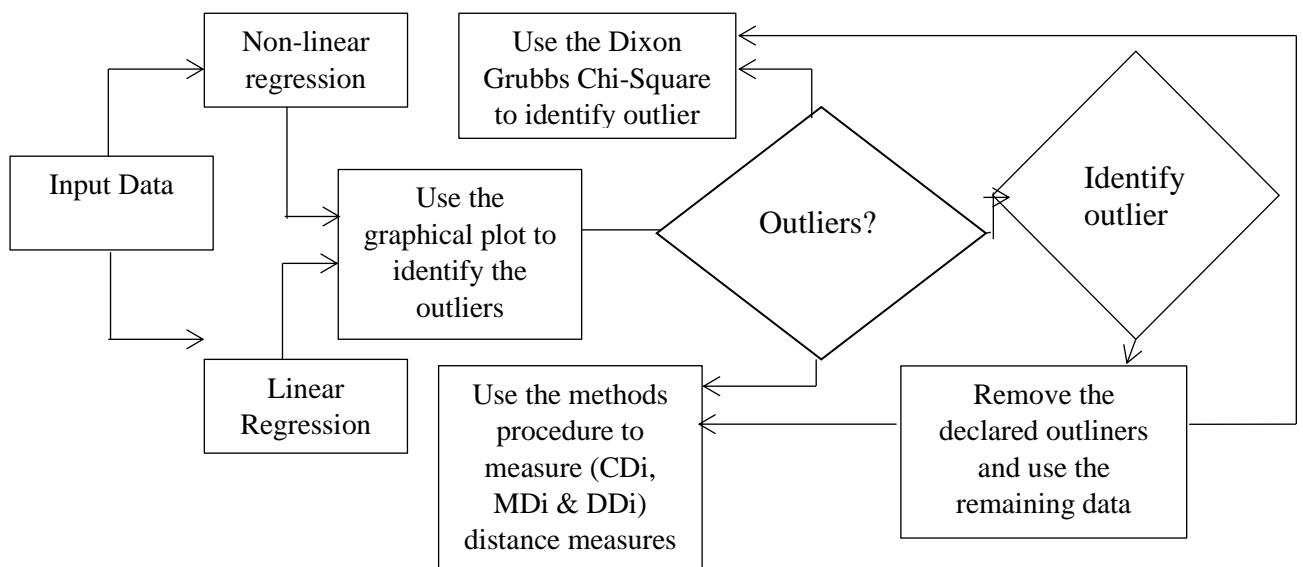


Fig. 1: Diagram for computational Procedure

Graphical Representation

Visualization of dataset is very important of any kinds of analysis. Researchers firstly want to show the data pattern and based on the data pattern they take the decision what they will want to do further. But it is very difficult task sometimes. One of the difficult tasks to detect the outliers in the dataset is very critical. Here, we have considered the graphical methods to suspect the presence and absence of unusual observations I the datasets. This is the preliminary process to progress the work and finally we will apply the analytical methods for outlier detection. The results of the graphical representation are following below.

Plot of Sample Data with outlier Contaminations when Sample Size is 10

Meanwhile, samples of data simulated that involve 1, 2, and 3 outliers using sample size of 10 are plotted and presented as follows:

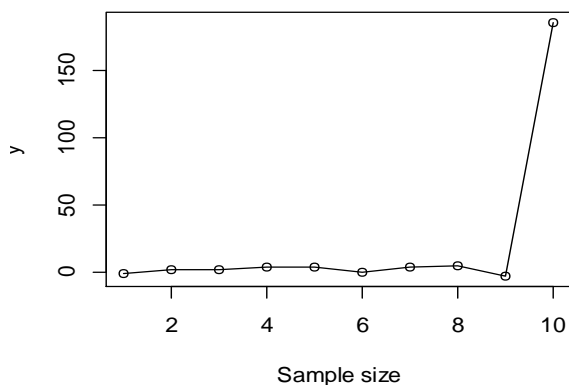


Fig. 2: Samples of Data Simulated with One Outlier and Sample size of 10

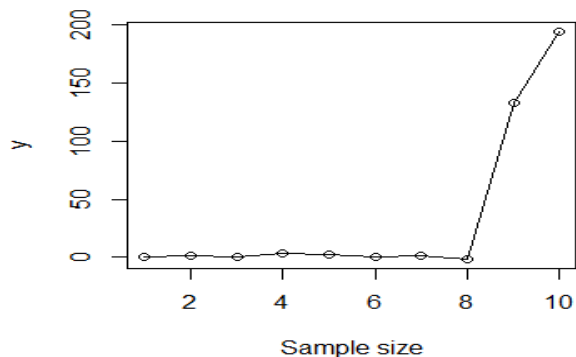


Fig. 3: Samples of Data Simulated with Two Outliers and Sample size of 10

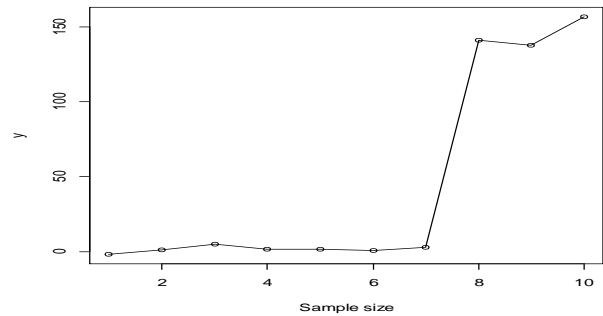


Fig. 4: Samples of Data Simulated with Three Outliers and Sample size of 10

Plot of Generated Data with Outlier Contamination When Sample Size is 20

Samples of data generated for outliers of 1, 2, and 3 at sample size of 20 are plotted and presented as follows

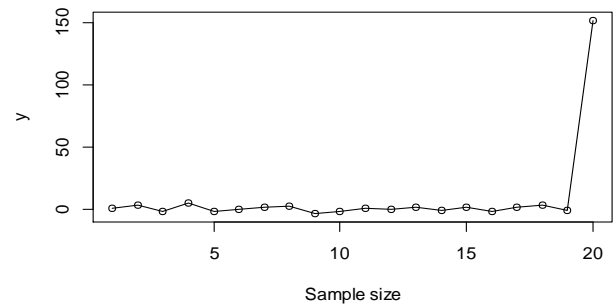


Fig. 5: Samples of Data Simulated with One Outlier and Sample size of 20

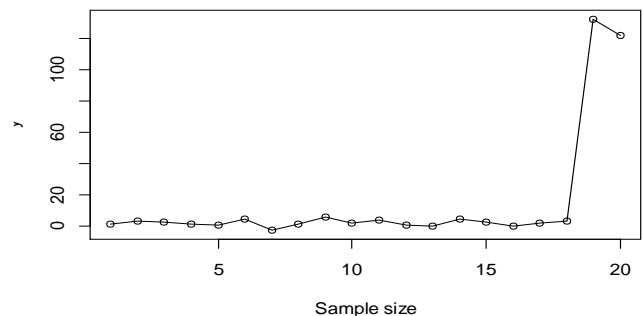


Fig. 6: Samples of Data Simulated with Two Outlier and Sample size of 20

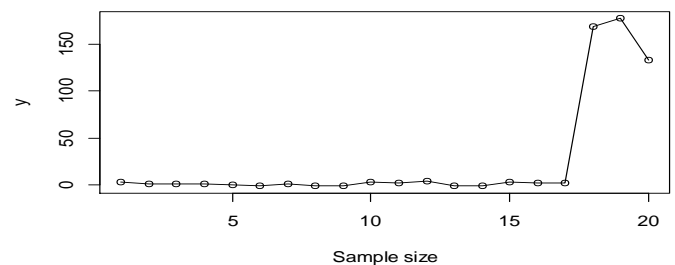


Fig. 7: Samples of Data Simulated with Three Outlier and Sample size of 20

Plot of Generated Data with Outlier Contamination When Sample Size is 100

Samples of data simulated that involve 1, 2, and 3 outliers with sample size of 100, are plotted and presented as follows:

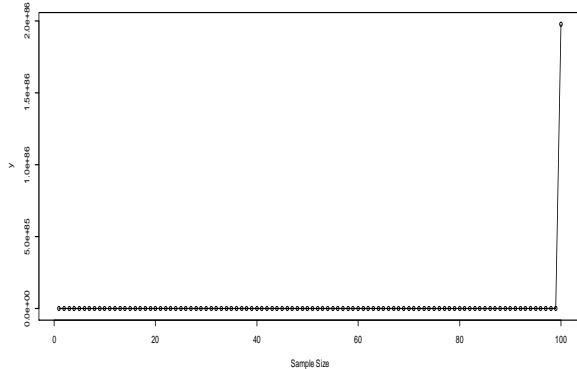


Fig. 8: Samples of Data Simulated with One Outlier and Sample size of 100

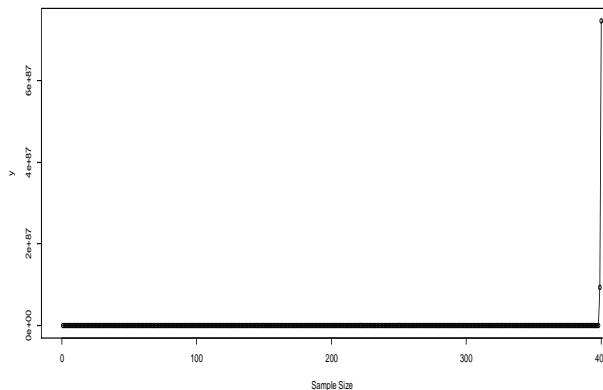


Fig. 9: Samples of Data Simulated with Two Outliers and Sample size of 100

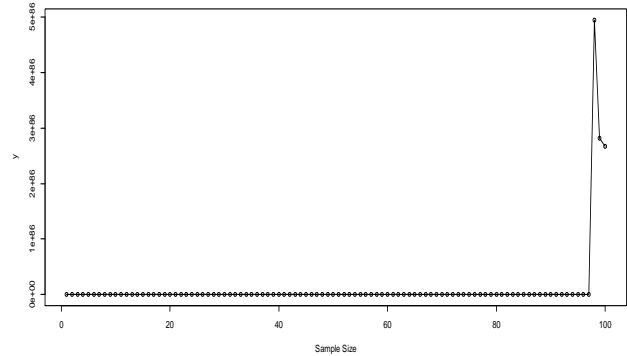


Fig. 10: Samples of Data Simulated with Three Outliers and Sample size of 100

RESULTS

Simulation Results

The sample of data generated at different categories and sample sizes are presented in graphs as discussed in the subsequent sections. The results of the three methods of outlier’s detection were presented in Table 3 - 8. In the first instance, 10% outlier was introduced to 10, 30 and 100 sample sizes of data generated; thereafter 20 and 30 percents of outlier were introduced respectively. Furthermore, the data simulated were analyzed by the three statistics (CDi, MDi and DDi). The experiment was repeated 1000 times for the three statistics and each sample size. Table 3, 4 and 5 showed the Probabilities of correctly identifying actual percentage number of Outliers at a higher level of X_1 , X_2 and $(X_1 \& X_2)$, Table 6, 7 and 8 show probability of correctly identifying actual percentage number of Outliers in at a lower level of X_1 , X_2 and $(X_1 \& X_2)$.

Table 3: probability of correctly identifying actual percentage number of Outliers at higher level in First Predictor X_1

Sample Size	outlier Percentage	CD ² _i		MD _i		DD _i	
		Dixon Statistic	P-value	Chi-sq. Statistic	P-value	Grub’s Statistic	P-value
10	10%	1	2.2e-16	8.1	0.0044	2.8460	2.2e-16
	20%	0.9430	2.2e-16	8.0738	0.0045	2.8414	1.5e-10
	30%	0.5548	0.0126	6.2113	0.0379	2.4922	0.0044
30	10%	0.9814	2.2e-16	28.011	1.206e-07	5.2925	2.2e-16
	20%	0.4381	2.2e-16	15.231	9.511e-05	3.9027	5.081e-05
	30%	0.5514	2.2e-16	12.646	0.0003	3.5560	0.0001
100	10%	2.5560	0.0421	46.511	9.112e-12	6.8198	1.221e-13
	20%	1.5560	0.0446	54.496	1.558e-13	7.3821	2.2e-16
	30%	2.5560	0.0279	48.419	3.442e-12	6.9583	2.22e-14

Source: Author’s Computation using R

Table 4: Probability of Correctly Identifying Actual Percentage Number of Outliers at higher level in Second Predictor X₂

CD ² i			MDi		DDi		
Sample size	Outlier	Dixon Statistic	P-value	Chi-sq. Statistic	P-value	Grubbs Statistic	P-value
10	10%	1	2.2e-16	8.1	0.0044	2.8460e+00	2.2e-16
	20%	0.9422	2.2e-16	8.0731	0.0044	2.8413	1.665e-10
	30%	0.1562	0.0161	4.1691	0.0411	2.0418	0.0975
	10%	0.8845	2.2e-16	26.752	2.313e-07	5.1722	2.2e-16
30	20%	0.7401	2.2e-16	16.186	5.741e-05	4.0232	1.67e-05
	30%	0.78224	2.2e-16	20.385	6.334e-06	4.5149	3.291e-08
100	10%	0.9761	2.2e-16	79.272	2.2e-16	8.9034	2.2e-16
	20%	0.9056	2.2e-16	26.978	2.058e-07	5.1940	1.053e-16
	30%	0.9112	2.2e-16	96.522	2.2e-16	9.8245	2.2e-16

Source: Author’s Computation using R

Table 5: Probability of Correctly Identifying Actual Percentage Number of Outliers at higher level in First and Second Predictors(X₁& X₂)

Sample Size	Outlier	CD ² i		MDi		DDi	
		Dixon Statistic	P-value	Chi-Sq. Statistic	P-value	Grubbs Statistic	P-value
10	10%	1	2.2e-16	8.1	0.0044	2.8460e+00	2.2e-16
	20%	0.8511	2.2e-16	7.9209	0.0048	2.8144	3.298e-07
	30%	0.7890	2.2e-16	7.7431	0.0053	2.7826	5.246e-06
30	10%	0.1755	9.67e-14	10.979	0.0009	3.3134	0.0032
	20%	0.8031	2.2e-16	23.683	1.136e-06	4.8664	1.14e-11
	30%	0.3779	9.07-14	10.337	0.0013	3.2150	0.0055
100	10%	0.9021	2.2e-16	53.046	3.259e-13	7.2832	2.2e-16
	20%	0.7890	2.2e-16	57.66	3.12e-14	7.5934	2.2e-16
	30%	0.1755	2.2e-16	72.687	2.2e-16	8.5256	2.2e-16

Source: Author’s Computation using R

Table 6: Probability of Correctly Identifying Actual Number of Outliers at lower level in First Predictors (X₁)

Sample Size	outlier	CD ² i		MDi		DDi	
		Dixon Statistic	P-value	Chi-Sq. Statistic	P-value	Grubbs Statistic	P-value
10	10%	1	2.2e-16	8.1	0.0044	2.8460e+00	2.2e-16
	20%	0.9208	2.2e-16	8.0493	0.0045	2.8371	2.096e-09
	30%	0.7536	2.2e-16	7.5606	0.0059	2.7496	2.764e-05
30	10%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
	20%	1	2.2e-16	24.386	7.886e-07	4.9381	9.526e-13
	30%	0.7293	2.2e-16	23.566	1.207e-06	4.8544	1.656e-11
100	10%	1	2.2e-16	98.01	2.2e-16	9.9000e+00	2.2e-16
	20%	1	2.2e-16	85.786	2.2e-16	9.2620	2.2e-16
	30%	1	2.2e-16	84.274	2.2e-16	9.1801	2.2e-16

Source: Author’s Computation using R

Table 7: Probability of Correctly Identifying Actual Number of Outliers at lower level in Second Predictors (X_2)

Sample Size	outlier	CD ² i		MDi		DDi	
		Dixon Statistic	P-value	Chi-Sq. Statistic	P-value	Grubbs Statistic	P-value
10	10%	1	2.2e-16	18.05	2.152e-05	4.2485e+00	2.2e-16
	20%	1	2.2e-16	18.05	2.152e-05	4.2485e+00	2.2e-16
	30%	1	2.2e-16	18.05	2.152e-05	4.2485e+00	2.2e-16
30	10%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
	20%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
	30%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
100	10%	1	2.2e-16	35.222	2.943e-09	5.9347	2.202e-09
	20%	1	2.2e-16	69.153	2.2e-16	8.3158	2.2e-16
	30%	1	2.2e-16	43.738	3.755e-11	6.6134	1.577e-12

Source: Author’s Computation using R

Table 8: Probability of Correctly Identifying Actual Number of Outliers at lower level in First and Second Predictors (X_1 and X_2)

Sample Size	Outlier	CD ² i		MDi		DDi	
		Dixon Statistic	P-value	Chi-Sq. Statistic	P-value	Grubbs Statistic	P-value
10	10%	1	2.2e-16	18.05	2.152e-05	4.2485e+00	2.2e-16
	20%	1	2.2e-16	18.05	2.152e-05	4.2485e+00	2.2e-16
	30%	1	2.2e-16	18.05	2.152e-05	4.2485e+00	2.2e-16
30	10%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
	20%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
	30%	1	2.2e-16	28.033	1.192e-07	5.2947e+00	2.2e-16
100	10%	1	2.2e-16	18.81	1.444e-05	4.3370	0.0002
	20%	1	2.2e-16	18.81	1.444e-05	4.3370	0.0002
	30%	1	2.2e-16	18.81	1.444e-05	4.3370	0.0002

Source: Author’s Computation using R

DISCUSSION

The actual percentage number of outliers in First Predictor was shown in table 3. For sample size ten (n=10), CDi has highest chance to detect the percentage of the outliers injected at 10% and 20% of lower sample size of 10, with values 2.2e-16 respectively which are the least p-values compare with 5% level of significance while the MDi is the highest chance at 30% with value 0.0379. At 20% of outliers, CDi performs best with probability 2.2e-16, at different sample sizes followed by DDi. CDi performance dropped to 0.0421, 0.0446 and 0.0279 at 10%, 20% and 30% of sample size 100 while DDi is the best detector with lowest p-values less than 5%. In table 4, which shows the actual percentage number of outliers in the Second Predictor. CDi has the highest probability to detect the actual number of the outliers injected at 10% and 20% for sample size of 10, 30 and 100. This is due to its p-values is far less than

5%. The accuracy of detection increased in the three test statistic at different percentages outlier levels.

Furthermore, Table 5, shows the actual percentage number of outliers in the first and Second Predictor. CDi has the highest probability to detect the actual number of the outliers injected at 10%, 20% and 30% followed by DDi for sample size of 10 and 30. At the largest sample size of 100, DDi has the same performance with CDi and the performances of the duo increase as sample size increase. Table 6, shows the actual number (1, 2 or 3) of outliers in the first Predictor. CDi has the highest probability to detect the actual number of the outliers injected over the sample size from the smallest to the highest. This was followed by DDi especially at the moderate sample of 30. This is due to its p-values is far less than 5%.

The accuracy of detection increased in the three test statistic when sample size becomes large.

In other way, table 7, shows the actual number (1, 2 or 3) of outliers in the first Predictor. CDi has the highest probability to detect the actual number of the outliers injected over the sample size from the smallest to the highest. This was followed by DDi especially at the small and moderate sample size of 10 and 30 respectively. The accuracy of detection also increased in the MDi when sample size becomes large. The Table 8 shows the probability of the test statistics to detect the presence of a number of outliers in the sample observations. The probability values obtained for CDi in all sample sizes shows the highest sensitivity in identifying outliers in small to large sample sizes at the three level of outliers' injection. DDi have the similar performance with CDi at sample level of 10 and 30 but it shows low sensitivity in detecting presence of outliers in large sample size(n=100) at all levels. The performance of MDi supersedes DDi as sample size increases.

Conclusion

Base on the results of the simulated data and analysis using R statistical software, the results show the appropriate and best statistic to be used for small medium and large sample sizes as well as the percentage of outlier contained in the sample. The outlier detections follow similar trend irrespective of which of the predictor variables contained the outliers (first, second predictors or first and second predictors).

CDi detects outliers more accurately in small sample size 10 and when the number (percentage) of outlier is small and (10%) while MDi performs better as proportion of outliers increases still with the same sample size in the first predictor. At 20% of outliers, CDi performs best with probability at different sample sizes followed by DDi. CDi performance dropped of sample size 100 while DDi is the best detector with lowest p-values less than 5%. For second and both predictors, CDi has the highest probability to detect the actual number of the outliers injected at 10% and 20% for sample size of 10, 30 and 100. This is due to its p-values is far less than 5%. The accuracy of detection increased in the three test statistic at different percentages outlier levels.

Furthermore, CDi has the highest probability to detect the actual number of the outliers injected

over the sample size from the smallest to the highest. The probability values obtained for CDi in all sample sizes shows the highest sensitivity in identifying outliers in small to large sample sizes at the three level of outliers' injection. DDi have the similar performance with CDi at sample level of 10 and 30 but it shows low sensitivity in detecting presence of outliers in large sample size(n=100) at all levels. The performance of MDi supersedes DDi as sample size increases in all predictor. The accuracy of detection also increased in the MDi when sample size becomes large.

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