

The Sequential Testing of Multiple Outliers in Linear Regression

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Abstract

In this paper we consider the problem of identifying and testing the outliers in linear regression. First we consider the problem for testing the null hypothesis of no outliers. The test based on the ratio of two scale estimates is proposed. We show the asymptotic distribution of the test statistic by Monte Carlo simulation and investigate its properties. Next we consider the problem of identifying the outliers. A forward sequential procedure based on the suggested test is proposed and shown to perform fairly well. The forward sequential procedure is unaffected by masking and swamping effects because the test statistic is based on robust estimate.

Keywords : Least median of squares, Outliers test, Forward sequential procedure.

1. Introduction

It is well known that outliers can have an extreme effect on the least squares estimation. Intuitively, an outlier is an observation $(x_{i1}, x_{i2}, \dots, x_{ip}, y_i)$ which deviate from the linear relation followed by the majority of the data. In the regression model,

$$y_i = \beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \dots + x_{ip}\beta_p + e_i, \quad i = 1, 2, \dots, n \quad (1)$$

where the error e_i is assumed to be normally distributed with mean zero and variance σ^2 , the outliers are classified into two categories, the outliers in y-direction and the outliers in the x-direction. Especially the outliers in x-direction are called leverage points. The non-outlying data will be referred to as the good data. It is assumed that good data contains more data than 50% of the observations in the sample.

In lower dimension, graphical technique can be used to detect the outliers. When the

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regression model has less than three independent variables, the outliers can be detected by scatter plots and spin plots. But the degree of outlyingness is based on the judgement of the researcher.

However, when the independent variable is more than two, it is difficult to detect the outliers by graphical tool. We have to resort to other methods.

There are two general approaches to dealing with the outliers, diagnostics test and robust methods. Each approach proceeds the same problem from opposite side. Since the advantages of one method tend to be the disadvantages of the other, we propose a diagnostic test by combining two methods, which is unaffected by masking and swamping effects.

In this paper, we propose a robust diagnostic tool to detect and test the outliers in linear regression. This tool is based on the ratio of a robust scale estimate and a non robust scale estimate. And then we propose the following forward sequential procedure for identifying the outliers. If the null hypothesis is rejected then the most extreme observation is removed and the test is applied again to the $n-1$ remaining observations. This procedure is applied iteratively and stops when the test is no longer significant. Since it is based on a robust estimate of scale, one expects that this procedure will not be affected by masking and swamping effects. This is confirmed by numerical examples.

The remaining of the paper is organized as follows. In Section 2 we introduce the test statistic and the forward sequential procedure. In Section 3 we derive that the asymptotic distribution of the test statistics by Monte Carlo simulation under the null hypothesis and calculate the critical values and powers of proposed test. In Section 4 the proposed test and the forward sequential procedure is applied to several real data sets and artificial data sets in order to show their performances. Section 5 contains some concluding remarks.

2. Testing Procedure for Detecting Multiple Outliers

In this section, we propose the test statistic for testing outliers in linear regression. The test statistic is defined as follows. Least median of squares estimator, suggested by Rousseeuw(1984), is known to be a highly robust method for estimating regression coefficient.

The least median of squares estimator $\hat{\beta}_{LMS}$ is given by

$$\text{Minimize med } r_i^2 \quad (2)$$

$$\hat{\beta}_J \quad i$$

where $r_i = y_i - \mathbf{x}_i^T \hat{\beta}_J$, $\hat{\beta}_J = (\mathbf{X}_J^T \mathbf{X}_J)^{-1} \mathbf{X}_J^T \mathbf{Y}_J$, $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{ip})$ and $J = \{i_1, i_2, \dots, i_p\}$ is a subset of $\{1, 2, \dots, n\}$ containing p indices. The breakdown point of least median of squares estimator is approximately 0.5. The residual is given by

$$r_{LMS_i} = y_i - \mathbf{x}_i^T \hat{\beta}_{LMS}. \quad (3)$$

The initial scale estimate s_0 for the least median squares regression is given by

$$s_0 = 1.4826(1 + 5/(n - p - 1))\sqrt{\text{med}_i(r_{LMS_i})^2}. \tag{4}$$

The initial scale estimate is then used to determine a weight w_i for the i th observation, namely

$$w_i = \begin{cases} 1 & \text{if } c \leq r_{LMS_i}/s_0 \leq d \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where $[c, d]$ is the inner fence of boxplot of r_{LMS_i}/s_0 .

By means of these weights, the final scale estimate s for the least median squares regression is given by

$$s = \sqrt{\sum_{i=1}^n w_i (r_{LMS_i})^2 / (\sum_{i=1}^n w_i - p - 1)}. \tag{6}$$

s also has a breakdown point 0.5, the highest possible value.

By contrast, the least squares estimator $\hat{\beta}_{LS}$ minimizes

$$\sum_{i=1}^n r_{LS_i}^2. \tag{7}$$

The breakdown point of least squares estimator is 0. The residual is given by

$$r_{LS_i} = y_i - \mathbf{x}_i^T \hat{\beta}_{LS}. \tag{8}$$

It is well known that outliers can have an extreme effect on the least squares estimator.

The scale estimate for the least squares regression is given by

$$\sigma = \sqrt{\sum_{i=1}^n (r_{LS_i})^2 / (n - p - 1)}. \tag{9}$$

The test statistics for testing the outliers is defined as

$$R = \sigma/s. \tag{10}$$

It tests the following hypothesis

$$H_0 : \text{no outlier in data } (x_{i1}, x_{i2}, \dots, x_{ip}, y_i), \quad i = 1, 2, \dots, n \tag{11}$$

$$H_1 : \text{some outliers in data } (x_{i1}, x_{i2}, \dots, x_{ip}, y_i), \quad i = 1, 2, \dots, n.$$

The null hypothesis is rejected for large R . However, if the null hypothesis is rejected, there is no indication of how many or which points are outliers. To solve this problem, we propose to apply the test sequentially in forward sequential procedure to identify the outliers. If the test rejects the null hypothesis then the point with the largest $D = |\text{sort}(r_{LMS_i}) - \text{Med}(r_{LMS_i})|$ is defined as an outlier. Where $\text{sort}(r_{LMS_i})$ is the sort of r_{LMS_i} , and $\text{Med}(r_{LMS_i})$ is the median of r_{LMS_i} . The observation detected as an outlier is removed and the test is applied again to the $n-1$ remaining observations. The procedure is repeated and stops when the test is no longer significant. The robust estimate of scale in the denominator is required to ensure that the test statistic is sensitive to outliers and that the

forward sequential procedure is not affected by possible masking swamping effects of several outliers.

3. Simulation and its Results

In this section we consider the properties of the proposed test. First we calculate the critical values for the test. For this purpose, we generate sample for various sample size up to 50 in the following situation,

$$y_i = x_{i1} + x_{i2} + \cdots + x_{ip} + e_i, \quad (12)$$

in which $e_i \sim N(0, 1)$ and the explanatory variables are generated as $x_{ij} \sim N(0, 49)$ for $j=1, 2, \dots, p$. Using 1000 replicates for each sampling situation we compute the critical values for the test. A summary of our results for $p=1, 2, 3, 4$ and sample size up to 50 is presented in the Table 1.

Next, we consider the power of the test for various situation. First, we generate a sample as $e_i \sim N(0, 1)$ and $x_{ij} \sim N(0, 49)$. Second, to construct outliers in the independent variables space, $(1-\alpha) \times 100\%$ of samples are as in the first. The remaining $\alpha \times 100\%$ are generated as $e_i \sim N(0, 1)$ and $x_{ij} \sim N(\mu, 49)$. Finally, we make the outliers in response variable space. For this purpose, $(1-\alpha) \times 100\%$ of the samples are as in the first. The remaining $\alpha \times 100\%$ are generated as $e_i \sim N(\mu, 1)$ and $x_{ij} \sim N(0, 49)$.

Using 1000 replicates for each sampling situation, we compute the power of the test. A summary of our results for a single outlier, various magnitude of outliers, $\mu=10, 20, 30, 40, 50, 60, 70, 80, 90, 100$, $p=1$ and sample sizes 25 and 40, are presented in the Table 2 and 3. The results for two outliers, various magnitude of outlier, $\mu=10, 20, 30, 40, 50, 60, 70, 80, 90, 100$, $p=1$ and sample size 25 are presented in the Table 4. The power of the test increases with sample size and magnitude of outliers.

Table 1. Critical values for the proposed test

Sample sizes	Number of explanatory variable											
	1			2			3			4		
	α level			α level			α level			α level		
	0.1	0.05	0.01	0.1	0.05	0.01	0.1	0.05	0.01	0.1	0.05	0.01
15	1.725	1.894	2.072	2.107	2.223	2.386	2.469	2.622	2.756	2.807	2.895	2.992
20	1.484	1.637	1.849	1.850	1.978	2.084	2.121	2.246	2.334	2.323	2.407	2.580
25	1.493	1.605	1.759	1.682	1.793	1.853	1.950	2.044	2.200	2.164	2.282	2.388
30	1.461	1.570	1.717	1.552	1.638	1.752	1.824	1.921	2.065	1.982	2.150	2.333
35	1.395	1.475	1.623	1.496	1.578	1.688	1.650	1.793	1.925	1.786	1.910	2.103
40	1.326	1.403	1.493	1.417	1.487	1.580	1.573	1.666	1.774	1.654	1.769	1.882
45	1.276	1.337	1.435	1.393	1.473	1.570	1.456	1.548	1.655	1.575	1.688	1.812
50	1.266	1.338	1.403	1.351	1.425	1.515	1.471	1.492	1.575	1.466	1.540	1.631

Table 2. Estimated power of the proposed test($n=25$, $p=1$, one outlier)

significant level	magnitude of outliers								
	20	30	40	50	60	70	80	90	100
0.1	0.955	0.997	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.05	0.949	0.996	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.01	0.941	0.995	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Table 3. Estimated power of the proposed test($n=40$, $p=1$, one outlier)

significant level	magnitude of outliers								
	20	30	40	50	60	70	80	90	100
0.1	0.974	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.05	0.972	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.01	0.965	0.999	1.00	0.999	1.00	1.00	1.00	1.00	1.00

Table 4. Estimated power of the proposed test($n=25$, $p=1$, two outliers)

magnitude of outliers	magnitude of outliers											
	20			30			40			50		
	significant level			significant level			significant level			significant level		
	0.1	0.05	0.01	0.1	0.05	0.01	0.1	0.05	0.01	0.1	0.05	0.01
20	0.965	0.943	0.938	0.995	0.993	0.988	0.998	0.997	0.996	1.00	1.00	1.00
30	0.966	0.955	0.944	0.996	0.994	0.99	0.999	0.998	0.997	1.00	1.00	1.00
40	0.969	0.957	0.950	1.00	0.999	0.995	1.00	1.00	1.00	1.00	1.00	1.00
50	0.970	0.962	0.954	1.00	0.999	0.995	1.00	1.00	1.00	1.00	1.00	1.00
60	0.973	0.966	0.958	1.00	1.00	0.996	1.00	1.00	1.00	1.00	1.00	1.00
70	0.975	0.973	0.963	1.00	1.00	0.997	1.00	1.00	1.00	1.00	1.00	1.00
80	0.977	0.975	0.967	1.00	1.00	0.998	1.00	1.00	1.00	1.00	1.00	1.00
90	0.983	0.977	0.972	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
100	0.991	0.985	0.983	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

continue(Table 4)

magnitude of outliers	magnitude of outliers											
	60			70			80			90		
	significant level			significant level			significant level			significant level		
	0.1	0.05	0.01	0.1	0.05	0.01	0.1	0.05	0.01	0.1	0.05	0.01
20	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
30	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
40	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
50	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
60	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
70	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
80	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
90	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
100	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Finally, we consider the asymptotic distribution of the test statistics. This is obtained by

the result of Monte Carlo simulation of 1000 replications under the null hypothesis. For various sample sizes and the number of explanatory variables, Q-Q plots of the test statistics are similar. So a Q-Q plot of the test statistic for sample size 100 in $p=3$ is shown only in Figure 1. Though the extreme quantiles for the test statistic is the greater spread, all of them appear to follow the normal distribution approximately.

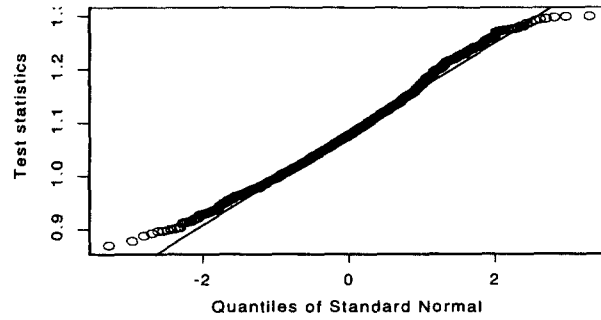


Figure 1. Normal probability plot of 1000 test statistics for size 100 in $p=3$

4. Applications of the proposed test

In this section, the proposed test is applied to several data sets for the purpose of testing and detecting outliers. The application begins by applying the test to the pilot-plant data given by Daniel and Wood(1971). Rousseeuw and Leroy(1987) used these data to illustrate the need for robust regression technique. Suppose now that one of the observations has been wrongly recorded. For example, the x -value of the sixth observation has been recorded as 370 instead of 37. This error produces an outlier in the independent variable space. The data appear in the Table 5. The results for the proposed test are in the Table 6.

Table 5. Pilot-Plant data set

index	Extraction(x)	Titration(y)	index	Extraction(x)	Titration(y)
1	123	76	11	138	82
2	109	70	12	105	68
3	62	55	13	159	88
4	104	71	14	75	58
5	57	55	15	88	64
6	370(37)	48	16	164	88
7	44	50	17	169	89
8	100	66	18	167	88
9	16	41	19	149	84
10	28	43	20	167	88

*(37) is original data of pilot-plant data set

Table 6. The proposed test applied to the contaminated pilot-plant data

sample size	observation selected	proposed test statistics	critical values		
			0.01	0.05	0.1
20	6	11.703	1.849	1.637	1.484
19	11	0.941	1.858	1.651	1.495

In the Table 6, the test is highly significant for observation 6 that wrongly recorded. When the test is applied to the remaining 19 observations, null hypothesis is not rejected. For this example, the proposed test yields a correct result.

The second application for testing and detecting outliers comes from the Brownlee(1965). The data is well-known stackloss data set. We have selected this example because it is a set of real data and it is examined by many statisticians. Most people concluded that observations 1, 3, 4, and 21 were outliers. Some people reported that observation 2 was outlier. The data are shown in the Table7. The result for the proposed test appear in the Table8. In the Table8, observation 4 is the most extreme followed by observation 21, observation 1, observation 3 and observation 2. The test identifies obseravtion 4, 21, 1, 3 and 2 as outliers. When the test is applied to the remaining 16 observations, null hypothesis is not rejected. Hence observation 13 is not a outlier. This result is the same to conclusion that most people reported.

Table 7. Stackloss data

index	rate (x1)	temper- ature(x2)	acid concen- tration(x3)	stackless (y)	index	rate (x1)	temper- ature(x2)	acid concen- tration(x3)	stackless(y)
1	80	27	89	42	12	58	17	88	13
2	80	27	88	37	13	58	18	82	11
3	75	25	90	37	14	58	19	93	12
4	62	24	87	28	15	50	18	89	8
5	62	22	87	18	16	50	18	86	7
6	62	23	87	18	17	50	19	72	8
7	62	24	93	19	18	50	19	79	8
8	62	24	93	20	19	50	20	80	9
9	58	23	87	15	20	56	20	82	15
10	58	18	80	14	21	70	20	91	15
11	58	18	89	14					

Table 8. The proposed test applied to the stackloss data

Sample size	observation selected	proposed test statistics	Critical Values		
			0.01	0.05	0.10
21	4	2.685	2.304	2.204	2.101
20	21	2.895	2.334	2.246	2.121
19	1	2.367	2.359	2.296	2.231
18	3	2.9067	2.384	2.346	2.321
17	2	2.610	2.421	2.396	2.384
16	13	2.326	2.634	2.583	2.421

Table 9 . Artificial data set of Hawkins, Bradu, and Kass

index	x1	x2	x3	y	index	x1	x2	x3	y
1	10.1	19.6	28.3	9.7	39	2.1	0.0	1.2	-0.7
2	9.5	20.5	28.9	10.1	40	0.5	2.0	1.2	-0.5
3	10.7	20.2	31.0	10.3	41	3.4	1.6	2.9	-0.1
4	9.9	21.5	31.7	9.5	42	0.3	1.0	2.7	-0.7
5	10.3	21.1	31.1	10.0	43	0.1	3.3	0.9	0.6
6	10.8	20.4	29.2	10.0	44	1.8	0.5	3.2	-0.7
7	10.5	20.9	29.1	10.8	45	1.9	0.1	0.6	-0.5
8	9.9	19.6	28.8	10.3	46	1.8	0.5	3.0	-0.4
9	9.7	20.7	31.0	9.6	47	3.0	0.1	0.8	-0.9
10	9.3	19.7	3.03	9.9	48	3.1	1.6	3.0	0.1
11	11.0	24.0	35.0	-0.2	49	3.1	2.5	1.9	0.9
12	12.0	23.0	37.0	-0.4	50	2.1	2.8	2.9	-0.4
13	12.0	26.0	34.0	0.7	51	2.3	1.5	0.4	0.7
14	11.0	34.0	34.0	0.1	52	3.3	0.6	1.2	-0.5
15	3.4	2.9	2.0	-0.4	53	0.3	70.4	3.3	0.7
16	3.1	2.2	0.3	0.6	54	1.1	3.0	0.3	0.7
17	0.0	1.6	0.2	-0.2	55	0.5	2.4	0.9	0.0
18	2.3	1.6	2.0	0.0	56	1.8	3.2	0.9	0.1
19	0.8	2.9	1.6	0.1	57	1.8	0.7	0.7	0.7
20	3.1	3.4	2.2	0.4	58	2.4	3.4	1.5	-0.1
21	2.6	2.2	1.9	0.9	59	1.6	2.1	3.0	-0.3
22	0.4	3.2	1.9	0.3	60	0.3	1.5	3.3	-0.9
23	2.0	2.3	0.8	-0.8	61	0.4	3.4	3.0	-0.3
24	1.3	2.3	0.5	0.7	62	0.9	0.1	0.3	0.6
25	1.0	0.0	0.4	-0.3	63	1.1	2.7	0.2	-0.3
26	0.9	3.3	2.5	-0.8	64	2.8	3.0	2.9	-0.5
27	3.3	2.5	2.9	-0.7	65	2.0	0.7	2.7	0.6
28	1.8	0.8	2.0	0.3	66	0.2	1.8	0.8	-0.9
29	1.2	0.9	0.8	0.3	67	1.6	2.0	1.2	-0.7
30	1.2	0.7	3.4	-0.3	68	0.1	0.0	1.0	0.6
31	3.1	1.4	1.0	0.0	69	2.0	0.6	0.3	0.2
32	0.5	2.4	0.3	-0.4	70	1.0	2.2	2.9	0.7
33	1.5	3.1	1.5	-0.6	71	2.2	2.5	2.3	0.2
34	0.4	0.0	0.7	-0.7	72	0.6	2.0	1.5	-0.2
35	3.1	2.4	3.0	0.3	73	0.3	1.7	2.2	0.4
36	1.1	2.2	2.7	-1.0	74	0.0	2.2	1.6	-0.9
37	0.1	3.0	2.6	-0.6	75	0.3	3.4	2.6	0.2
38	1.5	1.2	0.2	0.9					

Let us look at another example containing multidimensional artificial data. This data set generated by Hawkins, Brau, and Kass(1984) and consists of 75 observations in four dimensions. The first 10 observations are the bad leverage points and the next four points are good leverage points. This data is listed in the Table 9. Hawkins, Brau, and Kass(1984) mentioned that the M-estimator did not turn out the expected results because the first ten bad leverage points were masked by the effect of good leverage points and the four good leverage points were detected as outliers.

The classical standardized residuals, internally(t_i) or externally studentized residuals(t_i^*),

Cook's distance(D_i), DEFFITS, diagonal element of projection matrix, and Mahalanobis distance (MD_i) for the data set are shown in Table 10. The proposed test is shown in Table 11. In the Table 10, all diagnostics tool based on least squares method identified good leverage points 11, 12, 13, 14 as outliers because the first ten bad leverage points were masked by the effected of good leverage points. But in the Table 11, proposed test detected bad leverage points 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 as outliers.

Table 10 The results for outliers diagnostics(h_{ii} ; Squared Mahalanobis Distance(MD_i); Standardized(r_i/s), Studentized(t_i) and Jackknifed Ls Residuals($t_{(i)}$); $CD^2(i)$; DFFITS)

index	$h_{ii}(0.107)$	$MD_i(7.82)$	$r_i/s(2.50)$	$t_i(2.50)$	$t_{(i)}(2.50)$	$CD^2(i)(1.00)$	DFFITS (0.462)
1	0.063	3.674	1.50	1.55	1.57	0.040	0.404
2	0.060	3.444	1.78	1.83	1.86	0.053	0.470
3	0.086	5.353	1.33	1.40	1.41	0.046	0.430
4	0.081	4.971	1.14	1.19	1.19	0.031	0.352
5	0.073	4.411	1.36	1.41	1.42	0.039	0.399
6	0.076	4.606	1.53	1.59	1.61	0.052	0.459
7	0.068	4.042	2.01	2.08	2.13	0.079	0.575
8	0.063	3.684	1.71	1.76	1.79	0.052	0.464
9	0.080	4.934	1.20	1.26	1.26	0.034	0.372
10	0.087	5.445	1.35	1.41	1.42	0.048	0.436
11	0.094	5.986	-3.48	-3.66	-4.03	0.348	-1.30
12	0.144	9.662	-4.16	-4.50	-5.29	0.851	-2.168
13	1.109	7.088	-2.72	-2.88	-3.04	0.254	-1.065
14	0.564	40.725	-1.69	-2.56	-2.67	2.114	-3.030

Table 11. The results for the proposed test

Sample size	observation selected	proposed test statistics	Critical Values		
			0.01	0.05	0.10
75	7	3.606	1.407	1.344	1.291
74	3	3.446	1.413	1.346	1.293
73	8	3.301	1.419	1.349	1.294
72	2	3.419	1.425	1.350	1.295
71	10	3.358	1.431	1.351	1.296
70	5	3.130	1.437	1.353	1.297
69	9	3.093	1.443	1.358	1.303
68	4	2.859	1.449	1.363	1.309
67	6	2.458	1.455	1.369	1.315
66	1	2.083	1.460	1.374	1.321
65	53	0.878	1.464	1.379	1.330

The above examples demonstrate the performance of the proposed test and is unaffected by masking and swamping effects.

5. Concluding Remarks

It is very important to test and detect the multiple outliers in linear regression. Several diagnostic measures based on the resulting from the least squares estimate have been proposed to identify the multiple outliers. However, the accuracy of diagnostic measures is very suspect because these can be severely affected by the masking and swamping effects. This inaccuracy can seriously affect their performance.

In this paper, we proposed the forward sequential test for testing and detecting the multiple outliers. This was founded on a robust estimate of scale.

In principle, the forward sequential test set up a natural simple approach for identifying the multiple outliers. However, if the forward sequential test is founded on the resulting from the least squares estimate, it can be seriously affected by the masking and swamping effects. On the other hand, if the forward sequential test is founded on a robust estimate of scale, like the test proposed in this paper, the problem for the masking and swamping effects can be overcome.

We proved that the proposed forward sequential test was not affected by the masking and swamping effects through the Monte Carlo results and numerical examples. These suggest that the proposed test provides a conservative and fairly powerful method for the detection of the multiple outliers in linear regression.

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