

Multivariate Outlier Detection Technique Based on Normalizing Transformations for Non-Gaussian Data

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Метод Визначення Багатовимірних Викидів, що Базується на Нормалізуючих Перетвореннях для Негаусівських Даних

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Abstract—The statistical technique for detecting outliers in multivariate non-Gaussian data on the basis of normalizing transformations and a test statistic for the Mahalanobis squared distance (MSD), which has an approximate F distribution, is proposed. Application of the technique is considered for detecting outliers in the data of four-variate measurements.

Анотація—Пропонується статистичний метод для виявлення викидів в багатовимірних негаусівських даних на основі нормалізуючих перетворень і тестової статистики для

квадрата відстані Махаланобісу (MSD), який має наближений F розподіл. Розглянуто застосування цього методу для виявлення викидів за даними вимірювань чотирьох величин.

Keywords—outlier; normalizing transformation; multivariate non-Gaussian data; Mahalanobis squared distance; F distribution

Ключові слова—викид; нормалізуюче перетворення; багатовимірні негаусівські дані; квадрат відстані Махаланобісу; F -розподіл

I. INTRODUCTION

A very important step in data analysis and processing is the outlier detection. Today the problem of outlier detection in a multivariate data set is solved with different methods including statistical [1, 2]. However, well-known statistical methods (for example, multivariate outlier detection based on a test statistics for MSD, which have an approximate the Chi-Square distribution or F distribution) are used to detect outliers in a multivariate data set under the assumption that the data is generated by a Gaussian distribution. And this assumption is valid only in particular cases.

In [3] a statistical outlier detection technique for multivariate non-Gaussian data on the basis of normalizing transformations and MSD, which has an approximate the Chi-Square distribution, was proposed. However, the quantile of the Chi-Square distribution does not depend from the number of data. We propose a statistical outlier detection technique for multivariate non-Gaussian data on the basis of normalizing transformations and a test statistic for MSD, which has an approximate F distribution. At that the quantile of the F distribution depends from the number of data. The technique consists of two steps. In the first step, multivariate non-Gaussian data is normalized using a multivariate normalizing transformation. In the second step, MSD and a test statistic for MSD are calculated and compared with a quantile of the F distribution. The data values for which a value of test statistic for MSD is greater than the quantile of the F distribution are considered as outliers and these values are cut off. Two steps should be repeated for the data after outlier cutoff until all values of test statistic for MSD will be less than or equal to the quantile of the F distribution.

II. THE STATISTICAL TECHNIQUE

The outlier detection technique for multivariate non-Gaussian data is based on normalizing transformations and a test statistic for MSD, which has an approximate F distribution. Consider bijective multivariate normalizing transformation of non-Gaussian random vector $\mathbf{X} = \{X_1, X_2, \dots, X_m\}^T$ to Gaussian random vector $\mathbf{Z} = \{Z_1, Z_2, \dots, Z_m\}^T$ is given by

$$\mathbf{Z} = \psi(\mathbf{X}). \quad (1)$$

The values of the sample observations or multivariate data points $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_N$ are normalized using the transformation (1).

The Mahalanobis squared distance for each multivariate data point i , $i = 1, 2, \dots, N$, is denoted by d_i^2 and given by

$$d_i^2 = (\mathbf{z}_i - \bar{\mathbf{Z}})^T S_N^{-1} (\mathbf{z}_i - \bar{\mathbf{Z}}), \quad (2)$$

where $\bar{\mathbf{Z}}$ is the sample mean vector and S_N is the sample correlation matrix

$$S_N = \frac{1}{N} \sum_{i=1}^N (\mathbf{z}_i - \bar{\mathbf{Z}})(\mathbf{z}_i - \bar{\mathbf{Z}})^T. \quad (3)$$

A test statistic (TS) for d_i^2 can be created as follows [4]

$$(N-m)N d_i^2 / (N^2 - 1)m, \quad (4)$$

which has an approximate F distribution with m and $N - m$ degrees of freedom.

A test statistic for MSD (4) is compared with a quantile of the F distribution, which is noted as $F_{m, N-m, \alpha}$. Here α is significance level. We take α as 0.05. The data values for which a value of TS (4) is greater than the quantile of the F distribution are considered as outliers and these values are cut off. After outlier cutoff the reduced number of multivariate data points are normalized using the transformation (1) again until all values of TS (4) will be less than or equal to the quantile of the F distribution.

III. MULTIVARIATE NORMALIZING TRANSFORMATIONS

Some transformations have been proposed for normalizing multivariate non-Gaussian data, such as, transformation on the basis of the decimal logarithm, the Box-Cox transformation, the Johnson translation system and others. However, only a few normalizing transformations are bijective. Such bijective transformation is the transformation of S_U family of the Johnson translation system. The Johnson normalizing translation is given by [5]

$$\mathbf{Z} = \boldsymbol{\gamma} + \boldsymbol{\eta} \mathbf{h}[\boldsymbol{\lambda}^{-1}(\mathbf{X} - \boldsymbol{\varphi})] \sim N_m(0_m, \Sigma), \quad (5)$$

where Σ is the correlation matrix; $\boldsymbol{\gamma}$, $\boldsymbol{\eta}$, $\boldsymbol{\varphi}$ and $\boldsymbol{\lambda}$ are parameters of the Johnson normalizing translation; $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_m)^T$; $\boldsymbol{\eta} = \text{diag}(\eta_1, \eta_2, \dots, \eta_m)$; $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, \dots, \varphi_m)^T$; $\boldsymbol{\lambda} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)$; $\mathbf{h}[(y_1, y_2, \dots, y_m)] = \{h_1(y_1), h_2(y_2), \dots, h_m(y_m)\}^T$; $h_i(\cdot)$ is one of the translation functions

$$h = \begin{cases} \ln(y), & \text{for } S_L \text{ (log normal) family;} \\ \ln[y/(1-y)], & \text{for } S_B \text{ (bounded) family;} \\ \text{Arsh}(y), & \text{for } S_U \text{ (unbounded) family;} \\ y & \text{for } S_N \text{ (normal) family.} \end{cases}$$

$$\text{Here } y = (x - \varphi)/\lambda; \text{Arsh}(y) = \ln\left(y + \sqrt{y^2 + 1}\right).$$

IV. EXAMPLES

We consider the examples of detecting outliers in multivariate non-Gaussian data for two cases: the first, under the assumption that the data set is generated by a Gaussian distribution and, the second, this assumption is not valid. In [2]

example of detecting outliers in the lumber stiffness data (example 4.15, p.190) is presented. Table I contains the data on lumber, MSD and a test statistic for MSD for standardized measurements, which are

$$Z_{ki} = (X_{ki} - \bar{X}_k) / S_{X_k}, \quad k = 1, 2, 3, 4; \quad i = 1, 2, \dots, 30. \quad (6)$$

TABLE I. MSD for the standardized data

| i | X_1 | X_2 | X_3 | X_4 | d_i^2 | TS for MSD |
|-----|-------|-------|-------|-------|---------|------------|
| 1 | 1889 | 1651 | 1561 | 1778 | 0.61 | 0.13 |
| 2 | 2493 | 2048 | 2087 | 2197 | 7.48 | 1.62 |
| 3 | 2119 | 1700 | 1815 | 2222 | 7.85 | 1.70 |
| 4 | 1645 | 1627 | 1110 | 1533 | 5.23 | 1.13 |
| 5 | 1976 | 1916 | 1614 | 1883 | 1.44 | 0.31 |
| 6 | 1712 | 1712 | 1439 | 1546 | 2.27 | 0.49 |
| 7 | 1943 | 1685 | 1271 | 1671 | 5.17 | 1.12 |
| 8 | 2104 | 1820 | 1717 | 1874 | 1.34 | 0.29 |
| 9 | 2983 | 2794 | 2412 | 2581 | 12.37 | 2.68 |
| 10 | 1745 | 1600 | 1384 | 1508 | 0.78 | 0.17 |
| 11 | 1710 | 1591 | 1518 | 1667 | 2.05 | 0.44 |
| 12 | 2046 | 1907 | 1627 | 1898 | 0.5 | 0.11 |
| 13 | 1840 | 1841 | 1595 | 1741 | 2.78 | 0.60 |
| 14 | 1867 | 1685 | 1493 | 1678 | 0.12 | 0.03 |
| 15 | 1859 | 1649 | 1389 | 1714 | 1.11 | 0.24 |
| 16 | 1954 | 2149 | 1180 | 1281 | 17.53 | 3.80 |
| 17 | 1325 | 1170 | 1002 | 1176 | 3.63 | 0.79 |
| 18 | 1419 | 1371 | 1252 | 1308 | 4.08 | 0.89 |
| 19 | 1828 | 1634 | 1602 | 1755 | 1.48 | 0.32 |
| 20 | 1725 | 1594 | 1313 | 1646 | 1.48 | 0.32 |
| 21 | 2276 | 2189 | 1547 | 2111 | 10.25 | 2.22 |
| 22 | 1899 | 1614 | 1422 | 1477 | 4.8 | 1.04 |
| 23 | 1633 | 1513 | 1290 | 1516 | 0.8 | 0.17 |
| 24 | 2061 | 1867 | 1646 | 2037 | 2.64 | 0.57 |
| 25 | 1856 | 1493 | 1356 | 1533 | 4.33 | 0.94 |
| 26 | 1727 | 1412 | 1238 | 1469 | 3.37 | 0.73 |
| 27 | 2168 | 1896 | 1701 | 1834 | 2.13 | 0.46 |
| 28 | 1655 | 1675 | 1414 | 1597 | 2.93 | 0.64 |
| 29 | 2326 | 2301 | 2065 | 2234 | 6.76 | 1.47 |
| 30 | 1490 | 1382 | 1214 | 1284 | 2.67 | 0.58 |

These data consist of four different measures of stiffness X_1, X_2, X_3 and X_4 , on each $N = 30$ of boards. For significance level which equals to 0.05 the last column in Table

I reveals that specimen 16 is multivariate outlier, since $F_{m, N-m, \alpha} = 2.74$.

Table II contains the normalized data on lumber, MSD and a test statistic for MSD for normalized data. These data is normalized by S_U family of the transformation (5).

TABLE II. MSD FOR THE NORMALIZED DATA

| i | Z_1 | Z_2 | Z_3 | Z_4 | d_i^2 | TS for MSD |
|-----|---------|---------|---------|---------|---------|------------|
| 1 | 0.1984 | -0.1910 | 0.3966 | 0.3539 | 0.77 | 0.17 |
| 2 | 1.4562 | 1.0898 | 1.5843 | 1.2985 | 2.88 | 0.63 |
| 3 | 0.8508 | 0.0237 | 1.0712 | 1.3430 | 4.23 | 0.92 |
| 4 | -0.9978 | -0.3027 | -1.7482 | -0.4821 | 9.07 | 1.97 |
| 5 | 0.4882 | 0.7632 | 0.5598 | 0.6343 | 0.78 | 0.17 |
| 6 | -0.6296 | 0.0734 | -0.0412 | -0.4297 | 2.31 | 0.50 |
| 7 | 0.3859 | -0.0401 | -0.8259 | 0.0249 | 4.54 | 0.98 |
| 8 | 0.8177 | 0.4724 | 0.8404 | 0.6117 | 1.13 | 0.25 |
| 9 | 1.9326 | 2.1752 | 2.0416 | 1.8902 | 5.26 | 1.14 |
| 10 | -0.4518 | -0.4328 | -0.2728 | -0.5859 | 0.59 | 0.13 |
| 11 | -0.6406 | -0.4770 | 0.2530 | 0.0116 | 1.99 | 0.43 |
| 12 | 0.6799 | 0.7381 | 0.5977 | 0.6715 | 0.58 | 0.13 |
| 13 | 0.0031 | 0.5407 | 0.5029 | 0.2456 | 1.54 | 0.33 |
| 14 | 0.1139 | -0.0401 | 0.1644 | 0.0480 | 0.14 | 0.03 |
| 15 | 0.0819 | -0.2002 | -0.2507 | 0.1630 | 0.92 | 0.20 |
| 16 | 0.4209 | 1.2978 | -1.3383 | -1.7120 | 18.95 | 4.11 |
| 17 | -2.2232 | -2.2878 | -2.3454 | -2.3094 | 6.33 | 1.37 |
| 18 | -1.9595 | -1.5575 | -0.9289 | -1.5624 | 5.40 | 1.17 |
| 19 | -0.0488 | -0.2697 | 0.5241 | 0.2872 | 1.17 | 0.25 |
| 20 | -0.5587 | -0.4622 | -0.6080 | -0.0594 | 1.68 | 0.36 |
| 21 | 1.1474 | 1.3723 | 0.3511 | 1.1373 | 4.25 | 0.92 |
| 22 | 0.2352 | -0.3648 | -0.1103 | -0.7201 | 3.97 | 0.86 |
| 23 | -1.0620 | -0.8721 | -0.7256 | -0.5522 | 1.50 | 0.32 |
| 24 | 0.7172 | 0.6214 | 0.6518 | 0.9874 | 1.16 | 0.25 |
| 25 | 0.0697 | -0.9741 | -0.4000 | -0.4821 | 4.34 | 0.94 |
| 26 | -0.5479 | -1.3717 | -1.0063 | -0.7558 | 3.78 | 0.82 |
| 27 | 0.9523 | 0.7069 | 0.7996 | 0.5081 | 1.42 | 0.31 |
| 28 | -0.9435 | -0.0836 | -0.1435 | -0.2339 | 3.52 | 0.76 |
| 29 | 1.2270 | 1.5616 | 1.5482 | 1.3640 | 3.14 | 0.68 |
| 30 | -1.7150 | -1.5089 | -1.1418 | -1.6952 | 3.96 | 0.86 |

In these case the parameters are such: $\gamma_1 = -0.76817$, $\gamma_2 = -0.81796$, $\gamma_3 = -1.52027$, $\gamma_4 = -2.11559$, $\eta_1 = 1.01985$, $\eta_2 = 1.29026$, $\eta_3 = 1.58452$, $\eta_4 = 1.87154$, $\phi_1 = 1686.87$,

$\varphi_2 = 1523.59$, $\varphi_3 = 1148.94$, $\varphi_4 = 1209.93$, $\lambda_1 = 184.403$, $\lambda_2 = 252.185$, $\lambda_3 = 269.810$ and $\lambda_4 = 327.027$.

The sample correlation matrix (3) of the \mathbf{Z} is used as the approximate moment-matching estimator of correlation matrix Σ

$$S_N = \begin{pmatrix} 1.00000 & 0.85039 & 0.79001 & 0.82173 \\ 0.85039 & 1.00000 & 0.71725 & 0.73854 \\ 0.79001 & 0.71725 & 1.00000 & 0.87227 \\ 0.82173 & 0.73854 & 0.87227 & 1.00000 \end{pmatrix}.$$

In Table II the last column reveals that only specimen 16 is multivariate outlier, since $F_{m,N-m,\alpha} = 2.74$. We note the value of TS for MSD for the normalized data from Table II is greater than the same value for the data from Table I in this case.

Table III contains the normalized data on lumber and MSD for normalized data after outlier cutoff of specimen 16 (according Table II). These data is normalized by S_U family of the transformation (5). After outlier cutoff the parameters are such: $\gamma_1 = -0.70625$, $\gamma_2 = -0.62410$, $\gamma_3 = -0.70133$, $\gamma_4 = -21.2264$, $\eta_1 = 0.33081$, $\eta_2 = 0.23699$, $\eta_3 = 0.21906$, $\eta_4 = 6.20266$, $\varphi_1 = 1700.55$, $\varphi_2 = 1587.45$, $\varphi_3 = 1304.12$, $\varphi_4 = -181.883$, $\lambda_1 = 10.202$, $\lambda_2 = 2.123$, $\lambda_3 = 1.495$ and $\lambda_4 = 124.038$.

The sample correlation matrix (3) of the \mathbf{Z} is such

$$S_N = \begin{pmatrix} 1.00000 & 0.70699 & 0.74789 & 0.77134 \\ 0.70699 & 1.00000 & 0.72856 & 0.75745 \\ 0.74789 & 0.72856 & 1.00000 & 0.70002 \\ 0.77134 & 0.75745 & 0.70002 & 1.00000 \end{pmatrix}.$$

The last column in Table III reveals there are no multivariate outliers in the data, since $F_{m,N-m,\alpha} = 2.76$. We note, if the parametric anomaly detection technique [6] based on the Grubb test applies for detecting outliers in the normalized data from Table II and Table III then all data sample units do not appear to be an outlier in each of the univariate distributions.

Following [7] Mardia's multivariate kurtosis β_2 is calculated for the data from Table I, Table II and Table III as

$$\beta_2 = \frac{1}{N} \sum_{i=1}^N \left\{ (\mathbf{z}_i - \bar{\mathbf{z}})^T S_N^{-1} (\mathbf{z}_i - \bar{\mathbf{z}}) \right\}^2.$$

It is known that $\beta_2 = m(m+2)$ holds under multivariate normality. The given equality is a necessary condition for multivariate normality. In our case $\beta_2 = 24$. The values of multivariate kurtosis equal, respectively, 30.71, 23.84 and 23.78 for the data from Table I, Table II and Table III. These

values indicate that the necessary condition for multivariate normality is practically performed for the normalized data from Table II and Table III and does not hold for standardized data from Table I by the formula (6).

TABLE III. MSD FOR THE NORMALIZED DATA AFTER OUTLIER CUTOFF

| i | Z_1 | Z_2 | Z_3 | Z_4 | d_i^2 | TS for MSD |
|-----|---------|---------|---------|---------|---------|------------|
| 1 | 0.4880 | 0.3457 | 0.5780 | 0.1988 | 0.49 | 0.11 |
| 2 | 0.9629 | 0.8150 | 0.8221 | 1.3986 | 2.10 | 0.45 |
| 3 | 0.7517 | 0.4811 | 0.7286 | 1.4633 | 3.18 | 0.69 |
| 4 | -1.4990 | 0.2334 | -1.9193 | -0.6276 | 10.43 | 2.25 |
| 5 | 0.6135 | 0.7350 | 0.6191 | 0.5219 | 0.58 | 0.13 |
| 6 | -0.3870 | 0.5051 | 0.4369 | -0.5809 | 3.23 | 0.70 |
| 7 | 0.5713 | 0.4472 | -1.5320 | -0.1487 | 11.66 | 2.52 |
| 8 | 0.7397 | 0.6531 | 0.6819 | 0.4949 | 0.66 | 0.14 |
| 9 | 1.1222 | 1.0433 | 0.8982 | 2.3257 | 7.32 | 1.58 |
| 10 | 0.0142 | -0.0371 | 0.3221 | -0.7184 | 2.09 | 0.45 |
| 11 | -0.4323 | -0.3193 | 0.5379 | -0.1621 | 2.29 | 0.49 |
| 12 | 0.6883 | 0.7284 | 0.6281 | 0.5667 | 0.61 | 0.13 |
| 13 | 0.3886 | 0.6736 | 0.6052 | 0.0808 | 1.06 | 0.23 |
| 14 | 0.4470 | 0.4472 | 0.5106 | -0.1253 | 1.21 | 0.26 |
| 15 | 0.4308 | 0.3381 | 0.3354 | -0.0067 | 0.59 | 0.13 |
| 16 | -2.1285 | -2.0400 | -2.0162 | -2.0706 | 5.33 | 1.15 |
| 17 | -2.0332 | -1.8843 | -1.6313 | -1.4974 | 4.75 | 1.03 |
| 18 | 0.3589 | 0.2720 | 0.6104 | 0.1257 | 0.56 | 0.12 |
| 19 | -0.1743 | -0.1869 | -0.1577 | -0.2327 | 0.05 | 0.01 |
| 20 | 0.8571 | 0.8783 | 0.5657 | 1.1705 | 1.53 | 0.33 |
| 21 | 0.5051 | 0.1392 | 0.4073 | -0.8330 | 4.59 | 0.99 |
| 22 | -1.5628 | -1.6314 | -1.3458 | -0.6892 | 4.74 | 1.02 |
| 23 | 0.7024 | 0.6967 | 0.6406 | 0.9673 | 0.94 | 0.20 |
| 24 | 0.4244 | -1.6878 | 0.2276 | -0.6276 | 9.57 | 2.06 |
| 25 | -0.1502 | -1.8345 | -1.6834 | -0.8629 | 8.16 | 1.76 |
| 26 | 0.7883 | 0.7201 | 0.6733 | 0.3732 | 0.98 | 0.21 |
| 27 | -1.4346 | 0.4216 | 0.3920 | -0.4009 | 8.38 | 1.81 |
| 28 | 0.8847 | 0.9188 | 0.8159 | 1.4942 | 2.46 | 0.53 |
| 29 | -1.9372 | -1.8719 | -1.7512 | -1.5977 | 4.33 | 0.93 |

The F plots are computed for a test statistic for MSD from Table I, Table II and Table III. A F plot is similar to a Q-Q plot. The F plots for the test statistic for MSD (4) from Table I, Table II and Table III are shown on Fig. 1, Fig. 2 and Fig. 3.

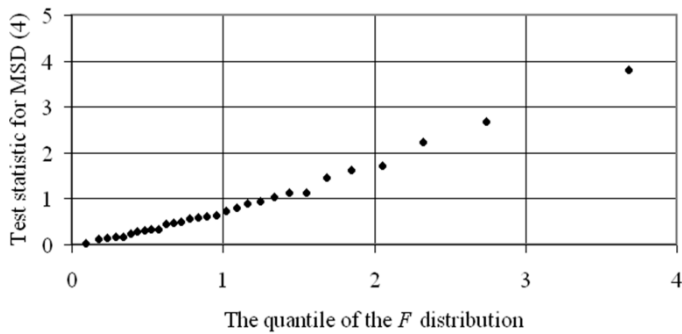


Fig. 1. F plot for a test statistic for MSD (4) from Table I

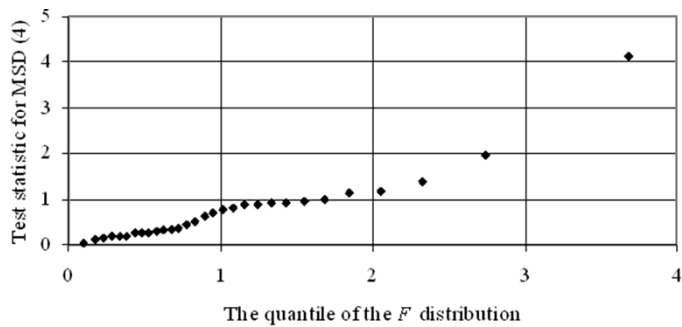


Fig. 2. F plot for a test statistic for MSD (4) from Table II

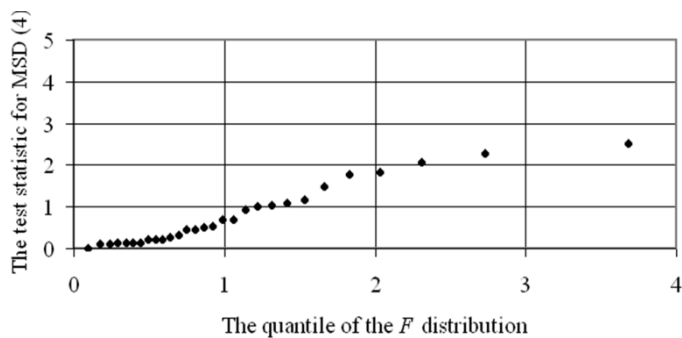


Fig. 3. F plot for a test statistic for MSD (4) from Table III

On Fig. 1 and Fig. 2 the quantiles of the F distribution are calculated for $m = 4$ and $N - m = 26$ degrees of freedom and the 30 probability levels, which are computed as $\frac{(1-0.5)}{30} = 0.0167$, $\frac{(2-0.5)}{30} = 0.05$, ..., $\frac{(30-0.5)}{30} = 0.9833$.

On Fig. 3 the quantiles of the F distribution are calculated for $m = 4$ and $N - m = 25$ degrees of freedom and the 29

probability levels, which are computed as $\frac{(1-0.5)}{29} = 0.0172$, $\frac{(2-0.5)}{29} = 0.0517$, ..., $\frac{(29-0.5)}{30} = 0.9828$.

It is necessary to check if points of the F plot approximately fall on a straight line. On Fig. 1 and Fig. 2 the one specimen with largest MSD is clearly removed from straight line pattern. We note on Fig. 1 and Fig. 2 the point with largest MSD is situated upper from an approximate straight line. On Fig. 3 all points do not appear to be an outlier. The same results were obtained by proposed technique for detecting outliers in multivariate non-Gaussian data.

V. CONCLUSIONS

From the examples we conclude that the proposed technique is promising, since, firstly, for multivariate outlier the value of test statistic for the Mahalanobis squared distance for the normalized data is greater than the same value for the standardized data and, secondly, the multivariate data point is not flagged as an outlier when we only consider the univariate data. However, some refinements may be necessary. We intend to try other normalizing transformations and test statistics for the Mahalanobis squared distance.

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