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ALTERNATIVE ESTIMATOR FOR MULTIVARIATE LOCATION AND SCATTER MATRIX IN THE PRESENCE OF OUTLIER

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ABSTRACT: It is generally known that in estimating location and scatter matrix of multivariate data when outliers are presents, the method of classical is not robust. The Maximum Likelihood Estimator (MLE) is always very sensitive to some deviations from the assumptions made on the data, especially, presence of outliers. To get over the above stated problem, many alternative estimators that are robust have been proposed in the last decades. Some of these estimators include the Minimum Covariance Determinant (MCD), the Minimum Volume Ellipsoid (MVE), S-Estimators, M-Estimators and Minimum Regularized Covariance Determinant (MRCD) among others. All the methods converged on tackling the problem of robust estimation by finding a sufficiently large subset of the data. In this paper, a robust method of estimating multivariate location and scatter matrix in the presence of outliers is proposed. The proposed estimator is obtained using the best units (samples) from the available data set that satisfied a set of three optimality criteria (C_A,C_H,C_G).The performance of the proposed robust method was compared with two of the existing robust methods (MCD and MVE) and the classical method with their application in Principal component analysis data simulation. The measure of performance used was the Mean Square Errors (MSE) of the characteristic roots (eigen-values) of the variance-covariance matrix. Generally, the proposed alternative method is better than other robust methods and classical method, when the level of magnitude of outliers is small and also performed considerably well with MCD and MVE when the level of magnitude is high at all percentages of outliers.

KEYWORDS: Eigen-values, Scatter matrix, Mean Square Errors, Outliers, Robust.

1. INTRODUCTION

In a large survey of observation, more often than none, there is the possibility that changes in the measurement process will bring about clusters of outliers. The standard multivariate analysis methods depend on the assumption of normality which requires the use of estimates for both the location and scatter parameters of the distribution. The presence of outliers in the observations may distort arbitrarily the values of the estimators and render meaningless the precision and accuracy of the results when these techniques are applied. Roche and Woodruff ([RW98]), opined that the problem of the joint estimation of location and scatter is one of the most challenged encounter in robust statistics.

In statistical data analysis, quite a large number of variables are usually sampled. The first step towards obtaining a coherent analysis that will lead to estimates with good precision and accuracy is to detect outlaying observations. Although outliers are usually regarded as disturbance error or noise that makes parameter estimates invalid, but it has important information which can stand as a measure of quality of data or observation. Detected outliers are instrument that corrupt data which would have adversely lead to model misspecification, biased parameter estimation, incorrect results, poor precision and inaccuracy. Outlier detection is one of the most important tasks in data analysis. The outliers describe the abnormality in data behaviour, such as data that deviate from the natural data variability. The cut-off value or threshold which divides anomalous and non-anomalous data numerically is often the basis for important decision. It is therefore important to identify the outlying observation before modelling and analysis of such data ([W+02], LSW04).

In this paper, an alternative robust method is proposed for estimating location and scatter matrix for multivariate data set and therefore contributes to the developments of aspects of robust estimation methods in the presence of outliers.

The minimum covariance determinant (MCD) method developed by Rousseuw ([Rou84]) is a highly robust estimator of multivariate location and scatter. Given an nxp data matrix x = (x_1, …, x_n) with x_i = (x_{i1}, …, x_{ip})^T, its objective is to find h observations with [(n+p+1)/2] ≤ h ≤ n whose covariance matrix has the lowest determinant. The minimum covariance determinant (MCD) estimate of location $\hat{\mu}$ is the average of these h points, and the scatter estimate $\hat{\Sigma}$ is a multiple of their covariance matrix. Butler et al. ([BDJ93]) had shown the consistency and asymptotic normality of the MCD estimator in their works, and also supported in the work of Carter and Lopuhaa ([CL10]). Croux and Haesbroech ([CH00]) argued that minimum covariance determinant (MCD) has a sounded influence function with highest possible breakdown value of 50% when h = [(n+p+1)/2], this is in line with Lopuhaa and Rousseeuw ([LR91]). The Minimum Covariance Determinant (MCD) is highly resistant to outliers and also possesses the characteristics of affine equivariant, that is, the estimates behave properly under affine transformations of the data.

Rousseeuw and Van Driessen ([RD99]) introduced Fast MCD as a fast resampling algorithm for the MCD. It starts by drawing initial random subsets of size p + 1 and performs so called concentration steps (C-steps) on them, yielding consecutive h-subsets with decreasing covariance matrix determinant. Since a random subset of size p + 1 is likely to contain outliers, many (by default 500) initial random subsets need to be considered to ensure that at least one of them is outlier free, which is computationally costly. To cut down on computation time, only C-steps are applied to each initial subset, and the 10 results with lowest determinant are kept. From these, C-steps are carried out until convergences, and again, the best solution is kept.

The minimum volume Ellipsoid estimator is first proposed by Rousseeuw ([Rou84]). It has been studied extensively for non-control charts settings and frequently used in detection of multivariate outliers. The mahalanobis distances based on Minimum volume Ellipsoid estimators proved to be very effective in detecting several outliers in a multivariate point cloud Rousseeuw and van Zomeren ([RZ93]). Vargas ([Var03]) suggested that if an unknown number of outliers are present, as is usual, in a multivariate data set, Minimum Volume Ellipsoid estimator is appropriate method that can consistently detect and identify them. Rousseeuw and van Zomeren ([RZ90]) recommended the application of the Minimum Volume Ellipsoid (MVE) when $n > 5p$.

The estimation seeks to find the Minimum Volume Ellipsoid that covers a subset of at least h data points. The subset of size h is called half set because h is often chosen to be just more than half of the n data points. The location estimator is the geometrical center of the ellipsoid and the estimator of the variance –covariance matrix defining the ellipsoid itself is multiplied by an appropriate constant to ensure consistency Rousseeuw and van Zomeren ([RZ90]), Rocke and Woodruff ([RW98]). Davies ([Dav97]) and Lopuhaa and Rousseeuw ([LR87]) proved that $h = \frac{n+p+1}{2}$ leads to maximum robustness (maximum breakdown point of $\frac{(n-p+1)/2}{n}$ which converges to 0.5 as $n \to \infty$).

However it was show by Davies ([Dav92]) that the Minimum Volume Ellipsoid (MVE) estimator is not $\sqrt{n}$ consistent.

Hampel et al. ([H+86]) pointed out that besides the breakdown point which is important robust measure; there is influence function which measures the effect on an estimator of adding a small mass at a specific point. Robust estimators ideally have a bounded influence function, which means that a small contamination at any point can only have a small effect on the estimator. Maronna ([Mar76]); Huber ([Hub81]) introduced M-estimator as the first class of bounded influence estimators for multivariate location and scatter. Tatsuoka and Tyler ([TT00]) introduced the multivariate MM-estimators as belonging to a broad class of estimators which they call Multivariate M- estimator with auxiliary scale. To estimate the scale by means of a very robust S-estimator and then estimate the location and shape using a different function is the idea behind its introduction that yields better efficiency at the central model. The breakdown points of the auxiliary scale were inherited by the location and shape estimates and can be seen as a generalization of the regression MM- estimators of Yohai ([Yoh87]). Another version of MM-estimators was proposed by Lupuhaa ([LR91]). He uses the entire initial covariance matrix (Σ_n) as an auxiliary statistic, instead of the scale $(\hat{\sigma}_n)$ only.

Tatsuoka and Tyler ([TT00]) work indicated that MM-estimators for multivariate location and scatter matrix inherited the breakdown point of the initial S-estimator and the asymptotic breakdown point was further investigated by Tyler ([Tyl02]). It was also shown in Tatsuoka and Tyler ([TT00]) that the MM-estimators for multivariate location and scatter are Fisher consistent for a broad class of distributions. In addition the MCD and other estimators equally have a bounded influence function. The first high-breakdown location and scatter estimator was proposed by Stahel ([Sta81]) and Donoho ([Don82]). The Stahel – Donoho estimates adopted weighted mean and covariance, the estimator has good robustness properties but it is computationally intensive which limits its use Tyler ([Tyl94]); Maronna and Yohoi ([MY95]). The Stahel Donolo estimator measures the outlyingness by examining at all univariate projection of the data, and it is related to projection pursuit methods in [FT74], [Hub85] and by Croux and Ruiz-Gazen ([CR05]).

Hubert et al ([H+14]) developed a new DetS and Det MM-estimator for multivariate location and scatter, the estimator combined the ideas from the deterministic DetMCD estimator with steps from the subsampling-based Fast S and Fast MM algorithms. The new DetS and Det MM-estimators performed similarly to FastS and Fast MM on low-dimensional data, where as in high dimentional data they are more robust. Their computational time is much lower than Fast S and Fast MM which allows to compute the estimate for a range of breakdown values. More also they are permutation invariant and very close to affine equvariant.

Kris Boudt et al ([B+18]) propose the Minimum Regularised Covariance Determinant (MRCD) approach, which differs from the MCD in that the subset- based covariance matrix is a convex combination of a target matrix and the sample covariance matrix. It is a data –driven procedures that sets the weight of the target matrix so that the regularization is only used when needed.

2. MEDODOLOGY

2.1 A proposed alternative robust estimator for multivariate location and scatter matrix

Let $X_n = x_{1,} \dots, x_n$ with $x_i \in \Re^p$ be the set of data with $X_i \sim N_p(\mu, \Sigma)$

It is assumed that the data are generated from an elliptical distribution i.e., a distribution whose density contours are ellipses.

The classical estimators for μ and Σ are the empirical mean and covariance matrix respectively where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_{i,} \qquad S_n = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(x_i - \bar{x})^1$$

Both the empirical mean and standard deviation are highly sensitive to outliers with Zero breakdown value and unbounded influence function (IF).

The proposed alternative robust method focused on the Eigen roots of variance covariance matrix. Given a P-dimensional multivariate normal data X_{pxm} with m observation $\{x_i\}_{i=1}^{m}$ The interest here is to obtain a subset of $\{x_i\}_{i=1}^{m}$ of size k =p+1 that satisfy some criteria stated below;

C_A= The minimum of the arithmetic mean of Eigen-roots; $\min\left\{\frac{\sum_{i=1}^{p}\lambda_{ij}}{p}, j = 1,2,3,,, C_k^m\right\}$.

C_H = The minimum of the harmonic mean of the Eigen- roots; $\min\{H(\lambda_{ij}), j = 1,2,3,,, C_k^m\}$, where $H(\lambda_{ij}) = \frac{p}{\sum_{i=1}^{p}\frac{1}{\lambda_{ij}}}$ is the harmonic mean λ's .

C_G = The minimum of the Geometric mean of the Eigen roots $\min\{G(\lambda_{ij}), j = 1,2,3,,, C_k^m\}$, where $G(\lambda_{ij}) = \sqrt[p]{\prod_{1=1}^{p}\lambda_{ij}}$ is the geometric mean of λ's .

A sample of size k from m is therefore drawn that will give C_{p+1}^m possible subsets of size p + 1. The variance-covariance matrix Σ_j is therefore estimated

as $\Sigma_j = \frac{1}{p+1}(x_j - \bar{x}_j)(x_j - \bar{x}_j)^T$

For each of the pxp matrix Σ_j, the eigen values $\lambda_{j1}, \lambda_{j2},,, \lambda_{jp}$ are obtained. from the egien values, the following is then obtained, the Arithmetic mean of the eigen value, the harmonic means of the eigen value and the geometric mean of the eigen value denoted by A, H and G respectively, from which the above optimality criteria is defined.

The objective here is to obtain data points whose variance –covariance matrix will satisfy at least two of the criteria taken in to consideration when the variance covariance matrix is from independent variables and also dependent variable (correlated variables).

The resulting covariance matrix will be inflated or deflated to accommodate good data points within the observed data.

2.2 Simulation procedures

P-variate multivariate data with m observation (P=2,3,4,5 and M = 10, 15,20,25,30,40, 50), taken *k= p+1* data points as many times as possible for independent variable and dependent variable.

Variance covariance matrix for each sample and the characteristic roots of such matrix are obtained from which the arithmetic, the harmonic mean and the geometric mean of the eigen values were obtained. The three optimality criteria (C_A,C_H,C_G) were also obtained.

From the simulation the following were observed, for various value of m (the population size) and p (the number of variables), whenever an appropriate no of sub-sample is taken, a set of data points obtained will satisfy at least two of the three criteria postulated except in some few cases where data point satisfied only one criteria both when the variance-covariance matrix is obtained from independent variables and correlated variables.

It is also observed that the criteria that was mostly satisfied were the harmonic and geometric mean except in some few cases where the data points satisfied the arithmetic and harmonic mean and also arithmetic and geometric mean.

It is also observed that taken excess subsample more than the required number of subsample (C_k^m) where k =p+1 does not change the data points that satisfied the criteria. This is true in the two cases. When equal number of sub-sample is taken for both independent and dependent variance-covariance matrixes the same data point satisfied at least two criteria except in some few instances.

Based on the Minimum Volume Ellipsoid (MVE) estimator, the k=p+1 of C_k^m sub- samples will form the basis for obtaining the Proposed estimator. The k+1 good data point that satisfy at least two of the optimality criteria is inflated or deflated to accommodate $h = \frac{m+p+1}{2}$ which is the half set of the data that are good from the whole data set.

2.3 Algorithm for obtaining proposed alternative estimator

Given a p-dimensional multivariate normal data X_{pxn} with n observations, $\{x_i\}_{i=1}^n$.

1. Decomposed the data using singular value decomposition(SVD)
2. From the n observations, take a subsample of size k = p + 1, C_k^n times
3. For each sample of p + 1, obtain the three optimality criteria $\{C_A, C_H, C_G\}$
4. Seek the sample points that satisfy at least two of the optimality criteria.
5. Obtain the classical mean vector and variance-covariance matrix;

$$\bar{x}_J = \frac{1}{p+1}\sum_{i\in J} x_i \quad \text{and}$$

$$S_J = \frac{1}{p}\sum_{i\in J}(x_i - \bar{x})(x_i - \bar{x})^T$$ respectively.

6. Use the estimates to obtain the mahalanobis distances;

$$d_j^2(i) = (x_i - \bar{x}_J)^T S_J^{-1}(x_i - \bar{x}_J),\ i = 1, 2, 3, \ldots, n$$

7. The mahalanobis distances are then ordered such that $d_1^2 \le d_2^2 \le d_3^2 \le,-,-,- \le d_n^2$
8. The p+2 points that correspond to the first p+2 ordered distances are picked to estimate the new estimates of mean vector and variance-covariance matrix.
9. Steps 4 and 5 are repeated until the selected sample points is h, where $h = \frac{n+p+1}{2}$.

The classical mean and variance-covariance matrix of the h points is the robust estimate of the vector of means and scatter matrix given as;

$$\bar{x}_{alternative} = \frac{1}{h}\sum_{i\in J} x_i \quad \text{and}$$

$$S_{alternative} = \frac{1}{h-1}\sum_{i\in h}(x_i - \bar{x}_{alternative})(x_i - \bar{x}_{alternative})^T \cdot (\chi^2_{j,0.025})^{\frac{1}{p}}$$

Where $(\chi^2_{j,0.025})^{\frac{1}{p}}$ is a correcting factor with p as the dimension, $j = \frac{(n+p+1)}{2}$

3. DATA ANALYSIS

3.1 Simulation study

Assuming we have a multivariate data set with number of observation n=20 and with number of variable p=3 such that $X_3 \sim N(\mu, \Sigma)$, where $\mu = [0,0,0]$ and $\sum$ is the variance co-variance matrix.

The data were contaminated at different percentages of 10%, 20%, 30% and 40%, with 2, 5, 10, 15, and 20 as magnitude of contamination/outliers introduced. The results obtained at various levels of magnitude with 100 iterations are shown in Table 1-7. The eigen roots were obtained based on the variance co-variance matrix estimated by;

- Classical methods
- Minimum covariance determinant
- Minimum volume Ellipsoid
- Proposed Alternative method

Let $\lambda_u = (\lambda_{1u}, \lambda_{2u}, \lambda_{3u})$ be the unique eigen roots from the variance co-variance matrix of an uncontaminated data set, and $\lambda_D = (\lambda_{1D}, \lambda_{2D}, \lambda_{3D},)$ be the eigen roots from variance co-variance matrix of a contaminated data,

Then the $MSE(\lambda_i) = \frac{1}{m}\sum_{i=1}^{m}(\lambda_i^{D(m)} - \lambda_i^{U(m)})^2$.

Eigen values obtained with 100 iterations, 20 sample sizes, varying values of magnitude of outliers and varying number of outliers in percentages is show in table 1-8 and Figure 1-8 below.

Table 1: Mean square error of eigen values when p=2 with magnitude of outlier equal 2

Outliers	Classical	MCD	MVE	Proposed
10%	1.3500	1.7316	1.5925	0.0792
20%	1.7154	1.8369	1.5862	0.0899
30%	1.7842	2.1104	2.0778	0.0792
40%	1.9813	1.8356	1.8621	0.0992

Table 2: Mean square error of eigen values when p=2 with magnitude of outlier equal 5

Outliers	Classical	MCD	MVE	Proposed
10%	3.2693	1.8798	1.8418	0.1358
20%	5.8193	2.7278	2.6426	0.1787
30%	7.8517	5.1762	5.2229	0.2654
40%	9.0334	7.1664	7.5409	0.3345

Table 3: Mean square error of eigen values when p=2 with magnitude of outlier equal 15

Outliers	Classical	MCD	MVE	Proposed
10%	30.2190	1.6184	1.6919	0.3168
20%	53.2135	1.8268	1.8048	1.0157
30%	71.1496	2.0284	1.9210	1.6828
40%	80.4882	1.6915	2.3246	2.7458

Table 4: Mean square error of eigen values when p=2 with magnitude of outlier equal 20

Outliers	Classical	MCD	MVE	Proposed
10%	53.8169	1.5563	1.6795	0.5628
20%	94.8856	1.6815	1.7317	1.8228
30%	125.3166	1.8165	1.8235	3.4305
40%	141.9813	1.7279	3.2213	4.1227

Table 5: Mean square error of eigen values when p=3 with magnitude of 2

Outliers in %	Classical	MCD	MVE	Proposed
10	2.4014	2.5273	2.4301	1.6145
20	2.5416	2.6252	2.4590	1.9464
30	2.7899	2.9080	3.0266	2.0748
40	2.6435	2.9061	2.6925	2.2844

Table 6: Mean square error of eigen values when p=3 with magnitude of 5

Outliers	Classical	MCD	MVE	Proposed
10%	4.2800	3.0759	2.7592	2.2351
20%	6.8054	3.5785	3.8392	3.2097
30%	9.2912	6.2077	7.1794	4.7297
40%	10.8962	9.5471	10.7504	5.9159

Table 7: Mean square error of eigen values when p=3 with magnitude of 15

Outliers	Classical	MCD	MVE	Proposed
10%	36.1450	2.6257	2.6926	5.3490
20%	64.3010	2.6227	2.6213	15.2456
30%	85.6156	3.0591	2.9265	30.7507
40%	98.3753	74.0571	81.9995	57.6168

Table 8: Mean square error of eigen values when p=3 with magnitude of 20

Outliers	Classical	MCD	MVE	Proposed
10%	65.8589	2.5202	2.5035	8.9354
20%	114.0941	2.4959	2.6193	32.3001
30%	152.1170	2.8316	2.8563	56.5233
40%	183.2250	83.0622	90.6226	62.2252

3.2 Discussion of results

When the magnitude of outliers is 2, the mean square error of the eigen values obtained with the Proposed method is the least at all percentages level of outliers, this is distantly followed by the Classical, MVE and MCD in that order at all percentage levels of outliers (Figure1).
When the magnitude of outliers is increased to 5 the MSE obtained using Proposed method is the least, distantly followed by that of the Classical, MVE and MCD in that order at all percentage levels of outliers (Figure 2).
When the magnitude of outliers is increased to 15 the MSE obtained using Proposed method is the least, but higher than that of the MVE and MVE at 40% level of outliers. The Classical method MSE is significantly high at all percentage levels of outliers compared to the other three methods (Figure 3).
When the magnitude of outliers is increased to 20 the MSE of the eigen value obtained using Proposed method is the least, but higher than that of the MVE and MVE at 30% and40% level of outliers. The Classical method MSE is significantly high at all percentage levels of outliers compared to the other three methods (Figure 4).
When the magnitude of outliers is 2 with p increased to 3 the MSE of the eigen values obtained using Proposed method is the least, closely followed by the classical method at all the percentage levels of outliers while the MVE and MVE followed in that order except at the 30% level of outlier where the MSE of MVE=3.0266 and MSE of MCD=2.9080 (Figure 5).
When the magnitude of outliers 5 and p=3 is introduced, the MSE obtained the eigen value using the Proposed method is the least at all percentage levels of the outliers this followed by the MSE of the MVE and MCD except at the percentage level of 30 and 40. The MSE of the eigen value by the Classical remain the highest at all the percentage levels (Figure 6).
When the magnitude of outliers introduced is 15 and p=3, the MSE of the eigen value obtained using the Proposed method is the least at the percentage levels of 40 while the MSE of the MCD is the least at 10 percentage level of outliers. The MSE of MVE is the least at 20 and 30 percentage levels. The MSE of the

eigen value by the Classical remain the highest at all the percentage levels (Figure 7).
When the magnitude of outliers introduced is increased to 20 at p=3, the MSE of the eigen value obtained using the Proposed method is the least at the percentage levels of 40 while the MSE of the MVE is the least at 10 percentage level of outliers. The MSE of MCD is the least at 20 and 30 percentage levels of outliers. The MSE of the eigen value by the Classical remain the highest at all the percentage levels (Figure 8).

4. CONCLUSION

Comparing the four methods with their application in obtaining eigen values of variance covariance matrix, using mean square error (MSE) of the eigen values, the Alternative Robust Methods was the least in almost all the cases considered. This implies that the Proposed Alternative Robust Method is insensitive to both percentage and magnitude of outliers than the Minimum Covariance Determinant (MCD) and the Minimum Volume Ellipsoid (MVE) methods, which are widely accepted to be robust methods and also more than classical method.
Generally, the Proposed Alternative Method is better than other robust methods and classical method, when the level of magnitude of outliers is small and also performed considerably well with MCD and MVE when the level of magnitude is high at all percentages of outliers.

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