Improving the Peña-Prieto “KSD” procedure

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Abstract

Peña and Prieto (2007) proposed the “Kurtosis plus specific directions” (KSD) method for robust multivariate location and scatter estimation and outlier detection. Maronna and Yohai (2017) employed it as an initial estimator for multivariate S- and MM-estimators, and their simulations showed that KSD generally outperforms initial estimators based on subsampling. However, further simulations show that KSD may become unstable and give wrong results in extreme situations when the contamination rate is “high” (≥ 0.2) and the ratio n/p of cases to variables is “low” (<10). Two simple modifications of the procedure are proposed, which greatly improve on the method’s performance as an initial estimator, with only a small increase in computational time.

1 The problem

Peña and Prieto (2007) developed an elaborate procedure for multivariate outlier detection and robust estimation of multivariate location and scatter, called “Kurtosis plus Specific Directions” (henceforth KSD). Maronna and Yohai (2017) have employed it as a starting estimator for robust multivariate estimators that are computed iteratively and need reliable initial values, and their simulations show that the initial values supplied by KSD generally yield better results than those based on subsampling, both in statistical performance and in computing speed.

However, it was observed by the author that in certain “difficult” cases KSD can be highly unstable and yield totally useless values. These cases occur when the contamination rate ε is “high” (≥ 0.2) and the ratio n/p of number of observations to number of variables is “low” (<10).

The problem was studied through simulated data with p between 10 and 50. Contaminated normal samples were generated as in (Maronna and Yohai 2017), namely: the “clean” observations \( \mathbf{x}_i \in \mathbb{R}^p \) \( i = 1, ..., n \) are generated as \( \mathcal{N}_p(\mathbf{0}, \mathbf{I}) \). Call respectively \( \varepsilon \), \( K \) and \( \gamma \) the contamination rate, the outlier size and the outliers’ dispersion and let \( m = \lfloor n\varepsilon \rfloor \). Then the data are contaminated by changing \( x_{i1} \) to \( \gamma x_{i1} + K \) for \( i = 1, ..., m \).
Since we are interested in the performance of KSD as a starting estimator, rather than the behavior of KSD itself, we use the output of KSD to start the iterations to compute Rocke’s (1996) $S$-estimator of location and scatter $\left(\hat{\mu}, \hat{\Sigma}\right)$.

The matrix $\hat{\Sigma}$ is corrected to make it consistent at the normal.

As an example, we generate $N = 200$ samples with $p = 30$, $n = 100$ and contamination rate $\varepsilon = 0.2$, and two values of $\gamma$: 0 and 0.5, corresponding to concentrated and moderately dispersed outliers. For each sample we compute Rocke’s location vector $\hat{\mu}$ and scatter matrix $\hat{\Sigma}$, and for each of them we compute its Kullback-Leibler divergence:

$$D(\hat{\mu}) = \|\hat{\mu}\|^2, \quad D(\hat{\Sigma}) = \text{trace}(\hat{\Sigma}) - \log\det(\hat{\Sigma}) - p.$$

In the following we concentrate on the scatter matrix $\hat{\Sigma}$, which appears to be more affected than $\hat{\mu}$ by this phenomenon. The next figure shows the ordered values of $D(\hat{\Sigma})$ for the $N$ Monte Carlo replications, corresponding to $K = 13$ with $\gamma = 0$ and $\gamma = 0.5$.

Ordered values of $D(\Sigma)$ of the Rocke estimator starting from the old version of KSD for $K = 13$

It is seen that the estimator is rather unstable and may yield very high values: for $\gamma = 0$ 30% of the values are below 8 and the rest are above 42; for $\gamma = 0.5$ roughly 20% of the values are below 8 and the rest are above 35.
2 The solution

We first need to give a brief description of KSD. It consists of three stages.

The data are first normalized to zero means and identity covariance matrix. Call \( z_i, i=1, \ldots, n \) the normalized data and \( Z \) the respective \( n \times p \) matrix.

In stage I, a number \( N_{\text{Kurt}} \) of directions \( u_k \) is derived, each of which yields a local maximum or minimum of the kurtosis of the projections \( Zu_k \).

In stage II a number \( N_{\text{SD}} \) of random “specific directions” \( v_k \) is computed, by a sort of stratified sampling procedure, which will hopefully have a higher probability of detecting outliers than simple random sampling.

Now the set of directions \( \mathcal{D} = \{ u_k, k=1, \ldots, N_{\text{Kurt}}, v_k, k=1, \ldots, N_{\text{SD}} \} \) is used in the same manner as in the Stahel (1981) -Donoho (1982) estimator to derive for each \( z_i \) an outlyingness measure \( t_i \).

In stage III the \( t_i \)s are used to make a preliminary classification of outliers. Suspect observations are temporarily deleted, and the procedure is repeated until no further changes occur.

The default values in the Matlab code kindly supplied by the authors are \( N_{\text{Kurt}}=2 \) and \( N_{\text{SD}}=10p \).

We now turn to fixing the problems shown in the former section. Experiments showed that dealing with the case of dispersed outliers required increasing \( N_{\text{SD}} \), and that a satisfactory choice was found to be

\[
N_{\text{SD}} = \max (Mp, 1000) \text{ with } M = 50. \tag{1}
\]

Larger values of \( M \) do not seem to yield an improvement.

This however did not fix the problem with concentrated outliers. Then the idea was to use the \( z_i \)’s themselves as directions, since if \( x_i \) is an outlier, one would expect \( z_i \) to point in the direction of \( x_i \). Adding the set of \( z_i \)’s to \( \mathcal{D} \) did in fact solve the problem. It may however become computationally expensive for large \( n \) since it is \( O \left( n^2 \right) \). It was observed that contrary to expectation, the outliers corresponded to the \( z_i \)’s with smallest norms. For this reason, rather than adding to \( \mathcal{D} \) the whole set of \( n \) \( z \)’s, it was decided to add the \( m \) with smallest and the \( m \) with largest norms, with \( m=\min \left( 5p, n/2 \right) \).

The next figure shows the results.
Ordered values of $D(\Sigma)$ of the Rocke estimator for $K = 13$, starting from the old (blue) and new (red) versions of KSD.

It is seen that for $\gamma = 0$ new version is very stable and yields much lower values than the old one; for $\gamma = 0.5$ it is more stable and its values are generally much lower than those from the old one.

To have a more complete picture, the simulation was performed for $K = 1, 2, ..., 30$. The next figure shows the mean $D(\hat{\Sigma})$ of the Rocke estimator, corresponding to the old and new versions of KSD.
Simulation for $p = 30$ : mean $D(\Sigma)$ starting from the old (blue) and new (red) versions of KSD.

It is seen that the new version is a represents a clear improvement over the old one. It may be argued that since for each $K$ the distribution of $D$ for each estimator is bimodal, the mean is not a representative value. However, using the median or a trimmed mean instead of the mean yields essentially the same qualitative conclusions.

### 3 Computing times

The average computing times of Rocke’s estimator based on the new to the old version was computed for $p$ between 10 and 50. The following table gives the results in seconds for the estimators computed in R on a PC with a 3.60 GHz Intel Core processor with 16 GB RAM.

| $p$ | $n$ | New   | Old   | new/old |
|-----|-----|-------|-------|---------|
| 20  | 100 | 0.030 | 0.008 | 3.750   |
|     | 400 | 0.036 | 0.015 | 2.400   |
| 50  | 250 | 0.134 | 0.056 | 2.393   |
|     | 1000| 0.181 | 0.121 | 1.496   |
| 100 | 500 | 0.737 | 0.526 | 1.402   |
|     | 2000| 0.970 | 0.871 | 1.113   |
It is seen that the improvement does not have a high cost in terms of computing performance. It is curious that the ratio new/old decreases with $n$ and with $p$. No explanation could be found for this fact.

4 References

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