Robust and efficient estimation of high dimensional scatter and location

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Abstract

We deal with the equivariant estimation of scatter and location for \( p \)-dimensional data, giving emphasis to scatter. It is important that the estimators possess both a high efficiency for normal data and a high resistance to outliers, that is, a low bias under contamination. The most frequently employed estimators are not quite satisfactory in this respect. The Minimum Volume Ellipsoid (MVE) and Minimum Covariance Determinant (MCD) estimators are known to have a very low efficiency. S-Estimators (Davies 1987) with a monotonic weight function like the bisquare behave satisfactorily for “small” \( p \), say \( p \leq 10 \). Rocke (1996) showed that their efficiency tends to one with increasing \( p \). Unfortunately, this advantage is paid with a serious loss of robustness for large \( p \).

We consider three families of estimators with controllable efficiencies: non-monotonic S-estimators (Rocke 1996), MM-estimators (Tatsuoka and Tyler 2000) and tau-estimators (Lopuhaä 1991), whose performance for large \( p \) has not been explored to date. Two types of starting estimators are employed: the MVE computed through subsampling, and a semi-deterministic procedure proposed by Peña and Prieto (2007) for outlier detection.

A simulation study shows that the Rocke and MM estimators starting from the Peña-Prieto estimator and with an adequate tuning, can simultaneously attain high efficiency and high robustness.

1 Introduction

Consider a sample \( \mathbf{X} = \{ \mathbf{x}_1, \ldots, \mathbf{x}_n \} \subset \mathbb{R}^p \). We look for substitutes \( \hat{\mu} \in \mathbb{R}^p \) and \( \hat{\Sigma} \in \mathbb{R}^{p \times p} \) of the sample mean vector and covariance matrix, that are resistant to atypical observations. We also want estimators that have a high efficiency for normal samples. As a measure of robustness we consider not only the breakdown point but also the maximum bias under contamination.

The most frequently employed estimators are not quite satisfactory in this respect. The Minimum Volume Ellipsoid (MVE) and Minimum Covariance Determinant (MCD) (Rousseeuw 1985) estimators are known to have a very...
low efficiency. S-Estimators (Davies 1987) with a monotonic weight function like
the bisquare behave satisfactorily for “small” $p$, say $p \leq 10$; but Rocke (1996)
showed that their efficiency tends to one with increasing $p$. Unfortunately, this
advantage is paid for with a serious loss of robustness for large $p$.

We restrict ourselves to equivariant estimators. There exist many non-
equivariant proposals; but the comparison between equivariant and non-equivariant
estimators is difficult. In particular, a non-equivariant estimator is more difficult
to tune for a given efficiency, since the latter depends on the correlations.

Among the published equivariant proposals, there are three families of esti-
mators with controllable efficiencies: non-monotonic S-estimators (Rocke 1996),
MM-estimators (Tatsuoka and Tyler 2000) and $\tau$-estimators (Lopuhaa 1991) but
their behavior for large dimensions has not been explored to date. We compare
their behaviors employing different loss functions. A simulation study shows
that the Rocke and MM estimators, with an adequate and an adequate tuning,
can simultaneously attain high efficiency and high robustness.

It will be seen below that if we have a good $\hat{\Sigma}$, it is easy to find a good
equivariant $\hat{\mu}$, but the converse is not true. For this reason we shall put more
emphasis on the estimation of the scatter matrix.

Since all the considered estimators are based on the iterative minimization of
a non-convex function, the starting values are crucial. Subsampling is the stan-
dard way to compute starting values; but we shall see that a semi-deterministic
equivariant procedure may yield both shorter computing times and better sta-
tistical performances.

In Section 2 we describe M-estimators; Section 3 deals with estimators based
on the minimization of a robust scale of Mahalanobis distances. Section 4
deals with MM estimators. In Section 5 the estimators are compared through
a simulation study. In Section 6 the estimators are applied to a real data
set. Finally Section 11 summarizes the results. The Appendix contains the
approximations for the tuning constants and some details on the Rocke and the
Peña-Prieto procedures.

2 M-estimators

For $x, \mu \in \mathbb{R}^p$ and $\Sigma \in \mathbb{R}^{p \times p}$ define the (squared) Mahalanobis distance as

$$d(x, \mu, \Sigma) = (x - \mu)' \Sigma^{-1} (x - \mu).$$

Let $W$ be a bounded nonincreasing “weight function”. Then M-estimators
(Maronna 1976) are defined as solutions of

$$\frac{1}{n} \sum_{i=1}^{n} W(d_i) (x - \mu) (x - \mu)' = \Sigma \quad (1)$$

$$\frac{1}{n} \sum_{i=1}^{n} W(d_i) (x - \mu) = 0 \quad (2)$$
where for brevity we put
\[ d_i = d(x_i, \mu, \Sigma). \]

The uniqueness of the solutions requires that \( W(d) \) be nondecreasing. Unfortunately, this implies (Maronna, 1976) that the breakdown point is \( \leq 1/(p+1) \), which makes these estimators unreliable except for small \( p \). Besides, this fact holds even if \( \mu \) is known, while the asymptotic breakdown point of \( \hat{\mu} \) with known \( \Sigma \) is 0.5 with an adequate \( W \). This shows that the main problem to attain high robustness is the scatter matrix.

3 Estimators based on the minimization of a robust scale

For \( d = (d_1, ..., d_n) \) let \( S(d) \) be a robust scale. Put
\[ d(\mu, \Sigma) = \{ d(x_1, \mu, \Sigma), ..., d(x_1, \mu, \Sigma) \} \]

A general family of estimators can be defined by
\[
\left( \hat{\mu}, \tilde{\Sigma} \right) = \arg \min S(d(\mu, \Sigma)), \ \mu \in \mathbb{R}^p, \ \Sigma \in \mathbb{R}^p, \ |\Sigma| = 1,
\]
where the condition \( |\Sigma| = 1 \) rules out trivial solutions with \( \Sigma \to \infty \).

If \( S(d) = \text{Median}(d) \) we have the “Minimum Volume Ellipsoid” (MVE) estimator, and if \( S \) is a trimmed mean, we have the “Minimum Covariance Determinant” (MCD) estimator, both proposed by Rousseeuw (1985). The first one is very robust, but has a null asymptotic efficiency; the second is very popular, but its asymptotic efficiency is very low; see (Paindaveine and Van Bever, 2014) and references therein, and its maximum contamination bias increases rapidly with \( p \) (Agostinelli et al, 2015, Table 1).

The condition \( |\Sigma| = 1 \) means that we estimate the “shape” of the scatter. Given the shape, the ”size” can easily estimated to yield consistency at the normal model (Maronna et al., Section 6.3.2). A simple way is to put
\[
\tilde{\Sigma} = \frac{\text{Median} \left( d \left( \hat{\mu}, \hat{\Sigma} \right) \right)}{\text{Median}(\chi^2_p)} \Sigma.
\]

Instead of the median, one could use more efficient scales, such as an M-scale, but exploratory simulations indicate that they do not yield better results.

3.1 S-estimators

Let \( S = S(d_1, ..., d_n) \) be a scale M-estimator defined as solution of
\[
\frac{1}{n} \sum_{i=1}^{n} \rho \left( \frac{d_i}{S} \right) = \delta,
\]

where \( \delta \in (0, 1) \) controls the breakdown point, and \( \rho (t) \in [0, 1] \) is smooth and nondecreasing in \( t \geq 0 \), with \( \rho (0) = 0 \) and \( \max \rho = 1 \). Then S-estimators (Davies 1987) are defined as solutions of (3) with \( S \) given by (5).

The maximum replacement breakdown point is given by

\[
\delta = 0.5 \left( 1 - \frac{p}{n} \right).
\]

See (Maronna et al., 2006, Section 6.4.2).

A popular \( \rho \) is the bisquare given by

\[
\rho (d) = \begin{cases} 
1 - (1 - d)^3 & \text{if } d \leq 1 \\
1 & \text{if } d > 1
\end{cases}
\]

Note that the usual bisquare \( \rho \) employed for regression is actually \( \rho_{\text{bis}} (t) = \rho (t^2) \). However, since we are dealing with the squared distances, we employ in (7) \( \rho_{\text{bis}} \left( \sqrt{d} \right) = \rho (d) \).

It is easy to show that S-estimators satisfy the “estimating equations”

\[
\frac{1}{n} \sum_{i=1}^{n} W \left( \frac{d_i}{S} \right) (x - \mu) (x - \mu)' = \Sigma
\]

\[
\frac{1}{n} \sum_{i=1}^{n} W \left( \frac{d_i}{S} \right) (x - \mu) = 0
\]

\[
\frac{1}{n} \sum_{i=1}^{n} \rho \left( \frac{d_i}{S} \right) = \delta
\]

with \( W = \rho' \). That is, they are M-estimators (1)-(2) with weight function \( W = \rho' \). Here, since \( \rho \) is bounded \( W (d) d \) is not a nondecreasing function, and therefore this case is different from the “monotonic” M-estimators in Section 2. In particular, the breakdown point is not bounded by \( (1 + p)^{-1} \); as shown by (6).

For the bisquare, the weight function is

\[
W(t) = 3 (1 - t)^2 I(t \leq 1)
\]

(where I(.) denotes the indicator), which is decreasing. It seems intuitive that the weights of the observations should decrease with their “outlyingness”. However it will be seen in the next Section that monotonicity is not necessarily favorable.

S-estimators with bisquare \( \rho \) have a reasonable efficiency and robustness for moderate \( p \), say \( p \leq 10 \); see (Maronna et al., 2006, Table 6.2, page 196).
| $p$  | 10   | 20   | 30   | 40   | 50   |
|------|------|------|------|------|------|
| Efficiency | 0.930 | 0.976 | 0.984 | 0.990 | 0.992 |

Table 1: Efficiencies of the S-estimator with bisquare weights for dimension $p$

### 3.2 S-estimators with a non-monotonic weight function

Rocke (1996) showed that if $W$ is nonincreasing, the efficiency of the estimator tends to one when $p \to \infty$. Table 1 shows the efficiencies (to be defined later) of the bisquare S-estimator of scatter for normal $p$-dimensional data.

However, it will be seen that the price for this increase in efficiency is a decrease in robustness. More precisely, although the breakdown point does not tend to zero with increasing $p$, the bias caused by contamination grows rapidly with $p$. This fact suggests that we need estimators with a controllable efficiency. But while in regression the efficiency has to be controlled to make it higher, here we need to prevent it from becoming “too high”.

Based on the fact that for large $p$ the $p$-variate standard normal distribution $N_p(\mathbf{0}, \mathbf{I})$ is concentrated “near” the spherical shell with radius $\sqrt{p}$, Rocke (1996) proposed estimators with non-monotonic weight functions. Maronna et al. (2006) proposed a modification of Rocke’s “biflat” function, namely

$$W(d) = \left[1 - \left(\frac{d - 1}{\gamma}\right)^2\right] I(1 - \gamma \leq d \leq 1 + \gamma)$$

(11)

with

$$\gamma = \min\left(1, \frac{\chi^2_p(1 - \alpha)}{p} - 1, 1\right),$$

(12)

where $\chi^2_p(\beta)$ is the $\beta$-quantile of the $\chi^2$ distribution with $p$ degrees of freedom, and $\alpha$ is “small” to control the efficiency.

Unfortunately Maronna et al (2006, Sec. 6.8) dealt only with location. The performance of the respective scatter matrix will be studied below.

### 3.3 $\tau$-estimators

$\tau$-estimators were proposed by Yohai and Zamar (1988) to obtain robust regression estimators with controllable efficiency, and later Lopuhaä (1991) employed the same approach for multivariate estimation. This approach requires two functions $\rho_1$ and $\rho_2$. For given $(\mu, \Sigma)$ call $\sigma_0(\mu, \Sigma)$ the solution of

$$\frac{1}{n} \sum_{i=1}^{n} \rho_1\left(\frac{d(x_i, \mu, \Sigma)}{\sigma_0}\right) = \delta.$$
Then the estimator minimizes the “τ-scale”

\[ \sigma(\mu, \Sigma) = \sigma_0(\mu, \Sigma) \frac{1}{n} \sum_{i=1}^{n} \rho_2 \left( \frac{d(x_i, \mu, \Sigma)}{\sigma_0(\mu, \Sigma)} \right). \]

Here

\[ \rho_2(t) = \rho_1 \left( \frac{t}{c} \right) \] (13)

where \( c \) is chosen to regulate the efficiency.

Originally, τ-estimators were proposed to obtain estimators with higher efficiency than S-estimators for small \( p \), which required \( c > 1 \); but for large \( p \) we need \( c < 1 \) in order to decrease the efficiency.

4 MM-estimators

MM-estimators were initially proposed by Yohai (1987) to obtain regression estimators with a controllable efficiency. This approach has been used in the multivariate setting by Lopuhaä (1992) and Tatsuoka and Tyler (2000). Here we give a simplified version of the latter.

Let \( (\tilde{\mu}_0, \tilde{\Sigma}_0) \) be an initial very robust although possibly inefficient estimator. We choose the MVE. Put

\[ d_i^0 = d \left( x_i, \tilde{\mu}_0, \tilde{\Sigma}_0 \right) \]

and call \( S \) the respective M-scale

\[ \frac{1}{n} \sum_{i=1}^{n} \rho \left( \frac{d_i^0}{S} \right) = \delta. \] (14)

The estimator is defined by \( \left( \tilde{\mu}, \tilde{\Sigma} \right) \) with \( |\tilde{\Sigma}| = 1 \) such that

\[ \sum_{i=1}^{n} \rho \left( \frac{d_i}{cS} \right) = \min, \] (15)

where \( d_i = d \left( x_i, \tilde{\mu}, \tilde{\Sigma} \right) \) and the constant \( c \) is chosen to control efficiency.

It can be shown that the solution satisfies the equations

\[ \frac{1}{n} \sum_{i=1}^{n} W \left( \frac{d_i}{cS} \right) (x - \mu) (x - \mu)' = \Sigma \] (16)

\[ \frac{1}{n} \sum_{i=1}^{n} W \left( \frac{d_i}{cS} \right) (x - \mu) = 0 \]

with \( W = \rho' \),
Actually, it is not necessary to obtain the absolute minimum in (15). Any solution of (16) for \( y \) with the objective function (15) is lower than for the initial estimator, has the same asymptotic behavior as the absolute minimum and has a breakdown point at least as high as the initial estimator.

Like \( \tau \)-estimators, MM estimators were originally proposed to obtain estimators with higher efficiency than S-estimators for small \( p \); but here for large \( p \) the constant has to chosen to prevent the efficiency becoming too high.

5 Choosing \( \rho \)

The most popular \( \rho \) in robust methods seems to be the bisquare. Yohai and Zamar (1997) proposed a \( \rho \) for regression with certain optimality properties. A simplified variant of this function is given by Muler et al (2002). Its version for multivariate estimation has weight function

\[
W(d) = \begin{cases} 
1 & \text{if } d \leq 4 \\
q(d) & \text{if } 4 < d \leq 9 \\
0 & \text{if } d > 9 
\end{cases},
\]

where

\[
q(d) = -1.944 + 1.728d - 0.312d^2 + 0.016d^3
\]

is such that \( W \) is continuous and differentiable at \( d = 4 \) and \( d = 9 \). The respective \( \rho \) function is

\[
\rho(d) = \frac{1}{6.494} \begin{cases} 
\frac{d}{6.494} & \text{if } d \leq 4 \\
\frac{s(d)}{6.494} & \text{if } 4 < d \leq 9 \\
6.494 & \text{if } d > 9 
\end{cases},
\]

where

\[
s(d) = 3.534 - 1.944d + 0.864d^2 - 0.104d^3 + 0.004d^4.
\]

Figure 1 shows the bisquare and “optimal” weight functions, scaled with their respective tuning constants for the MM-estimator with 90% efficiency and \( p = 30 \). It is seen that the optimal \( \rho \) yields a smaller cutoff point.

6 Computing issues

All estimators described above are computed as iterative reweighted means and covariances, starting from an initial estimator. For S-, \( \tau \)- and MM estimators this algorithm ensures that the objective function descends at each iteration. This need not happen with the Rocke estimator, which has a non-monotonic weight function. Maronna et al. (2006, Section 6.4.4) describe an algorithm which ensures attaining a local minimum.

The (approximate) MVE is computed with 1000 subsamples and using the improvement described in (Maronna et al., 2006, Section 6.7.3).
Since in all cases we attempt to minimize a non-convex function, the initial estimator is an essential part of the procedure. The standard way to obtain a robust and equivariant starting point is subsampling. However, ensuring a high enough breakdown point with large $p$ may require an impractically large number of subsamples. Besides, our experiments indicate that the breakdown point may be much lower than expected when $n/p$ is “small” (say, $\leq 5$), which is not uncommon with high-dimensional data sets. For these reasons we need a faster and more reliable starting point.

Peña and Prieto (2007) proposed an equivariant and semi-deterministic procedure for outlier detection, based on finding directions that maximize or minimize the kurtosis of the respective projections, plus a set of random “specific directions” aimed at detecting outliers. Here we employ this procedure (which they call “kurtosis plus specific directions”, henceforth abbreviated as “KSD”) as an estimator by itself. In the present setting it would not be competitive with

![Figure 1: Bisquare and “optimal” weight functions.](image)
the other estimators because its efficiency cannot be tuned (see Table 2 below), but we shall use it as an initial estimator competing with the sampling-based MVE.

There are no theoretical results on the breakdown point of KSD. However, the simulations in (Peña and Prieto 2007, table 4) suggest that it can yield reliable results even with 40% of outliers. A limited theoretical result is given in Section 12.

7 Comparing the estimators

As a reference distribution we take the \( p \)-variate normal \( N_p (\mu_0, \Sigma_0) \). In order to measure the performance of a given estimator \( \hat{\mu}, \hat{\Sigma} \) we need a measure of “distance” between an estimator and the true value. Recall that the Kullback-Leibler divergence between densities \( f_1 \) and \( f_2 \) is

\[
d_{\text{KL}} (f_1, f_2) = \int_{-\infty}^{\infty} \log \left( \frac{f_1(z)}{f_2(z)} \right) f_1(z) \, dz.
\]

If both densities belong to the same parametric model with parameter vector \( \theta: f_j (z) = f(z, \theta_j) \), then \( d_{\text{KL}} \) induces a “distance” between parameters:

\[
D(\theta_1, \theta_2) = d_{\text{KL}} (f(., \theta_1), f(., \theta_1)).
\]

In the normal family, for \( \mu \) with known \( \Sigma \) we have

\[
D = (\hat{\mu} - \mu_0)' \Sigma_0^{-1} (\hat{\mu} - \mu_0),
\]

and for \( \Sigma \) with known \( \mu \) we have

\[
D = \text{trace} \left( \Sigma_0^{-1} \hat{\Sigma} \right) - \log |\Sigma_0^{-1} \hat{\Sigma}| - p
\]

Since all estimators are equivariant we may take without loss of generality \( (\mu_0, \Sigma_0) = (0, I) \).

8 Simulation

Each estimator is evaluated by \( \overline{D} = \text{Monte Carlo average of the Kullback-Leibler divergences} \) \( D \) given in (17)-(18).

We generate \( N = 500 \) samples \( \mathbf{X} = [x_{ij}] \) of size \( n \) from \( N_p (0, I) \).

The estimators compared are:

- Rocke with tuning constant \( \alpha \); see (12)
- MM with bisquare and “optimal” \( \rho \), with tuning constant \( c \); see (16)
- \( \tau \) with bisquare and “optimal” \( \rho \), with tuning constant \( c \); see (13)
• The S-estimator (S-E) with \( \delta = 0.5 \) in \( \text{[5]} \), as well as the MVE and KSD estimators are also added for completeness.

All scatter estimators are corrected for “size” by means of \( \text{[6]} \).

The tuning constants were chosen to attain an efficiency of 0.9 (see below).

For all estimators we employed both the MVE and KSD estimators as starting values.

### 8.1 No contamination

Call \( C \) the sample covariance matrix. For each estimator \( \hat{\Sigma} \) we define

\[
\text{efficiency} = \frac{D(C)}{D(\hat{\Sigma})}.
\]

The constants for each estimator are chosen to attain finite-sample efficiencies of 0.90. To this end we computed for each estimator its tuning constants for \( n = Kp \) with \( K = 5, 10 \) and 20 and \( p \) between 10 and 100, and then fitted the constants as functions of \( n \) and \( p \).

The simulation showed the efficiency cannot be controlled in all cases, namely

• For \( p = 15 \) the maximum efficiency of the Rocke estimator is 0.876 for all \( \alpha \)s, and is still lower for smaller \( p \). The explanation is that when \( \alpha \) tends to zero, the estimator does not tend to the covariance matrix unless \( p \) is large enough.

• The minimum efficiency of the \( \tau \) -estimators over all constants \( c \) tends to one with increasing \( p \), for both \( \rho \) -functions. In particular, it is >0.95 for \( p \geq 50 \). The reason is that when \( c \) is small, the \( \tau \) -scale approaches the M-scale, and therefore the \( \tau \) -estimators approaches the S-estimator.

Therefore, in order to be able to compare all estimators with the same efficiency, we limit the simulations to \( p \) between 15 and 30.

Table \( \text{[2]} \) shows the efficiencies of the KSD estimator.

It seen that the efficiency depends heavily on the ratio \( n/p \) and can be rather low for \( n/p = 5 \).

### 8.2 Contamination

We deal first with shift contamination. For contamination rate \( \varepsilon \), let \( m = \lfloor n\varepsilon \rfloor \).

Given \( K \), we replace the first coordinate:

\[
x_{1i} \leftarrow \gamma x_{1i} + K, \quad i = 1, \ldots, m
\]
Table 2: Efficiencies of the KSD estimator

| $p$ | $n$ | Scatter | Location |
|-----|-----|---------|----------|
| 10  | 50  | 0.40    | 0.62     |
| 100 |     | 0.70    | 0.85     |
| 200 |     | 0.86    | 0.95     |
| 20  | 100 | 0.44    | 0.62     |
| 200 |     | 0.80    | 0.89     |
| 400 |     | 0.90    | 0.95     |
| 50  | 250 | 0.47    | 0.58     |
| 500 |     | 0.82    | 0.85     |
| 1000|     | 0.93    | 0.96     |

The outlier size $K$ is varied in order to find the maximum $\overline{D}$. The constant $\gamma$ determines the scatter of the outliers. We employed the values $\gamma = 0$ and 0.5.

The simulations were run for $n = 15, 20$ and 30. Since the results for the three cases are qualitatively similar, we give them just for $p = 20$. Tables 3 and 4 show the results for $\varepsilon = 0.10$ and 0.20 respectively.

Comments

- KSD is always much better than MVE as a starting estimator.
- The “optimal” $\rho$ is always better than the bisquare $\rho$ in both MM and $\tau$.
- MM is generally better than $\tau$.
- The Rocke estimator starting with KSD clearly outperforms all other estimators; the MM estimator also does a good job.
- The price paid for the high efficiency of S-E is a large loss of robustness.

Figure 2 shows the values of $\overline{D}$ as a function of the outlier size $K$ for some of the estimators in the case $n = 200$ and $\gamma = 0$. Here “MM-Opt+KSD” stands for “MM estimator with optimal $\rho$ starting from KSD”.

The plot confirms the superiority of Rocke+KSD.

We now deal with radially distributed contamination. For contamination rate $\varepsilon$, let $m = \lfloor n\varepsilon \rfloor$. Given $K$, for $i = 1,...,m$ we replace $x_i$ with $Kx_i$. The “inflation” $K$ is varied in order to find the maximum $\overline{D}$. The simulations were run for $n = 15, 20$ and 30. Since the results for the three cases are qualitatively similar, we give them just for $p = 20$. Tables 5 and 6 show the results for $\varepsilon = 0.10$ and 0.20 respectively.
It is seen that all estimators have roughly the same performances, with the exception of the S estimator with KSD start when $\varepsilon = 0.2$.

### 8.3 Comparison with a non-equivariant estimator

Recently Hubert et al. (2015) proposed two deterministic estimators, called DetS and DetMM, of which the latter has a tuneable efficiency. We compare it with Rocke+SD. The nominal efficiency of DetMM is chosen as 0.90. The scenario is the same as above. However, since DetMM is not equivariant, the model is now $N_p(0, \Sigma_0)$ where $\Sigma_0$ has unit diagonal elements and all non-diagonal elements equal to $\rho$. We chose the extreme cases $\rho = 0$ and $\rho = 0.9$. Since both yield qualitatively similar results, we show in Table 7 only the results from the first case.
The performance of DetMM is clearly poor. We have not been able to find an explanation for this disappointing behavior.

The simulation was also performed with radial contamination. In this case both estimators yielded similar results.

9 A real example

We deal with the well-known wine data set, available at the UCI machine learning repository: https://archive.ics.uci.edu/ml/datasets/Wine, which has been employed as a benchmark data set for pattern recognition; see e. g. (Aeberhard et al, 1994), and consists of three classes with 13 variables. The estimators were applied to the data of class 3, with \( n = 48 \) and \( p = 13 \). Since KSD and MVE yielded similar results as initial estimators, we show only the results corresponding to the former. Figures 3 and 4 contain the QQ-plots of the (squared) Mahalanobis distances for the different estimators.

Rocke, MM and DetMM pinpoint respectively 8, 6 and 5 possible outliers, while S-E and Tau behave like the classical estimator, showing no suspicious points. Some subject-matter knowledge would be necessary to decide how atypical the suspicious points are.

10 Computing times

We compare the computing times of the Rocke estimator with MVE and KSD starts, and of DetMM. The results are the average of 10 runs with normal samples, on a PC with Intel TM12 Duo CPU and 3.01 GHz. The values of \( n \) were \( 5p, 10p \) and \( 20p \), with \( p \) between 10 and 100. The number of subsamples for the MVE was made to increase slowly as \( 50p \). Table 8 displays the results, where for brevity we show only the values for \( p = 20, 50, 80 \) and 100.

It is seen that Rocke+KSD is faster than DetMM for \( p \leq 80 \), and Rocke+MVE. However it is slower than DetMM for \( p = 100 \). This rapid increase in computing time is probably due to the optimization procedure employed by KSD, and may be improved upon by choosing a more efficient optimizer.

11 Conclusions

The Rocke estimator has a controllable efficiency for \( p \geq 15 \). With equal efficiencies, the Rocke estimator with KSD start outperforms all its competitors for shift contamination, and has a similar performance for radial contamination. Its computing time is competitive for \( p < 100 \), and can probably be improved upon. It can therefore be recommended for estimation with high-dimensional data.
Figure 3: Wine data: Ordered Mahalanobis distances vs. $\chi^2_p$-quantiles.

12 Appendix

12.1 Approximations for the tuning constants

For the MM estimator, the constant $c$ in (15) is approximated by

$$c = \left( a + \frac{b}{p} + \frac{c}{p^2} \right) \left( d + \frac{e}{n} \right)$$

where the coefficients depend on $\rho$ and the starting values as follows:

| $\rho$     | Start | $a$     | $b$     | $c$     | $d$     | $e$     |
|------------|-------|---------|---------|---------|---------|---------|
| Bisquare   | MVE   | 0.5404  | 3.5383  | -7.5046 | 1.1142  | -0.9682 |
| Optimal    | MVE   | 0.4690  | 3.1577  | -0.9279 | 1.1665  | -1.6979 |
| Bisquare   | KSD   | 0.5404  | 3.5383  | -7.5046 | 1.2256  | -1.0848 |
| Optimal    | KSD   | 0.4016  | 4.0164  | 3.5499  | 1.1874  | -2.1418 |
Figure 4: Wine data: Ordered Mahalanobis distances vs. $\chi^2_p$-quantiles.

For the Rocke estimator, the value of $\alpha$ in (12) which yields 90% efficiency for the Rocke estimator starting from KSD is approximated for $p \geq 15$ by

$$\alpha = ap^b n^c$$

with

| Start  | $a$   | $b$   | $c$  |
|--------|-------|-------|------|
| MVE    | 0.00436 | -0.5030 | 0.4214 |
| KSD    | 0.00216 | -1.0078 | 0.8156 |

Finally, for the $\tau$-estimator the constant $c$ in (13) which yields 90% efficiency is approximated for both MVE and KSD starts by

$$c = ap^b$$
with

|     |  $\rho$  | $a$   | $b$   |
|-----|---------|-------|-------|
| Bisquare | 6.2984 | -0.8458 |       |
| Optimal  | 2.9987 | -0.4647 |       |

12.2 Computing the Rocke Estimator

Given a starting point, the Rocke estimate is computed iteratively as described in Section 9.6.3 of (Maronna et al., 2006).

The form of the weight function ensures that for normal data sets, most of the data have positive weights. Since real data are seldom normal, it may happen that for data sets with large $p$ and low ratio $n/p$ the proportion of data with positive weights is small. If the data set is nearly collinear, this may cause $\Sigma$ to be ill-conditioned, which affects the computation of Mahalanobis distances. For this reason, if at the first iteration the number of data with positive weights is less than $2p$, the tuning constant is enlarged until this number is $\geq 2p$.

12.3 The breakdown point of the KSD estimator

The KSD procedure is defined in the same way as the Stahel-Donoho estimator, but with a different set of directions. The population version is as follows. Let $x$ be a random vector with distribution $F$. Let $U \subset \mathbb{R}^p$ be a set of directions $u$ with $\|u\| = 1$. Let $\mu$ and $\sigma$ be univariate robust location and scale estimators. The outlyingness of a point $z \in \mathbb{R}^p$ is defined as

$$OL(z) = \max_{u \in U} \frac{|u'z - \mu_F(u'x)|}{\sigma_F(u'x)}.$$  

The location and scale estimators are defined as weighted means and covariance matrix with weights $W(OL(x))$ where $W(t) \geq 0$ is a nonincreasing function for $t \geq 0$.

For a sample, the estimator is defined as above with $F$ the empirical distribution. In the (theoretical) Stahel-Donoho estimator, $U$ is the set of all directions, and $W$ is a smooth function; in actual practice, a finite set of directions obtained by subsampling is employed.

The KSD procedure employs two sets of directions: $U = U_1 \cup U_2$. The first one is deterministic, and consists of a set of $p$ orthogonal directions maximizing the kurtosis of $u'x$ and $p$ directions minimizing it. The other is a set of random “specific directions” obtained through a stratified sampling. We shall deal only with the first one. Besides, $W$ is of “hard rejection” type: $W(t) = 1 (t \leq \beta)$ where $\beta$ depends on $p$.

Theoretical calculations with KSD seem extremely difficult, and for this reason we will limit ourselves to a very simplified case. We consider only the population case with point-mass contamination; furthermore we assume that the uncontaminated data are elliptically distributed. It will be shown that if $\mu$ and $\sigma$ have breakdown 0.5, so has the KSD estimator.
Let $F_0$ be an elliptical distribution with fourth moments and consider the contaminated distribution $F = (1 - \varepsilon) F_0 + \varepsilon \delta_{x_0}$ with $\varepsilon < 0.5$. Because of the estimator’s equivariance it may be assumed that $F_0$ is radial, with zero means and identity covariance matrix, and that $x_0 = K b_1$ where $b_1$ are the elements of the canonical base and $K > 0$. Put $A = E F_0 x_1^4$, where $x_1$ is the first coordinate of $x$. The rotational symmetry implies that $A = E F_0 (u' x)^4$ for all $u = (u_1, ..., u_p)'$ with $\|u\| = 1$.

We will show that the direction of the contamination, i.e., $u = b_1$, is always included in the set. It is straightforward to show that the kurtosis of a projection $u' x$ under $F$ is

$$Kurt_F (u' x) = g(s) = \frac{a + bsK^2 + cs^2K^4}{(1 + \varepsilon sK^2)},$$  \hspace{1cm} (19)

where $s = u_1^2$ and

$$a = (1 - \varepsilon) A, \quad b = 6 (1 - \varepsilon) \varepsilon^2, \quad c = \varepsilon \left( 1 - 4\varepsilon + 6\varepsilon^2 - 3\varepsilon^3 \right)$$

It follows that $Kurt_F (u' x)$ depends on $u$ only through $s = u_1^2 \in [0, 1]$. A laborious but straightforward calculation shows that the derivative of $g(s)$ has the form $g'(s) = u(s) v(s)$, where $u(s) > 0$ does not depend on $K$, and

$$v(s) = (1 - \varepsilon) (3\varepsilon - A) + sK^2 (1 - 4\varepsilon + 3^2).$$

The location of the extrema depends only on the sign of $v$. To simplify the analysis we consider only the case $A > 1.5$, and we assume $K^2 > A$. There are two cases. If $\varepsilon \geq 1/3$, then $v(s) < 0$ for $s \in [0, 1]$, and therefore $u = b_1$ is a minimizer of $Kurt_F (u' x)$. If $\varepsilon < 1/3$ there are maxima at $s = 1$ and $s = 0$, and therefore the set of maximizing directions contains $b_1$ and a set of orthogonal $u$’s which are orthogonal to $b_1$.

It follows that

$$OL (x_0) \geq \frac{|K - \mu(x_1)|}{\sigma(x_1)}.$$

Note that $\mu(x_1)$ and $\sigma(x_1)$ depend on $K$, but since $\varepsilon < 0.5$ they are bounded. Therefore for $K$ large enough, $OL (x_0)$ will be larger than the cutoff value $\beta$ and will therefore have null weight. This finishes the proof.

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| $\gamma$ | Start | Scatter | Location |
|--------|-------|---------|----------|
| $n =$ |       |         |          |
| 0      | S-E   | MVE     | 12.30    | 11.03   | 10.69   | 1.91     | 1.79     | 1.71     |
|        | S-E   | KSD     | 10.78    | 10.03   | 10.06   | 1.86     | 1.72     | 1.64     |
|        | MM-Bisq. | MVE  | 8.82     | 8.14    | 7.93    | 1.83     | 1.72     | 1.65     |
|        | MM-Bisq. | KSD    | 7.71     | 7.41    | 7.56    | 1.60     | 1.59     | 1.50     |
|        | MM-Opt.  | MVE   | 5.78     | 4.16    | 3.52    | 0.66     | 0.59     | 0.56     |
|        | MM-Opt.  | KSD    | 6.21     | 3.85    | 3.19    | 0.63     | 0.56     | 0.54     |
|        | $\tau$-Bisq. | MVE | 14.23    | 14.11   | 13.65   | 2.98     | 2.94     | 2.68     |
|        | $\tau$-Bisq. | KSD  | 13.58    | 12.93   | 12.56   | 2.95     | 2.68     | 2.52     |
|        | $\tau$-Opt. | MVE | 6.42     | 5.08    | 4.58    | 0.80     | 0.74     | 0.73     |
|        | $\tau$-Opt. | KSD  | 5.91     | 4.59    | 4.10    | 0.74     | 0.68     | 0.68     |
|        | Rocke   | MVE     | 4.81     | 2.90    | 1.80    | 0.45     | 0.30     | 0.17     |
|        | Rocke   | KSD     | 4.01     | 2.49    | 1.14    | 0.39     | 0.28     | 0.11     |
|        | KSD     |         | 10.47    | 6.69    | 2.35    | 1.63     | 1.52     | 1.49     |
|        | MVE     |         | 11.01    | 6.20    | 3.79    | 0.82     | 0.55     | 0.37     |
| 0.5    | S-E   | MVE     | 15.00    | 9.78    | 9.02    | 1.98     | 1.50     | 1.49     |
|        | S-E   | KSD     | 9.97     | 9.21    | 9.05    | 1.48     | 1.43     | 1.41     |
|        | MM-Bisq. | MVE  | 17.17    | 11.07   | 8.19    | 2.65     | 1.89     | 1.56     |
|        | MM-Bisq. | KSD    | 7.12     | 6.36    | 6.38    | 1.18     | 1.12     | 1.10     |
|        | MM-Opt.  | MVE   | 13.26    | 8.22    | 5.86    | 1.67     | 1.11     | 0.88     |
|        | MM-Opt.  | KSD    | 7.52     | 4.45    | 3.48    | 0.81     | 0.66     | 0.62     |
|        | $\tau$-Bisq. | MVE | 16.97    | 11.95   | 10.82   | 2.61     | 2.09     | 2.02     |
|        | $\tau$-Bisq. | KSD  | 11.14    | 9.84    | 9.62    | 1.81     | 1.76     | 1.70     |
|        | $\tau$-Opt. | MVE | 13.11    | 8.16    | 5.84    | 1.66     | 1.11     | 0.88     |
|        | $\tau$-Opt. | KSD  | 5.75     | 4.41    | 3.92    | 0.73     | 0.66     | 0.65     |
|        | Rocke   | MVE     | 12.08    | 7.27    | 5.01    | 1.41     | 0.90     | 0.68     |
|        | Rocke   | KSD     | 4.77     | 3.23    | 2.28    | 0.55     | 0.43     | 0.36     |
|        | KSD     |         | 10.45    | 3.78    | 2.55    | 1.63     | 1.53     | 1.49     |
|        | MVE     |         | 23.32    | 13.14   | 8.03    | 2.29     | 1.51     | 1.01     |

Table 3: Simulation with shift contamination: Maximum mean $D$ for scatter and location with $p = 20$ and 10% contamination
| $\gamma$ | Start | Scatter | Location |
|------|-------|---------|----------|
|      |       | n = 100 | 200 | 400 | 100 | 200 | 400 |
| 0    | S-E   | MVE 36.13 | 35.50 | 32.4 | 13.83 | 12.71 | 11.60 |
|      | S-E   | KSD 27.25  | 25.31 | 25.48 | 12.24 | 11.95 | 10.64 |
|      | MM-Bisq. | MVE 40.38 | 38.61 | 34.9 | 17.34 | 16.76 | 16.20 |
|      | MM-Bisq. | KSD 22.49  | 16.86 | 16.18 | 8.59 | 7.57 | 7.38 |
|      | MM-Opt.  | MVE 25.9  | 23.3 | 20.33 | 6.97 | 6.33 | 5.92 |
|      | MM-Opt.  | KSD 23.55  | 10.18 | 8.41 | 5.40 | 2.89 | 2.75 |
|      | $\tau$-Bisq. | MVE 42.40 | 40.6 | 38.66 | 20.22 | 19.95 | 19.02 |
|      | $\tau$-Bisq. | KSD 35.82  | 34.95 | 34.15 | 19.59 | 18.24 | 17.57 |
|      | $\tau$-Opt. | MVE 26.75  | 25.36 | 21.39 | 7.86 | 7.06 | 6.39 |
|      | $\tau$-Opt. | KSD 16.60  | 12.62 | 11.11 | 4.17 | 3.92 | 3.6 |
|      | Rocke  | MVE 5.89   | 3.47 | 2.62 | 0.53 | 0.28 | 0.25 |
|      | Rocke  | KSD 6.70   | 3.17 | 2.21 | 0.52 | 0.35 | 0.24 |
|      | KSD    | 24.12     | 14.83 | 13.8 | 9.08 | 6.04 | 6.35 |
|      | MVE    | 56.38     | 55.81 | 41.6 | 20.88 | 18.15 | 14.97 |
| 0.5  | S-E    | MVE 53.9  | 52.0 | 51.1 | 15.26 | 17.78 | 17.49 |
|      | S-E    | KSD 27.2    | 23.98 | 23.80 | 9.9 | 8.72 | 8.18 |
|      | MM-Bisq. | MVE 65.1  | 64.7 | 63.4 | 26.9 | 25.70 | 25.05 |
|      | MM-Bisq. | KSD 20.18  | 19.50 | 18.7 | 8.82 | 8.25 | 7.84 |
|      | MM-Opt.  | MVE 47.23  | 46.63 | 45.78 | 14.67 | 13.81 | 13.35 |
|      | MM-Opt.  | KSD 20.7   | 14.03 | 14.18 | 5.30 | 4.99 | 4.62 |
|      | $\tau$-Bisq. | MVE 64.71  | 63.58 | 63.18 | 27.61 | 26.95 | 26.71 |
|      | $\tau$-Bisq. | KSD 29.57  | 28.72 | 28.29 | 14.83 | 13.41 | 12.42 |
|      | $\tau$-Opt. | MVE 47.06  | 46.44 | 45.78 | 14.86 | 13.82 | 13.44 |
|      | $\tau$-Opt. | KSD 15.75  | 12.76 | 12.26 | 4.77 | 4.03 | 3.95 |
|      | Rocke  | MVE 36.97  | 35.31 | 34.21 | 7.69 | 7.41 | 7.23 |
|      | Rocke  | KSD 12.53  | 9.35 | 8.54 | 2.38 | 1.96 | 1.86 |
|      | KSD    | 19.94     | 16.57 | 10.7 | 7.73 | 7.58 | 3.54 |
|      | MVE    | 65.7      | 64.06 | 50.84 | 18.39 | 16.73 | 13.88 |

Table 4: Simulation with shift contamination: Maximum mean $D$ for scatter and location with $p = 20$ and 20% contamination
Table 5: Simulation with radial contamination: Maximum mean $D$ for scatter and location with $p = 20$ and 10% contamination

|       | Start | Scatter | Location |
|-------|-------|---------|----------|
| $n = $ | 100   | 200     | 400      | 100 | 200 | 400 |
| S-E   | MVE   | 2.81    | 1.47     | 0.85 | 0.23 | 0.12 | 0.057 |
| S-E   | KSD   | 2.74    | 1.27     | 0.61 | 0.22 | 0.11 | 0.056 |
| MM-Bisq. | MVE | 2.93    | 1.55    | 0.89 | 0.23 | 0.12 | 0.060 |
| MM-Bisq. | KSD | 2.91    | 1.53   | 0.88 | 0.23 | 0.12 | 0.058 |
| MM-Opt. | MVE | 2.88    | 1.51   | 0.87 | 0.23 | 0.12 | 0.56 |
| MM-Opt. | KSD | 3.96    | 1.73   | 0.92 | 0.26 | 0.13 | 0.060 |
| $\tau$-Bisq. | MVE | 2.87  | 1.53 | 0.89 | 0.23 | 0.12 | 0.059 |
| $\tau$-Bisq. | KSD | 2.88    | 1.52   | 0.88 | 0.23 | 0.12 | 0.059 |
| $\tau$-Opt. | MVE | 2.81  | 1.49  | 0.86 | 0.22 | 0.11 | 0.057 |
| $\tau$-Opt. | KSD | 2.80    | 1.48   | 0.86 | 0.23 | 0.11 | 0.057 |
| Rocke | MVE   | 2.95    | 1.55   | 0.89 | 0.23 | 0.12 | 0.058 |
| Rocke | KSD   | 2.91    | 1.53   | 0.90 | 0.45 | 0.12 | 0.059 |
| KSD   |       | 7.10    | 1.85   | 0.91 | 0.45 | 0.24 | 0.142 |
| MVE   |       | 8.82    | 3.92   | 2.21 | 0.69 | 0.13 | 0.059 |

Table 6: Simulation with radial contamination: Maximum mean $D$ for scatter and location with $p = 20$ and 20% contamination

|       | Start | Scatter | Location |
|-------|-------|---------|----------|
| $n = $ | 100   | 200     | 400      | 100 | 200 | 400 |
| S-E   | MVE   | 4.78    | 2.84    | 2.15 | 0.26 | 0.13 | 0.063 |
| S-E   | KSD   | 3.40    | 1.43    | 0.68 | 0.25 | 0.13 | 0.063 |
| MM-Bisq. | MVE | 4.39    | 2.89    | 2.18 | 0.25 | 0.13 | 0.065 |
| MM-Bisq. | KSD | 4.37    | 2.89    | 2.17 | 0.25 | 0.13 | 0.064 |
| MM-Opt. | MVE | 4.37    | 2.84    | 2.16 | 0.26 | 0.12 | 0.063 |
| MM-Opt. | KSD | 4.35    | 2.91    | 2.17 | 0.27 | 0.12 | 0.065 |
| $\tau$-Bisq. | MVE | 4.35   | 2.87   | 2.17 | 0.25 | 0.13 | 0.064 |
| $\tau$-Bisq. | KSD | 4.35    | 2.87    | 2.17 | 0.25 | 0.13 | 0.064 |
| $\tau$-Opt. | MVE | 4.56    | 2.15    | 0.86 | 0.26 | 0.13 | 0.063 |
| $\tau$-Opt. | KSD | 4.55    | 2.14    | 0.86 | 0.26 | 0.13 | 0.063 |
| Rocke | MVE   | 4.48    | 2.19    | 0.89 | 0.27 | 0.13 | 0.065 |
| Rocke | KSD   | 4.48    | 2.20    | 0.90 | 0.47 | 0.13 | 0.0565 |
| KSD   |       | 9.47    | 2.28    | 0.91 | 0.71 | 0.25 | 0.142 |
| MVE   |       | 21.70   | 2.27    | 2.21 | 0.36 | 0.15 | 0.067 |

Table 5: Simulation with radial contamination: Maximum mean $D$ for scatter and location with $p = 20$ and 10% contamination

Table 6: Simulation with radial contamination: Maximum mean $D$ for scatter and location with $p = 20$ and 20% contamination

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Table 7: Simulation with shift contamination: Maximum mean D for $\rho = 0$

| $\varepsilon$ | $\gamma$ | $n$ = | Scatter | Location |
|--------------|----------|-------|---------|----------|
| 0.1          | 0        | Rocke+KSD | 3.96    | 0.39    | 0.19    |
|              |          | DetMM    | 26.97   | 5.93    | 5.32    |
| 0.5          | 0        | Rocke+KSD | 4.73    | 0.54    | 0.36    |
|              |          | DetMM    | 18.01   | 3.46    | 3.18    |
| 0.2          | 0        | Rocke+KSD | 10.62   | 1.47    | 0.73    |
|              |          | DetMM    | 213.66  | 118.79  | 111.87  |

Table 8: Mean computing times of estimators in seconds

| $p$ | $n$ | Rocke+MVE | Rocke+KSD | DetMM |
|-----|-----|-----------|-----------|-------|
| 20  | 100 | 0.62      | 0.06      | 0.20  |
|     | 200 | 0.98      | 0.079     | 0.30  |
|     | 400 | 1.31      | 0.15      | 0.54  |
| 50  | 250 | 5.03      | 0.51      | 1.61  |
|     | 500 | 6.54      | 1.22      | 3.11  |
|     | 1000| 12.72     | 3.07      | 6.51  |
| 80  | 400 | 14.55     | 6.43      | 5.97  |
|     | 800 | 22.46     | 14.90     | 12.23 |
|     | 1600| 65.45     | 22.48     | 26.64 |
| 100 | 500 | 26.86     | 59.18     | 11.79 |
|     | 1000| 74.01     | 91.63     | 24.47 |
|     | 2000| 152.06    | 113.54    | 47.41 |

Table 8: Mean computing times of estimators in seconds