

covMcd() – Considerations about Generalizing the FastMCD

Martin Mächler

July 1, 2024

1 Introduction

The context is robust multivariate “location and scatter” estimation, which corresponds to estimating the first two moments in cases they exist. We assume data and a model

$$x_i \in \mathbb{R}^p, \quad i = 1, 2, \dots, n \quad (1)$$

$$x_i \sim \mathcal{F}(\mu, \Sigma), \quad \text{i.i.d.}; \quad \mu \in \mathbb{R}^p, \quad \Sigma \in \mathbb{R}^{p \times p}, \quad \text{positive definite}, \quad (2)$$

where a conceptual null model is the p -dimensional normal distribution. One typical assumption is that \mathcal{F} is a mixture with the majority component (“good data”) being $\mathcal{N}_p(\mu, \Sigma)$ and other components modeling “the outliers”.

In other words, we want estimates $(\hat{\mu}, \hat{\Sigma})$ which should be close to the true “good data” (μ, Σ) — and do not say more here.

2 MCD and “the Fast” MCD (= fastmcd) Algorithm

The `robustbase` R package has featured a function `covMcd()` since early on (Feb. 2006) and that has been an interface to the Fortran routine provided by the original authors and (partly) described in [Rousseeuw and van Driessen \(1999\)](#). We describe shortly how the algorithm works, partly building on the documentation provided in the source (R, S, and Fortran) codes:

The minimum covariance determinant estimator of location and scatter (MCD) implemented in `covMcd()` is similar to R function `cov.mcd()` in `MASS`. The (“theoretical”) MCD looks for the $h = h_\alpha (> 1/2)$ out of n observations whose classical covariance matrix has the lowest possible determinant. In more detail, we will use $h = h_\alpha = h(\alpha, n, p) \approx \alpha \cdot (n + p + 1)$, where as [Rousseeuw and van Driessen \(1999\)](#) mainly use (the default) $\alpha = \frac{1}{2}$, where $h = h(1/2, n, p) = \lfloor \frac{n+p+1}{2} \rfloor$. For general $\alpha \geq \frac{1}{2}$, the R implementation (derived from their original S code) uses $h = h(\alpha, n, p) = \text{h.alpha.n}(\text{alpha}, n, p)$ (function in `robustbase`), which is

$$h = h_\alpha = h(\alpha, n, p) := \lfloor 2n_2 - n + 2\alpha(n - n_2) \rfloor, \quad \text{where } n_2 := \lfloor \frac{n + p + 1}{2} \rfloor. \quad (3)$$

The fraction $\alpha \geq \frac{1}{2}$ can be chosen by the user, where $\alpha = \frac{1}{2}$ is the most robust, and indeed, $h_{1/2} = n_2 = \lfloor \frac{n+p+1}{2} \rfloor$. Even in general, as long as $n \gg p$, α is approximately the *proportion* of the subsample size h in the full sample (size n):

$$h \approx \alpha \cdot n \iff \alpha \approx \frac{h}{n}, \quad (4)$$

```
> require(robustbase)
> n <- c(5, 10, 20, 30, 50, 100, 200, 500)
> hmat <- function(alpha, p) cbind(n, h.alpha = h.alpha.n(alpha, n, p),
+   h. = floor(alpha * (n + p + 1)), alpha.n = round(alpha * n))
> hmat(alpha = 1/2, p = 3)
```

	n	h.alpha	h.	alpha.n
[1,]	5	4	4	2
[2,]	10	7	7	5
[3,]	20	12	12	10
[4,]	30	17	17	15
[5,]	50	27	27	25
[6,]	100	52	52	50
[7,]	200	102	102	100
[8,]	500	252	252	250

```
> hmat(alpha = 3/4, p = 4)
```

	n	h.alpha	h.	alpha.n
[1,]	5	5	7	4
[2,]	10	8	11	8
[3,]	20	16	18	15
[4,]	30	23	26	22
[5,]	50	38	41	38
[6,]	100	76	78	75
[7,]	200	151	153	150
[8,]	500	376	378	375

The breakdown point (for $h > \frac{n}{2}$) then is

$$\epsilon_* = \frac{n - h + 1}{n}, \quad (5)$$

which is less than but close to $\frac{1}{2}$ for $\alpha = \frac{1}{2}$, and in general, $h/n \approx \alpha$, the breakdown point is approximately,

$$\epsilon_* = \frac{n - h + 1}{n} \approx \frac{n - h}{n} = 1 - \frac{h}{n} \approx 1 - \alpha. \quad (6)$$

The raw MCD estimate of location, say $\hat{\mu}_0$, is then the average of these h points, whereas the raw MCD estimate of scatter, $\hat{\Sigma}_0$, is their covariance matrix, multiplied by a consistency factor `.MCDcons(p, h/n)` and (by default) a finite sample correction factor `.MCDcnp2(p, n, alpha)`, to make it consistent at the normal model and unbiased at small samples.

In practice, for reasonably sized n , p and hence h , it is not feasible to search the full space of all $\binom{n}{h}$ h -subsets of n observations. Rather, the implementation of `covMcd` uses the Fast MCD algorithm of [Rousseeuw and van Driessen \(1999\)](#) to approximate the minimum covariance determinant estimator, see [Section 3](#).

Based on these raw MCD estimates, $(\hat{\mu}_0, \hat{\Sigma}_0)$, a reweighting step is performed, i.e., $\mathbf{V} \leftarrow \text{cov.wt}(\mathbf{x}, \mathbf{w})$, where \mathbf{w} are weights determined by “outlyingness” with respect to the scaled raw MCD, using the “Mahalanobis”-like, robust distances $d_i(\hat{\mu}_0, \hat{\Sigma}_0)$, see [\(7\)](#). Again, a consistency factor and a finite sample correction factor are applied. The reweighted covariance is typically considerably more efficient than the raw one, see [Pison et al. \(2002\)](#).

The two rescaling factors for the reweighted estimates are returned in `cnp2`. Details for the computation of the finite sample correction factors can be found in [Pison et al. \(2002\)](#).

3 Fast MCD Algorithm – General notation

Note: In the following, apart from the mathematical notation, we also use variable names, e.g., `kmini`, used in the Fortran and sometimes R function code, in R package `robustbase`.

Instead of directly searching for h -subsets (among $\binom{n}{h} \approx \binom{n}{n/2}$) the basic idea is to start with small subsets of size $p+1$, their center μ and covariance matrix Σ , and a corresponding h -subset of the h observations with smallest (squared) (“Mahalanobis”-like) distances

$$d_i = d_i(\mu, \Sigma) := (x_i - \mu)' \Sigma^{-1} (x_i - \mu), \quad i = 1, 2, \dots, n, \quad (7)$$

and then use concentration steps (“C steps”) to (locally) improve the chosen set by iteratively computing μ , Σ , new distances d_i and a new set of size h with smallest distances $d_i(\mu, \Sigma)$. Each C step is proven to decrease the determinant $\det(\Sigma)$ if μ and Σ did change at all. Consequently, convergence to a local minimum is sure, as the number of h -subsets is finite.

To make the algorithm *fast* for non small sample size n the data set is split into “groups” or “sub-datasets” as soon as

$$n \geq 2n_0, \text{ where } n_0 := \mathbf{nmini} \text{ (} = 300, \text{ by default)}. \quad (8)$$

i.e., the default cutoff for “non small” is at $n = 600$. The *number* of such subsets in the original algorithm is maximally 5, and we now use

$$k_M = \mathbf{kmini} \text{ (} = 5, \text{ by default)}, \quad (9)$$

as upper limit. As above, we assume from now on that $n \geq 2n_0$, and let

$$k := \left\lfloor \frac{n}{n_0} \right\rfloor \geq 2 \quad (10)$$

and now distinguish the two cases,

$$\begin{cases} A. & k < k_M \iff n < k_M \cdot n_0 \\ B. & k \geq k_M \iff n \geq k_M \cdot n_0 \end{cases} \quad (11)$$

In case A k (= \mathbf{ngroup}) subsets aka “groups” or “sub datasets” are used, $k \in \{2, 3, \dots, k_M - 1\}$, of group sizes n_j , $j = 1, \dots, k$ (see below). Note that case A may be empty because of $2 \leq k < k_M$, namely if $k_M = 2$. Hence, in case A, we have $k_M \geq 3$.

in case B k_M (= \mathbf{ngroup}) groups each of size n_0 are built and in the first stage, only a *subset* of $k_M \cdot n_0 \leq n$ observations is used.

In both cases, the disjoint groups (“sub datasets”) are chosen at random from the n observations. For the group sizes for case A, n_j , $j = 1, \dots, k$, we have

$$n_1 = \left\lfloor \frac{n}{k} \right\rfloor = \left\lfloor \frac{n}{\left\lfloor \frac{n}{n_0} \right\rfloor} \right\rfloor \quad (\geq n_0) \quad (12)$$

$$n_j = n_1, \quad j = 2, \dots, j_* \quad (13)$$

$$n_j = n_1 + 1, \quad j = j_* + 1, \dots, k, \quad (14)$$

$$\text{where } j_* := k - r \in \{1, \dots, k\}, \quad (15)$$

$$\text{and } r := n - kn_1 = n - k \left\lfloor \frac{n}{k} \right\rfloor \in \{0, 1, \dots, k - 1\}, \quad (16)$$

where the range of j_* , $1, \dots, k$ in (15) is a consequence of the range of the integer division remainder $r \in \{0, 1, \dots, k - 1\}$ in (16). Consequently, (14) maybe empty, namely iff $r = 0$ ($\iff n = k \cdot n_1$ is a multiple of k): $j_* = k$, and all $n_j \equiv n_1$.

Considering the range of n_j in case A, the minimum $n_1 \geq n_0$ in (12) is easy to verify. What is the maximal value of n_j , i.e., an upper bound for $n_{\max} := n_1 + 1 \geq \max_j n_j$? Consider $n_{1,\max}(k) = \max_{n, \text{ given } k} n_1 = \max_{n, \text{ given } k} \left\lfloor \frac{n}{k} \right\rfloor$. Given k , the maximal n still fulfilling $\left\lfloor \frac{n}{n_0} \right\rfloor = k$ is $n = (k+1)n_0 - 1$ where $\left\lfloor \frac{n}{n_0} \right\rfloor = k + \left\lfloor 1 - \frac{1}{n_0} \right\rfloor = k$. Hence, $n_{1,\max}(k) = \left\lfloor \frac{(k+1)n_0 - 1}{k} \right\rfloor = n_0 + \left\lfloor \frac{n_0 - 1}{k} \right\rfloor$,

and as $k \geq 2$, the maximum is at $k = 2$, $\max n_1 = \max_k n_{1,\max}(k) = n_0 + \lfloor \frac{n_0-1}{2} \rfloor = \lfloor \frac{3n_0-1}{2} \rfloor$. Taken together, as $n_j = n_1 + 1$ is possible, we have

$$\begin{aligned} n_0 \leq n_1 &\leq \left\lfloor \frac{3n_0 - 1}{2} \right\rfloor \\ n_0 \leq n_j &\leq \left\lfloor \frac{3n_0 + 1}{2} \right\rfloor, \quad j \geq 2. \end{aligned} \tag{17}$$

Note that indeed, $\lfloor \frac{3n_0+1}{2} \rfloor$ is the length of the auxiliary vector `subndex` in the Fortran code.

References

- Pison, G., S. Van Aelst, and G. Willems (2002). Small sample corrections for lts and mcd. *Metrika* 55(1-2), 111–123.
- Rousseeuw, P. J. and K. van Driessen (1999, August). A fast algorithm for the minimum covariance determinant estimator. *Technometrics* 41(3), 212–223.