HUBER'S M-ESTIMATOR ON UNDERDETERMINED PROBLEMS^{*1)}

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Abstract

After surveying the theoretical aspects of Huber's M-estimator on underdetermined problems, two finite algorithms are presented. Both proceed in a constructive manner by moving from one partition to an adjacent one. One of the algorithm, which uses the tuning constant as a continuation parameter, also has the facility to simultaneously estimate the tuning constant and scaling factor. Stable and efficient implementation of the algorithms is presented together with numerical results. The L_1 -norm problem is mentioned as a special case.

1. Introduction

Huber's M-estimator on overdetermined problems has been surveyed by many authors such as $\text{Clark}^{[3,4]}$, Madsen and Nielsen^[12,13] using various schemes. But the underdetermined problems have not attracted much attention, although they are often met in engineering problems. Here we want to use the most popular approaches on the basis of iterative schemes to solve this kind of problems. In the algorithm a scaling factor can be estimated either at the beginning of the computation or by the algorithm at each iteration.

We are concerned with the following problem:

Problem 1.

min
$$f(X) = ||X||_2 = \sum_{i=1}^n x_i^2$$
, (1)

s.t.
$$AX = b$$
, (2)
 $A \in R^{m \times n}, m < n$.

The estimator X is called the least square or L_2 -estimator and was shown by Gauss^[6] in 1821 to be the most probable value under the assumption that the model has independent identical normal distribution. However, as illustrated by Tuckey^[15] in

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1960, the L_2 estimator is very sensitive to quite small deviation from that assumption, and, in particular, a few gross errors can have a marked effect.

In an effect to find a more robust estimator, Huber^[10] suggested replacing the square terms in (1) with a less rapidly increasing function:

$$\rho(x_i) = \begin{cases} \frac{1}{2}x_i^2 & \text{for } |x_i| \le \gamma \\ \gamma |x_i| - \frac{1}{2}\gamma^2 & \text{for } |x_i| > \gamma \end{cases} \tag{3}$$

where γ is a parameter to be estimated from the data. The resulting estimator was shown by Huber [10] to be a maximum likelihood estimator for a perturbed normal distribution and has become known as Huber's *M*-estimator.

Many iterative methods can be used to obtain the *M*-estimator. Among those are Huber's method^[10], Newton method^[12], Beaton and Tuckey's method^[15], Clark's method^[4]. We find the last one most attractive because of its efficiency and finiteness.

Now, let us consider Problem 1 with the replacement of (3) for the estimator. Then Problem 1 becomes

Problem 2.

min
$$F(X) = \sum_{i=1}^{n} \rho(x_i) = \frac{1}{2} \sum_{\sigma} x_i^2 + \sum_{\sigma_+} (\gamma x_i - \frac{1}{2}\gamma^2) + \sum_{\sigma_-} (-\gamma x_i - \frac{1}{2}\gamma^2) ,$$
 (4)

s.t.
$$AX = b$$
, (5)
 $A \in R^{m \times n}, m \le n$.

where $\sigma = \{i | | |x_i| \le \gamma\}, \sigma_- = \{i | x_i < -\gamma\}, \sigma_+ = \{i | x_i > \gamma\}.$

To solve this problem, Lagrange multiplier is used to transform the constrained problem into an unconstrained one:

$$F(X,\Lambda) = \sum_{\sigma} \frac{1}{2}x_i^2 + \sum_{\bar{\sigma}} \left(|x_i|\gamma - \frac{1}{2}\gamma^2 \right) + \Lambda^T (AX - b)$$

where Λ is a Lagrange multiplier and $\bar{\sigma} = \sigma_+ \cup \sigma_-$.

Since $F(X, \Lambda)$ is convex, the necessary and sufficient condition of minimum is

$$\nabla F(X,\Lambda) = 0$$

while

$$\nabla F(X,\Lambda) = \begin{pmatrix} D_{\sigma} & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} X^* \\ \Lambda^* \end{pmatrix} + \begin{pmatrix} \gamma e_{\sigma} \\ -b \end{pmatrix}$$

where D_{σ} is a diagonal matrix,

$$(D)_{ii} = \begin{cases} 1, \text{ if } i \in \sigma \\ 0, \text{ if } i \in \bar{\sigma} \end{cases} \qquad (e_{\sigma})_i \begin{cases} = 0, & \text{ if } i \in \sigma \\ = \theta_i, & \text{ if } i \in \bar{\sigma}, x_i^* \neq 0 \\ \in [-1, 1], & \text{ if } i \in \bar{\sigma}, x_i^* = 0 \end{cases}$$

and $\theta_i = sign(x_i), X^*, \Lambda^*$ are the optimum.

Because the minimizing partition is not known, the search for *M*-estimator is a search for the correct partition. We find the correct partition by regarding X as a function of γ . Starting with the L_2 estimator $X(\infty)$ we prove that X is a piecewise linear function of γ , when one or more components change status.

Another estimator which has received a great deal of attention in the quest for robustness is the L_1 estimator.

Problem 3.

$$\sum_{i=1}^{n} |x_i| = \min,$$

s.t. $AX = b$

The solution of the above problem can be described variously as the robust estimator in some sense^[8,17], or as the L_1 estimator^[17] by partition of N into $\sigma = \{i|x_i = 0\}$, $\bar{\sigma} = \{i|x_i \neq 0\}$, so that

$$\begin{pmatrix} e_{\sigma} + A^T \Lambda^* \\ AX^* - b \end{pmatrix} = 0$$

where

$$(e_{\sigma})_i \begin{cases} = \theta_i \ , & \text{ if } x_i^* \neq 0 \ , \\ \in [-1,1] \ , & \text{ if } x_i^* = 0 \ . \end{cases}$$

It seems that the partition approach should throw light onto the relationship between the L_1 and *M*-estimator.

2. Definitions and Conventions

A partition P is splitting of the set $N = \{1, 2, ..., n\}$ into disjoint complementary subsets σ and $\bar{\sigma}$. The function associated with P is

$$F(X,\Lambda) = \frac{1}{2} \sum_{\sigma} x_i^2 + \sum_{\bar{\sigma}} (\gamma |x_i| - \frac{1}{2}\gamma^2) + \Lambda^T (AX - b).$$

 X^* or Z denotes the minimizer of F, and $F(Z, \Lambda)$ is called the value of the partition. Define a feasible region $FR = \{X | AX = b, X \in \mathbb{R}^n\}$, and note if $X \in FR$, $F(X, \Lambda) = F(X)$.

A partition is σ -feasible if $|z_i| \leq \gamma$, $i \in \sigma$, or $\bar{\sigma}$ -feasible if $i \in \bar{\sigma}, |z_i| > \gamma$ and the components are of assumed signs.

A partition is feasible if it is σ -feasible and $\bar{\sigma}$ -feasible.

 θ_i will denote the sign of the *i*th component, $\theta_i = sign(x_i)$.

Adjacent partitions P_a and P_b satisfy $\sigma_a = \sigma_b \cup \{k\}$ or $\sigma_a = \sigma_b/\{k\}$.

An outlier is a component x_j such that $j \in \bar{\sigma}$.

A degeneracy problem is that more than two components are involved in changing status. $(T_{1}, T_{2}, \dots, T_{n})$

Define $H_{\sigma} = \begin{pmatrix} D_{\sigma} & A^T \\ A & 0 \end{pmatrix}, H = \begin{pmatrix} I & A^T \\ A & 0 \end{pmatrix}$. Then $H_{\sigma}^{-1} = \begin{pmatrix} G & T^T \\ T & U \end{pmatrix}_{\sigma}$ (see Fletcher [5]) where G, U are symmetric matrixes.

Subset σ after a component z_k changes status is denoted by σ^+ .

3. Theorems

First we prove several lemmas and theorems to survey the theoretical aspect of M-estimator on underdetermined problems. Then, we use these theorems to build up our continuation algorithm.

Lemma 1. The minimum of

$$F(X,\Lambda) = \frac{1}{2}\sum_{\sigma} x_i^2 + \sum_{\bar{\sigma}} (\gamma |x_i| - \frac{1}{2}\gamma^2) + \Lambda^T (AX - b)$$

is characterized by

$$H_{\sigma}\begin{pmatrix} X^*\\ \Lambda^* \end{pmatrix} = \begin{pmatrix} -\gamma e_{\sigma}\\ b \end{pmatrix}.$$

Lemma 2. If P_a , P_b are adjacent partitions with $\sigma_a = \sigma_b \cup \{k\}$ for any X satisfying $|x_k| = \gamma$, then $F_a(X, \Lambda) = F_b(X, \Lambda)$.

Proof. The proof follows directly from

$$\frac{1}{2}x_k^2 = \gamma |x_k| - \frac{1}{2}\gamma^2.$$

Lemma 3. If P_a, P_b are adjacent partitions with $\sigma_a = \sigma_b \cup \{k\}$ for which a minimizer Z of one of the partitions has $|z_k| = \gamma$, then Z also minimizes the other partition.

Proof. Let us assume Z is the optimum of P_a . Then from Lemma 1,

$$H_{a}\begin{pmatrix} Z\\\Lambda^{*} \end{pmatrix} = \begin{pmatrix} -\gamma e_{a}\\b \end{pmatrix} \Longrightarrow H_{b}\begin{pmatrix} Z\\\Lambda^{*} \end{pmatrix} + \begin{pmatrix} 0\\\vdots\\z_{k}\\\vdots\\0 \end{pmatrix} = \begin{pmatrix} -\gamma e_{a}\\b \end{pmatrix}$$
$$\Longrightarrow H_{b}\begin{pmatrix} Z\\\Lambda^{*} \end{pmatrix} = \begin{pmatrix} -\gamma e_{b}\\b \end{pmatrix}$$

where e_a and H_a denote e_{σ} and H_{σ} for partition P_a ; e_b and H_b denote e_{σ} and H_{σ} for partition P_b .

A similar proof will show that if Z is the optimum of P_b, Z is also an optimum of P_a .

Lemma 4. If $\sigma_a = \sigma_b \cup S$, then $F_a(X, \Lambda) \ge F_b(X, \Lambda)$ with equality holding only when $|x_i| = \gamma, i \in S$.

Proof. The proof follows directly from

$$\frac{1}{2}x_i^2 \ge \gamma |x_i| - \frac{1}{2}\gamma^2.$$

the inequality being strict unless $|x_i| = \gamma$.

Lemma 5. Let P_a, P_b be adjacent partitions with unique minima Z_a, Z_b respectively, and let $\sigma_a = \sigma_b \cup \{k\}$. Then

i)
$$|(Z_a)_k| > \gamma \iff |(Z_b)_k| > \gamma$$

ii) $|(Z_a)_k| \le \gamma \iff |(Z_b)_k| \le \gamma$

Proof. Assume $|(Z_a)_k| > \gamma$ and $|(Z_b)_k| \le \gamma$ or $|(Z_a)_k| \le \gamma$ and $|(Z_b)_k| > \gamma$. Define $X = \alpha Z_a + (1 - \alpha) Z_b, 0 \le \alpha \le 1$ such that $|x_k| = \gamma$. Then from in turn Lemma 3, Z_a minimizes F_a , Lemma 2 and convexity, we have

$$F_b(Z_a) \le F_a(Z_a) \le F_a(X) = F_b(X) \le \alpha F_b(Z_a) + (1 - \alpha)F_b(Z_b).$$
 (6)

If $\alpha = 1$, from Lemma 3, Z_a minimizes F_b , and if $\alpha < 1$, (6) implies $F_b(Z_a) \leq F_b(Z_b)$ and again Z_a minimizes F_b . This contradicts the assumption of the uniqueness of the minimizer of F_b .

Next, we want to present the first algorithm in which the solution is a continuous piecewise linear function of γ . We first have to prove that Z is continuous with γ . Let

$$F_{\gamma}(X,\Lambda) = \frac{1}{2}X^T D_{\sigma}X - \gamma e_{\sigma}^T X - \sum_{\bar{\sigma}} \frac{1}{2}\gamma^2 + \Lambda^T (AX - b)$$
(7)

and

$$Y = \begin{pmatrix} X \\ \Lambda \end{pmatrix}, \quad Y^* = \begin{pmatrix} Z \\ \Lambda^* \end{pmatrix}; \qquad F_{\gamma}(X, \Lambda) = F(Y).$$

Theorem 1. If H_{σ} is invertible, then the minimum of (7) is continuous with γ . *Proof.* Define

$$G(\gamma, Y) = \frac{\partial}{\partial Y} F(Y) = H_{\sigma} Y + \begin{pmatrix} \gamma e_{\sigma} \\ -b \end{pmatrix}$$

If Z is the optimum, from Lemma 1, $G(\gamma, Y) = 0$ must hold. From the Implicit Function Theorem(Th5.2.4, Ortega[14]), if $\frac{\partial}{\partial Y}G(\gamma, Y)$ is invertible, $\frac{\partial Y}{\partial \gamma}$ exists, and

$$\frac{\partial Y}{\partial \gamma} = -\left(\frac{\partial G}{\partial Y}\right)^{-1} \frac{\partial G}{\partial \Lambda}.$$

But from the assumption, $\frac{\partial}{\partial Y} G(\gamma, Y) = H_{\sigma}$ is invertible, so we have shown the theorem.

Theorem 2. If H_{σ} is nonsingular for a partition, then the minimizer Z is a linear function of γ .

Proof. Differentiating (7) with respect to Y gives

$$H_{\sigma}Y + \begin{pmatrix} \gamma e_{\sigma} \\ -b \end{pmatrix} = 0. \tag{8}$$

Since H_{σ} is nonsigular, and $(H_{\sigma})^{-1} = \begin{pmatrix} G & T^T \\ T & U \end{pmatrix}_{\sigma}$, $Z = \gamma G_{\sigma} e_{\sigma} - T^T b$ is a linear function of γ .

Theorem 3. Let P_a be a feasible partition at $\gamma \geq \overline{\gamma}$, but infeasible at $\gamma < \overline{\gamma}$, which is caused by the size of a single component $(Z_a)_k$. Then the partition $\sigma_b = \sigma_a \setminus \{k\} (k \in \sigma_a)$ or $\sigma_b = \sigma_a \cup \{k\} (k \in \overline{\sigma}_a)$ is feasible for some $\gamma < \overline{\gamma}$.

Proof. For $\gamma < \bar{\gamma}$,

$$|(Z_a)_k| > \gamma(k \in \sigma_a) \text{ or } |(Z_a)_k)| \le \gamma(k \in \bar{\sigma}_a).$$

So by Lemma 5 and observing that $k \in \sigma_a(\bar{\sigma}_a) \Longrightarrow k \in \bar{\sigma}_b(\sigma_b)$,

$$|(Z_b)_k| > \gamma(k \in \overline{\sigma}_b) \text{ or } |(Z_b)_k| \le \gamma(k \in \sigma_b).$$

Thus, if the reduction in γ is slight enough so that $|(Z_b)_i| \neq \gamma, i \neq k, P_b$ is a feasible partition.

Theorem 4. If H_{σ} is nonsingular, then the *M*-estimator *Z* is a continuous piecewise linear function of γ .

Proof. For any feasible partition, Z is a linear function of γ , and P will remain feasible for a range of values of γ . Moreover, at the end of the feasible range of γ , $|Z_k| = \gamma$. The result now follows from Lemma 3, Theorem 2 and Theorem 3.

4. The Continuation Algorithm

4.1. General description

Our continuation algorithm depends on the behavior of the *M*-estimator as γ is varied. We have shown in Section 3 that it is a continuous piecewise linear function of γ . As for γ large enough, the *M*-estimator is the *LS*-estimator: this is taken as the starting point and the value of γ is reduced until the size of some components of *Z* is equal to γ . At this point the partition changes, and the rate of the *M*-estimate with respect to γ has to be recalculated. Piecewise linearity now gives the estimate on the new partition until a new tie occurs. This process is repeated until either a predetermined number of outliers is identified or a desired value of γ is reached. The algorithm can thus be thought of as a continuation algorithm with parameter γ . The choice of stopping value is discussed in Section 4.6.

As γ is reduced, the normal pattern is that a component changes status from being $\leq \gamma$ to becoming $> \gamma$ in size. Occasionally, the opposite situation may occur, so that a component, which was an outlier at one range of value of γ , is not one for small γ . Further, it is theoretically possible that more than one component could be involved in changing status at the same value of γ . The resolution of this problem, analogous to degeneracy in linear programming, has led to the algorithm described in Appendix.

4.2. Updating at the change of partition

When a new range of γ is entered, there will be a change of status of one or more components. Here we show how to update $\frac{dZ}{d\gamma}$ in the usual case where only one component, say z_k , is involved in changing status when Z is piecewise linear in γ . It is well known that the LS solution of Problem 1 using Lagrange multiplier is:

$$X = -A^T (AA^T)^{-1}b, \quad \Lambda = -(AA^T)^{-1}b.$$

This is just the solution of Problem 2 corresponding to $\sigma = \{1, \dots, n\}, D_{\sigma} = I, e_{\sigma} = 0.$ Differentiating (8) with respect to γ , we have

$$H_{\sigma}\frac{dY}{d\gamma} = \begin{pmatrix} -e_{\sigma} \\ 0 \end{pmatrix}.$$

If H_{σ} is invertible,

$$\frac{dY}{d\gamma} = \begin{pmatrix} \frac{dZ}{d\gamma} \\ \frac{d\Lambda^*}{d\gamma} \end{pmatrix} = H_{\sigma}^{-1} \begin{pmatrix} -e_{\sigma} \\ 0 \end{pmatrix} = \begin{pmatrix} G & T^T \\ T & U \end{pmatrix}_{\sigma} \begin{pmatrix} -e_{\sigma} \\ 0 \end{pmatrix},$$
$$\left(\frac{dZ}{d\gamma}\right)_{\sigma} = -G_{\sigma}e_{\sigma}.$$

If only one component z_k changes status, i.e. $\sigma^+ = \sigma \cup \{k\}$ or $\sigma^+ = \sigma \setminus \{k\}$, that is, only one diagonal element in D_{σ} changes status, let us denote the new matrix by H_{σ^+} ,

$$H_{\sigma^+} = H_{\sigma} \pm e_k e_k^T.$$

We may use the Sherman-Morrison formula to revise matrix H_{σ}^{-1} in order to obtain the new inverse:

$$H_{\sigma^+}^{-1} = H_{\sigma^-}^{-1} \mp \frac{H_{\sigma^-}^{-1} e_k e_k^T H_{\sigma^-}^{-1}}{1 \pm e_k^T H_{\sigma^-}^{-1} e_k}$$

and

$$G_{\sigma^+} = G_{\sigma} \mp \frac{G_{\sigma} e_k e_k^T G_{\sigma}}{1 \pm e_k^T G_{\sigma} e_k}.$$

In the same while only one component of e_{σ} change status. So

$$\left(\frac{dZ}{d\gamma}\right)_{\sigma^+} = -G_{\sigma^+}e_{\sigma^+} = -\left(G \mp \frac{G_{\sigma}e_k e_k^T G_{\sigma}}{1 \pm e_k^T G_{\sigma} e_k}\right)e_{\sigma^+} \tag{9}$$

As the search direction is determined, we need to know how long we can walk along this direction until one component changes status.

Let z_i be the *i*th component of Z in a certain iteration. We denote z_i^+ as the corresponding component in the next iteration, and η as the distance that γ moves. $\gamma^+ = \gamma - \eta$.

Let

a) $\forall z_i, i \in \sigma_+$, let $z_i^+ \in (\sigma^+)_+$. That is

$$z_i^+ = z_i - \eta \frac{dz_i}{d\gamma} > \gamma - \eta$$

if
$$\frac{dz_i}{d\gamma} \le 1$$
, the inequality always holds.
if $\frac{dz_i}{d\gamma} > 1$, let

$$\eta_1 = \min_i \left\{ \frac{z_i - \gamma}{\frac{dz_i}{d\gamma} - 1} | i \in \sigma_+, \frac{dz_i}{d\gamma} > 1 \right\}.$$
(10)

b) $\forall z_i, i \in \sigma_-$, we let $z_i^+ \in (\sigma^+)_-$,

$$\eta_2 = \min_i \left\{ \frac{z_i + \gamma}{1 + \frac{dz_i}{d\gamma}} | i \in \sigma_-, \frac{dz_i}{d\gamma} < -1 \right\}.$$
(11)

c) $\forall z_i, i \in \sigma$, we let $z_i^+ \in \sigma^+$, that is

$$-(\gamma - \eta) \le z_i^+ = z_i - \eta \frac{dz_i}{d\gamma} \le \gamma - \eta,$$

$$\eta_3 = \min_i \left\{ \frac{\gamma + z_i}{1 + \frac{dz_i}{d\gamma}} | i \in \sigma, \frac{dz_i}{d\gamma} > -1 \right\},\tag{12}$$

$$\eta_4 = \min_i \left\{ \frac{\gamma - z_i}{1 - \frac{dz_i}{d\gamma}} | i \in \sigma, \frac{dz_i}{d\gamma} < 1 \right\}.$$
(13)

 Set

$$\eta = \min\{\eta_1, \eta_2, \eta_3, \eta_4\}.$$

In the case that only one element, say η_k , let the equality hold, this is only one component is involved in changing status, then

$$z_i^+ = z_i - \frac{dz_i}{d\gamma}\eta.$$

4.3. The algorithm

Step 1. Set
$$j \leftarrow 1$$
(counter)
Find the LS estimator Z_0
Set $\frac{dZ}{d\gamma} \leftarrow 0$
Determine $k = \arg\max_i \{|z_i|\}$
Let $P = \{N \setminus \{k\}\}$ and $\gamma_1 = |z_k|$
If the stop criterion is satisfied, stop
Otherwise
Step 2. Update $\frac{dZ}{d\gamma}$ using (9)

Compute $\eta_1, \eta_2, \eta_3, \eta_4$ using (10),(11),(12) and (13) Let $\eta = \min\{\eta_1, \eta_2, \eta_3, \eta_4\}$ Calculate $Z(\gamma_{j+1}) = Z(\gamma_j) - \eta \frac{dZ}{d\gamma}$

- Step 3. If the stop criterion is satisfied, stop Otherwise
- Step 4. If only one component z_k is involved in changing status,

define the new partition by

$$\sigma_{j+1} = \sigma_j \cup \{k\} (k \in \bar{\sigma})$$

$$\sigma_{j+1} = \sigma_j \setminus \{k\} (k \in \sigma)$$

If more than one component is involved in changing status,

define the new partition as in the last section.

 $j \leftarrow j + 1$

Goto Step 2.

4.4. Finiteness

In order to demonstrate that the algorithm is finite, we need to show that

i) cycling dose not occur at the change of partition;

ii) the number of ranges of γ is finite.

That cycling does not occur when only one component is involved in changing status is a consequence of Theorem 3 and $Z = \gamma G_{\sigma} e_{\sigma} - T^T b$.

We now show that the number of ranges of γ is finite.

Theorem 5. The number of ranges of γ is finite.

Proof. For any partition P, if H_{σ} is nonsingular, $Z(\gamma, P)$ is a linear function of γ . Hence as γ decreases, once a given component has changed status, it cannot return to its original status. The results now follow from the finiteness of the number of partitions.

4.5. Choise of scaling factor and tuning constant

In the definition of F(X) of Problem 2, we must assume that the vector model X is an unbiased estimator. In fact, it is not always true. So a scaling factor should be adopted to avoid the disadvantage of the above algorithm.

Problem 4.

min
$$F(X) = \sum_{i=1}^{n} \rho\left(\frac{x_i}{\tau}\right)$$

s.t. $AX = b$,
 $A \in \mathbb{R}^{m \times n}, m \le n$.

Huber^[10] suggests that in the location case the best estimate of scale is given by

$$\tau = \operatorname{med}_i\{|x_i - \operatorname{med}_j x_j|\}.$$

However, in the regression case the analogue of the median, the L_1 estimator, requires calculation of complexity similar to that of the *M*-estimate itself. Holland and Welsch^[9] suggest

$$\tau = 1.48 \operatorname{med}_i\{|x_i - \operatorname{med}_j x_j|\} = 1.48\mu \tag{14}$$

introducing the factor 1.48 to give an approximately unbiased estimate of scale when the vector model is Gaussian. This factor is also cited by $\operatorname{Birch}^{[2]}$ as a popular choice.

The γ is taken as 1.345 by Holland and Welsh^[9] as giving 95% asymptotic efficiency at Gaussion distribution.

Most algorithms estimate τ only once, using (14) at the initial point which is usually the *LS* estimator. However, as we shall see, we can estimate τ iteratively in our continuation algorithm with minimal extra effort.

If τ is not assumed to be unity in Problem 4, the definition of σ becomes $i \in \sigma \leftrightarrow |z_i/\tau| \leq \gamma$ or $i \in \sigma \leftrightarrow |z_i| \leq \gamma \tau$. This suggests that we can use $\delta = \gamma \tau$ as our continuation parameter. We have $\frac{dZ}{d\delta} = \frac{1}{\tau} \frac{dZ}{d\gamma}$. Thus the rate of change of Z is calculated as before and divided by Z.

The stopping rule now becomes $\delta' > 1.48 * 1.345\mu'$ at the beginning of a range and $\delta'' < 1.99\mu''$ at the end of the range. Choose the final value of δ as $\delta' + (\delta' - \delta'')(1.99\mu'' - \delta'')/(\delta' - \delta'')$ and $Z = \alpha Z(\gamma_j) + (1 - \alpha)Z(\gamma_{j+1})$ where $\alpha = \frac{1.99\mu_{j+1} - \gamma_{j+1}}{\gamma_j - 1.99\mu_j}$.

The approach has two important advantages. First, although the scale factor is estimated at each iteration, its use in the algorithm only affects the stopping rule. This means the problem of convergence of τ is sidestepped. (This contrasts with the difficulty of simultaneously estimating Z and τ in the iterative schemes; see for example the method of Dutter^[10] when τ is defined by Huber's proposal 2 ^[11]. Indeed, when τ is defined as in (14), a scheme such as Dutter's need not converge.)

Secondly, although we have chosen (14) for τ , other choices of scaling factor can easily be incorporated. In particular, methods of determining scale by satisfying an auxiliary equation of the form $F(X, \tau, \gamma) = 0$, such that the Huber's proposal 2, may be used.

4.6. Stopping rules

Several stopping rules can be used:

- 1. The algorithm is processed until a predetermined number of outliers is identified, or a desired value of γ is reached. Especially, for L_1 -estimator, the predetermined number is usually m, and the desired value of γ is 0.
- 2. A predetermined percentage of outliers is identified for the M-estimator.
- 3. The stopping rule described in Section 4.5.

These rules are selected according to problems and aims.

4.7. Implementation

A decomposition method with row pivot for the singular matrix (see Golub^[7], algorithm 6.4-1) is used to obtain the LS solution. The decomposition needs $2mnr - r^2(m+n) + 2r^3/3$ computer operations, where r = rank(A),

$$\Pi A = RQ,$$

 $A \in \mathbb{R}^{m \times n}$; $\Pi \in \mathbb{R}^{m \times m}$ is a permutation matrix; $R \in \mathbb{R}^{m \times n}$ is a left-triangular matrix; $Q \in \mathbb{R}^{n \times n}$ is an orthogonal matrix.

One advantage of the QR decomposition is its stability. We can eliminate dependent rows, if some diagonal elements of R are small enough. The LS solution is

$$Z_{LS} = -A^T (AA^T)^{-1}b = -A^T (\Pi^T R Q Q^T R^T \Pi)^{-1}b = -(\Pi A)^T (RR^T)^{-1} (\Pi b).$$

During this stage we must calculate R^{-1} for further use. So we need another $\frac{1}{6}(m^3 - m + 3) + m(m + 1) + nm$ multiplications in order to obtain Z_{LS} .

When we find a component changing status, we use the Sherman-Morricon Formula to revise matrix G. After $\frac{dZ}{d\gamma}$ and η are computed. Z^+ can be obtained easily.

Because we start from the LS solution, we have $D_{\sigma} = I$ at this time. Then

$$H = \begin{pmatrix} I & A^T \\ A & 0 \end{pmatrix}, \qquad H^{-1} = \begin{pmatrix} G & T^T \\ T & U \end{pmatrix}.$$

From R. Fletcher[3] Section 10.3,

$$G = I - A^{T} (AA^{T})^{-1}A = I - (\Pi A)^{T} R^{-T} R^{-1} (\Pi A).$$

We require $\frac{1}{2}mn(m+1) + \frac{1}{2}mn(n+1)$ multiplications in this stage.

Now we have to begin the iteration stage. We only need $n^2 + 1$ multiplications to update $\frac{dZ}{d\gamma}$ [see (9)] and at most 2n divisions to obtain η [see (10),(11),(12)and(13)]. So the total computer work in every iteration is $(n^2 + 1) + 2n + n$.

If $l \leq m$ outliers are identified, i.e. normally l iterations are needed, the total work l iterations require is $l(n^2 + 3n + 1)$.

Practically, we need m iterations to obtain the L_1 solution and the program will terminate automatically before or when we reach the L_1 solution. So the work amount to obtain M-estimator is at most

$$(m^{2}n - \frac{1}{3}m^{3}) + (\frac{1}{6}m^{3} + nm + m^{2} + \frac{5}{6}m + \frac{1}{2}) + \frac{1}{2}mn(m + n + 2) + m(n^{2} + 3n + 1) = O(\frac{3}{2}mn^{2} + \frac{3}{2}m^{2}n - \frac{1}{6}m^{3})$$

multiplications totally.

4.8. Numerical results and conclusions

Our program is performed on IBM 386 with both testing problems and pratical problems. The continuation algorithm appears to be suitable for most situations. The given implementation is stable and efficient for all real models, particularly when there are relatively few outliers expected.

Testing problem 1.

$$\min \|X\|$$

s.t.
$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0.5 & 0.5 & 0.5 & 0.5 \end{pmatrix} X = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}$$
$$X_{LS} = (1, 1, 1, 1), \qquad X_{L_1} = (1, 1, 1, 1).$$

Testing problem 2.

min ||X||

s.t.
$$\begin{pmatrix} 2 & 0 & 2 & 1 \\ 2 & 2 & 2 & 2 \\ 1 & 2 & 2 & 4 \end{pmatrix} X = \begin{pmatrix} -2 \\ 2 \\ 7 \end{pmatrix}$$

 $X_{LS} = (-1.38, 1.09, -0.57, 1.83), \qquad X_{L_1} = (-1.8, 1.2, 0, 1.6).$

Testing problem 3.

min ||X||

s.t.
$$\begin{pmatrix} 2 & 0 & -2 & 1 \\ 2 & -2 & 2 & 2 \\ 1 & 2 & 2 & 4 \end{pmatrix} X = \begin{pmatrix} 4 \\ 6 \\ 9 \end{pmatrix}$$

 $X_{LS} = (1.294, 0.202, 0.165, 1.743), \qquad X_{L_1} = (1, 0, 0, 2).$

Testing problem 4.

min ||X||

s.t.
$$x_1 + 2x_2 + 3x_3 = 6$$

 $X_{LS} = (3/7, 6/7, 9/7), \qquad x_{L_1} = (0, 0, 2).$

Results of the Continuation Algorithm

PROBLEM	LS SOLUTION	L1-NORM SOLUTION	
	ACCURACY	ACCURACY	NUMBER OF ITERATION
1	$< 1.0 \mathrm{E}{-15}$	$< 1.0 \mathrm{E} - 15$	0
2	< 1.0 E - 10	< 1.0 E - 10	3
3	$< 1.0 \mathrm{E}{-10}$	< 1.0 E - 07	2
4	$< 1.0 \mathrm{E}{-15}$	$< 1.0 \mathrm{E} - 15$	1

Appendix: The Partitioning Algorithm

In step 4 of our continuation algorithm we may meet the case that at least two components are involved in changing status. This is difficult to handle by the continuation algorithm. But we can deal with it by using the partition algorithm.

Althought the degeneracy problem can be given constructively, it arises scarcely in practice. As no example has been found, we give only the theoretical conclusion and the algorithm without numerical results.

This partition algorithm is designed to find a feasible partition starting from an arbitrary partition and proceeding only by adjacent partition changes.

The partitioning algorithm:

Step 1. Starting from an initial partition do until P_j is $\bar{\sigma}$ – feasible $\sigma' = \sigma \cup \{k\}$ where $k \in \bar{\sigma}$ and $|(Z^j)_k| \leq \gamma$ Set $j = 1, \sigma_j = \sigma'$. Step 2. While P_j is $\bar{\sigma}$ – feasible do If P_j is feasible then stop; else do $\sigma_{j+1} = \sigma_j \setminus \{k\}$ where $k \in \sigma_j$ and $|Z^j)_k| > \gamma, k \in \bar{\sigma}_j$, j = j + 1. Step 3. $Y^{j-1} = Z^{j-1}(Z^{j-1} \text{ satisfies } |(Z^{j-1})_k| > \gamma, k \in \bar{\sigma}_j)$ Until P_j is $\bar{\sigma}$ -feasible do find $Y^j = \alpha Z_j + (1 - \alpha)Y^{j-1}, 0 \leq \alpha < 1 \text{ to satisfy}$ $|(Y^j)_i| > \gamma, i \in \bar{\sigma}_j \text{ and } |(Y^j)_k| = \gamma \text{ for at least one } k \in \bar{\sigma}_j$ $\sigma_{j+1} = \sigma_j \cup \{k\}$ j = j + 1Goto Step 2.

Here, $(Z^j)_k$ denotes the kth component of Z in the *j*th iteration.

Theorem 6. The partition algorithm terminates finitely with a feasible partition. Proof. The proof is analogous to that of Theorem 3.3 of Clark [4] which must show no cycling occur in step 1 and step 2 and then show the function values of these partitions in step 2 and step 3 decrease monotonically. Concisely, we mention it here as a conclusion.

References

A.E. Beaton and J.W. Tuckey, The fitting of power series, meaning polynomials, illustrated on band-spectroscopic data, *Tecnometrics*, 16 (1974), 523–531.

- [2] J.B. Birch, Some convergence properties of iterated reweighted least square in the location model, *Comm. Statis.*, B9(4) (1980), 359–369.
- [3] D.I. Clark, The mathematical structure of Huber's M-estimator, SIAM J. Sci. Stat. Comp., 6 (1985), 209–219.
- [4] D.I. Clark and M.R. Osborne, Finite algorithms for Huber's M-estimator, SIAM J. Sci. Stat. Comp., 7 (1986), 72–85.
- [5] R. Fletcher, Practical Methods of Optimization, 2nd ed. (1987).
- [6] C.F. Gauss, Göttingische Gelhrte Anzeigen, (1821), 321–327.
- [7] G.H. Golub and C.F. Van Loan, Matrix Computation, The John Hopkings University Press, USA (1983).
- [8] F.R. Hampel, Robust estimation: a condensed patial survey, Z. Wahrsch. Verw., Geb 27 (1973), 84–104.
- [9] P.W. Holland and R.E. Welsh, Robust regression using iteratively reweighted least squares, Comm. Statist., A6(9) (1977), 813–827.
- [10] P.J. Huber, Robust Regression: Asymptotics, Conjectures and Monte Carlo, Ann. Statist., 1, (1973), 799–821.
- [11] P.J. Huber, Robust estimation of a location parameter, Ann. Math. Stat., 35 (1964), 73–101.
- [12] K. Madsen and H.B. Nielsen, Finite algorithm for robust linear regression, BIT, 30 (1990), 682–699.
- [13] K. Madsen and H.B. Nielsen, A Finite Smoothing Algorithm for Linear L_1 Estimator. Revised version, March 1992.
- [14] J.M. Ortega and W.C. Rheinboldt, Iterative Solution of Nonlinear Equations in Several Variables, Academic Press, New York and London (1970).
- [15] J.W. Tuckey, A Survey of Sampling from Contaminated Distributions, Contributions to Probability and Statistics, I Olkin, ed., Stanford Univ., Press. Stanford, CA (1960).
- [16] G. Watson, Approximation Theory and Numerical Methods, John Wiley, New York, 1980.
- [17] Robust Statistical Procedures, CBMS Regional Conference Series in Applied Mathematics 27, Society for Industrial and Applied Mathematics, Philadelphia, 1977.