An Introduction to Robust Estimation with R Functions

Ruggero Bellio

Department of Statistics, University of Udine
ruggero.bellio@dss.uniud.it

Laura Ventura

Department of Statistics, University of Padova
ventura@stat.unipd.it

October 2005

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1 Introduction

Since 1960, many theoretical efforts have been devoted to develop statistical procedures that are resistant to small deviations from the assumptions, i.e. robust with respect to outliers and stable with respect to small deviations from the assumed parametric model. In fact, it is well-known that classical optimum procedures behave quite poorly under slight violations of the strict model assumptions.

It is also well-known that to screen the data, to remove outliers and then to apply classical inferential procedures is not a simple and good way to proceed. First of all, in multivariate or highly structured data, it can be difficult to single out outliers or it can be even impossible to identify influential observations. Second, in place of rejecting an observation, it could be better to down-weight uncertain observations, although we may wish to reject completely wrong observations. Moreover, rejecting outliers reduces the sample size, could affect the distribution theory, and variances could be underestimated from the cleaned data. Finally, empirical evidence shows that good robust procedures behave quite better than techniques based on the rejection of outliers.

Robust statistical procedures focus in estimation, testing hypotheses and in regression models. There exist a great variety of approaches toward the robustness problem. Among these, procedures based on M-estimators (and gross error sensitivity) and high breakdown point estimators (and breakdown point) play an important and complementary role. The breakdown point of an estimator is the largest fraction of the data that can be moved arbitrarily without perturbing the estimator to the boundary of the parameter space: thus the higher the breakdown point, the more robust the estimator against extreme outliers. However, the breakdown point is not enough to assess the degree of robustness of an estimator. Instead, the gross error sensitivity gives an exact measure of the size of robustness, since it is the supremum of the influence function of an estimator, and it is a measure of the maximum effect an observation can have on an estimator. There are some books on robust statistics. Huber (1981) and Hampel et al. (1986) are the main theoretical ones; see also Staudte and Sheather (1990). Rousseeuw and Leroy (1987) is more practical.

At present, the practical application of robust methods is still limited and the proposals concern mainly a specific class of applications (typically estimation of scale and regression models, which include location and scale models). In view of this, a considerable amount of new programming in R is requested. Two books about practical application of robust methods with S and R functions are Marazzi (1993) and Venables and Ripley (2002).

An example: Chushny and Peebles data

The data plotted in Figure 1 concern n = 10 observations on the prolongation of sleep by means of two drugs (see Chushny and Peebles, 1905, and Hampel *et al.*, 1986, chap. 2). These data have been used by Student as the first illustration of a t-test, to investigate whether a significant difference existed between the observed effect of both drugs.

```
> xdat <- c(0.0,0.8,1.0,1.2,1.3,1.3,1.4,1.8,2.4,4.6)
> boxplot(xdat)
```

The boxplot is a useful plot since it allows to identify possible outliers and to look at the overall shape of a set of observed data, particularly for large data sets.

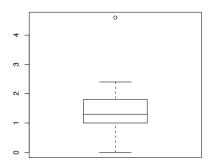


Figure 1: Chushny and Peebles data.

Most authors have considered these data as a normally distributed sample and for inferential purposes have applied the usual *t*-test. For instance, to test for a null mean or to give a confidence interval for the mean, the function t.test can be used.

```
> t.test(xdat)
        One Sample t-test
data: xdat
t = 4.0621, df = 9, p-value = 0.002833
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
 0.7001142 2.4598858
sample estimates:
mean of x
     1.58
> mean(xdat)
[1] 1.58
> sd(xdat)
[1] 1.229995
> t.test(xdat)$conf.int
[1] 0.7001142 2.4598858
attr(, "conf.level")
[1] 0.95
```

However, the boxplot in Figure 1 reveals that the normality assumption could be questionable, and the value 4.6 appears to be an outlier. An outlier is a sample value that cause surprise in relation to the majority of the sample. If this value is not considered in the analysis, the value of the arithmetic mean changes (the mean is shifted in the positive direction of the outlier), but the relevant effect is mainly on the classical estimate of the scale parameter (see, for example, the 95 percent confidence interval).

```
[1] 0.0004766165
> mean(xdat[1:9])
[1] 1.244444
> sd(xdat[1:9])
[1] 0.6597558
> t.test(xdat[1:9])$conf.int
[1] 0.7373112 1.7515777
attr(,"conf.level")
[1] 0.95
```

In this situation, the value 4.6 is considered as an outlier for the Gaussian model, but there is no so much information (only n = 10 observations) to assume a longer tailed distribution for the data. In this case, robust methods for estimation of the scale and location parameters could be useful.

An example: Regression model

Suppose that the points in Figure 2 represent the association between vacation expenses and wealth of n = 13 fictitious individuals (see Marazzi, 1993). Three different models are considered: the first one (fit1) is based on all the observations, the second one (fit2) considers also a quadratic term in x in the linear predictor, and the last one (fit3) is without the leverage observation.

```
> xx <- c(0.7,1.1,1.2,1.7,2,2.1,2.1,2.5,1.6,3,3.2,3.5,8.5)
> yy <- c(0.5,0.6,1,1.6,0.9,1.6,1.5,2,2.1,2.5,2.2,3,0.5)
> plot(xx,yy,xlim=c(0,10),ylim=c(0,6))
> fit1 <- lm(yy~xx)
> abline(fit1$coef,lty=1)
> fit2 <- lm(yy~xx+I(xx^2))
> xx1 <- seq(0,10,length=50)
> lines(xx1,fit2$coef[1]+fit2$coef[2]*xx1+fit2$coef[3]*I(xx1^2),lty=3)
> fit3 <- lm(yy~xx,subset=c(-13))
> abline(fit3$coef,lty=5)
> legend(6, c("fit1", "fit2", "fit3"),lty = c(1,3,5))
```

The choice between the fitted models depends on many things, among which are the purposes of the description and the degree of reliability on the leverage point: in fact, this point may be correct. Of course, the choice of the fitted model has a great impact of the resulting inference, such as in the estimation of predicted values based on the linear model.

```
> new <- data.frame(xx=6)
> predict.lm(fit1,new,se.fit=T)
$fit
[1] 1.524642
$se.fit
[1] 0.4840506
$df
[1] 11
```

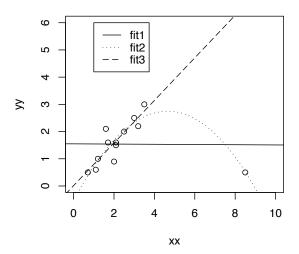


Figure 2: Fictitious data: (fit1) with all data, (fit2) with a quadratic term, and (fit3) without the leverage observation.

```
$residual.scale
[1] 0.8404555
> predict.lm(fit2,new,se.fit=T)
$fit
[1] 2.47998
$se.fit
[1] 0.2843049
$df
[1] 10
$residual.scale
[1] 0.4097049
> predict.lm(fit3,new,se.fit=T)
$fit
[1] 4.709628
$se.fit
[1] 0.543763
$df
[1] 10
$residual.scale
[1] 0.3890812
```

In regression models, especially when the number of regressors is large, the use of the residuals is important for assessing the adequacy of fitted models. Some patterns in the residuals are evidence of some form of deviation from the assumed model, such as the presence of outliers or incorrect assumptions concerning the distribution of the error term. Informal graphical procedures, such as the boxplot or the normal QQ-plot of the residuals, can be useful (see Figure 3).

```
> par(mfrow=c(1,3))
```

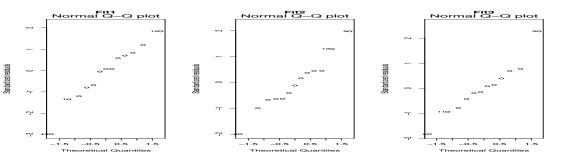


Figure 3: Fictitious data: normal QQ-plots.

```
> plot(fit1,2)
> title("Fit1")
> plot(fit2,2)
> title("Fit2")
> plot(fit3,2)
> title("Fit3")
```

Moreover, leverage points can be identified using the diagonal elements h_{ii} of the orthogonal projector matrix onto the model space (or hat matrix) $H = X(X^{T}X)^{-1}X^{T}$, where X is a known $(n \times p)$ -matrix of full rank. The trace of X is equal to p, the number of regression parameters in the model, so that the average leverage is p/n: an observation whose leverage is much in excess of this deserves attention.

```
> x.mat <- model.matrix(fit1)
> hat(x.mat)
[1] 0.15065351 0.12226880 0.11624530 0.09256387 0.08350386 0.08134200
[7] 0.08134200 0.07698528 0.09644201 0.08119348 0.08588026 0.09612846
[13] 0.83545118
> p.over.n <- ncol(x.mat)/nrow(x.mat)
> p.over.n
[1] 0.1538462
```

The last observation is clearly a leverage point.

An observation is said to be *influential* if it has a big effect on the fitted model. A direct method for assessing influence is to see how an analysis changes when single observations are deleted from the data. The overall influence that an observation has on the parameters estimates is usually measured by Cook's distance, given by $c_i = r_i^2 h_{ii}/(ps^2(1-h_{ii})^2)$, where r_i is the *i*-th residual, i = 1, ..., n, and s^2 is the usual unbiased estimate of the scale parameter. In practice, a large value of c_i arises if an observation has high leverage or presents a large value of the corresponding standardized residual, or both. A useful plot, in addition to the plot of the residuals, for pointing out influential observations is based on the comparison of c_i versus $h_{ii}/(1-h_{ii})$. In fact, this plot helps to distinguish the nature of the observations: a simple rule is that an observation with residual satisfying $|r_i| > 2$ or with leverage $h_{ii} > 2p/n$ deserves attention, such as an observation with $c_i > 8/(n-2p)$.

The Cook's distance plot (see Figure 4) can be obtained with:

```
> par(mfrow=c(1,3))
```

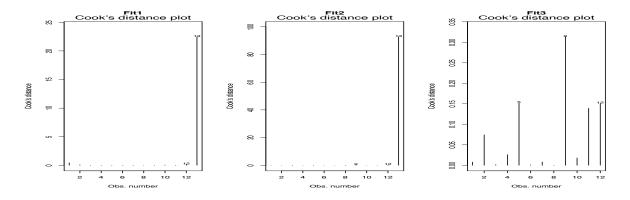


Figure 4: Fictitious data: Cook distance plot for fit1, fit2 and fit3.

- > plot(fit1,4)
- > title("Fit1")
- > plot(fit2,4)
- > title("Fit2")
- > plot(fit3,4)
- > title("Fit3")

Since large values of c_i identify observations whose deletion has the greatest influence on the estimation of the regression parameters, we note that the last observation will merit careful inspection in the first two models considered. Also in this case robust methods could be useful.

In general (see e.g. Figure 2), anomalous observations may be dealt with by a preliminary screening of the data, but this is not possible with influential observations which can only be detected once the model has been fitted or when p is very large. In the light of the amount of data available nowadays and the automated procedures used to analyze them, robust techniques may be preferable as they automatically take possible deviations into account. Moreover, the diagnostic information provided by these techniques can be used by the analyst to identify deviations from the model or from the data.

2 Estimation in scale and location models

This Section describes the functions given by R for the analysis of scale and location models. Consider the following framework of a scale and location model, given by

$$x_i = \mu + \sigma \epsilon_i \;, \quad i = 1, \dots, n \;, \tag{1}$$

where $\mu \in \mathbb{R}$ is an unknown location parameter, $\sigma > 0$ a scale parameter and ϵ_i are independent and identically distributed random variables according to a known density function $p_0(\cdot)$. If $p_0(x) = \phi(x)$, i.e. the standard Gaussian distribution, the classical inferential procedures based on the arithmetic mean, standard deviation, t-test, and so on, are the most efficient. Unfortunately, they are not robust when the Gaussian distribution is just an approximate parametric model. In this case, it may be preferable to base inference on procedures that are more resistant (see Huber, 1981; Hampel et al., 1986).

Given a random sample $x = (x_1, \ldots, x_n)$, it is typically of interest to find an estimate (or to test an hypothesis) of the location parameter μ , when σ can be known or a nuisance

parameter. In this setting, probably the most widely used estimator (least squares) for a location parameter is the sample mean $\bar{x} = (1/n) \sum_{i=1}^{n} x_i$ and for the scale parameter is the standard deviation $s^2 = (1/(n-1) \sum_{i=1}^{n} (x_i - \hat{\mu}_m)^2)^{1/2}$. However, it is well known that the sample mean is not a robust estimator in the presence of deviant values in the observed data, since can be upset completely by a single outlier. One simple step toward robustness is to reject outliers and the trimmed mean has long been in use.

2.1 The function mean for a trimmed mean

A simple way to delete outliers in the observed data x is to compute a trimmed mean. A trimmed mean is the mean of the central $1-2\alpha$ part of the distribution, so αn observations are removed from each end. This is implemented by the function mean with the argument trim specifying α . The usage of the function mean to compute a trimmed mean is:

```
mean(x, trim = 0)
```

where the arguments are an R object x (a vector or a dataframe) and trim, which indicates the fraction (0 to 0.5) of observations to be trimmed from each end of x before the mean is computed. If trim is zero (the default), the arithmetic mean \bar{x} of the values in x is computed. If trim is non-zero, a symmetrically trimmed mean is computed with a fraction of trim observations deleted from each end before the mean is computed.

Example: Chushny and Peebles data

Consider the n = 10 observations on the prolongation of sleep by means of two drugs.

```
> xdat
  [1] 0.0 0.8 1.0 1.2 1.3 1.3 1.4 1.8 2.4 4.6
> mean(xdat)
[1] 1.58
> mean(xdat,trim=0.1)
[1] 1.4
> mean(xdat,trim=0.2)
[1] 1.333333
> mean(xdat[1:9])
[1] 1.244444
```

Summarizing these results, it can be noted that the robust estimates are quite different both from the arithmetic mean and from the sample mean computed without the value 4.6.

Example: the USArrests data

The data set USArrests is a data frame of n=50 observations on 4 variables, giving the number in arrests per 100000 residents for assault, murder, and rape in each of the 50 US states in 1973. Also given is the percent of the population living in urban areas. The boxplot of this dataset is given in Figure 5 (a). One can compute the ordinary arithmetic means or, for example, the 20%-trimmed means: one starts by removing the 20% largest and the 20% smallest observations, and computes the mean of the rest.

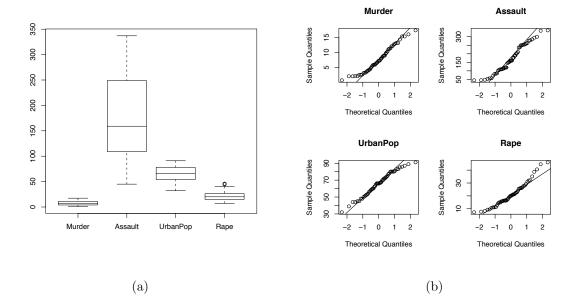


Figure 5: USA arrests data.

```
> data(USArrests)
> boxplot(USArrests)
> mean(USArrests)
  Murder
          Assault UrbanPop
                                 Rape
   7.788
          170.760
                     65.540
                              21.232
> mean(USArrests, trim = 0.2)
  Murder
          Assault UrbanPop
                                 Rape
    7.42
           167.60
                      66.20
                                20.16
```

Summarizing these results, we note that all the trimmed estimates do not leave a clearly gap up to the corresponding arithmetic means. This is not in general true, and they can give different answers. From the normal QQ-plots in Figure 5 (b) is can be noted that in this case a robust estimator for location with respect to small deviation from the Gaussian model could be preferable.

> par(mfrow=c(2,2))
> qqnorm(USArrests\$Murder,main="Murder")
> qqline(USArrests\$Murder)
> qqnorm(USArrests\$Assault,main="Assault")
> qqline(USArrests\$Assault)
> qqnorm(USArrests\$UrbanPop,main="UrbanPop")
> qqline(USArrests\$UrbanPop)
> qqnorm(USArrests\$Rape,main="Rape")
> qqline(USArrests\$Rape)

2.2 The functions median and mad

Two simple robust estimators of location and scale parameters are the median and the MAD (the median absolute deviation), respectively. They can be computed using the median and mad functions. In particular, the median function computes the sample median $\hat{\mu}_{me}$ of the vector of values \mathbf{x} given as its argument. It is a Fisher consistent estimator, it is resistant to gross errors and it tolerates up to 50% gross errors before it can be made arbitrarily large (the mean has breakdown point 0%). The usage of the function median is:

```
median(x, na.rm = FALSE)
```

The na.rm argument is a logical value indicating whether NA values should be stripped before the computation proceeds.

In many applications, the scale parameter is often unknown and must be estimated too. The are several robust estimators of σ , such as the interquartile range and the MAD. The simpler but less robust estimator of scale is the interquartile range, that can be computed with the IQR function. Also the MAD is a simple robust scale estimator, given by $\hat{\sigma}_{MAD} = k \ med(|x_i - \hat{\mu}_{me}|)$, where $(x_i - \hat{\mu}_{me})$ denotes the *i*-th residual. Both are very resistant to outliers but not very efficient.

The mad function computes the MAD, and (by default) adjust it by a suitable constant k for asymptotically normal consistency. The usage of the mad function is:

```
mad(x, center = median(x), constant = 1.4826, na.rm = FALSE)
```

The arguments are:

- x: a numeric vector;
- center: optionally, a value for the location parameter (the default is the sample median, but a different value can be specified if the location parameter is known);
- constant: the scale factor k (the default value $k = 1 \Phi(3/4) \cong 1.4826$ makes the estimator Fisher consistent at the normal model $\Phi(x)$);
- na.rm: logical value indicating whether NA values should be stripped before the computation proceeds.

The variance of $\hat{\mu}_{me}$ can be estimated by $\hat{V}(\hat{\mu}_{me}) = (\pi/2)(\hat{\sigma}_{MAD}^2/n)$ and an approximate $(1-\alpha)$ confidence interval for μ can be computed as $\left(\hat{\mu}_{me} \pm z_{1-\alpha/2}\sqrt{\hat{V}(\hat{\mu}_{me})}\right)$, where $z_{1-\alpha/2}$ is the $(1-\alpha/2)$ -quantile of the standard normal distribution.

Example: The rivers data

The rivers dataset gives the lengths (in miles) of n=141 rivers in North America, as compiled by the US Geological Survey (McNeil, 1977). Plots and standard location estimates can be obtained using the following functions:

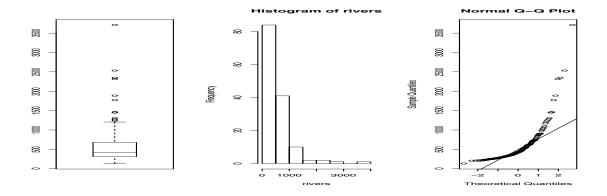


Figure 6: Rivers data.

```
> data(rivers)
> par(mfrow=c(1,3))
> boxplot(rivers)
> hist(rivers)
> qqnorm(rivers)
> qqline(rivers)
> median(rivers)
[1] 425
> summary(rivers)
   Min. 1st Qu.
                  Median
                            Mean 3rd Qu.
                                             Max.
  135.0
          310.0
                   425.0
                           591.2
                                    680.0
                                           3710.0
```

The plots in Figure 6 indicate that the distribution appears asymmetric and in this case $\hat{\mu}_{me}$ is preferable to $\hat{\mu}_{m}$. Scale estimators can be computed using:

```
> mad(rivers)
[1] 214.977
> IQR(rivers)
[1] 370
```

An approximate 0.95 confidence interval for μ can be computed and it is quite different from the standard confidence interval based on the sample mean.

```
> se.med <- sqrt((pi/2)*(mad(rivers)^2/length(rivers)))
> median(rivers)-qnorm(0.975)*se.med
[1] 380.5276
> median(rivers)+qnorm(0.975)*se.med
[1] 469.4724
> t.test(rivers)$conf.int
[1] 508.9559 673.4129
attr(,"conf.level")
[1] 0.95
```

2.3 The huber and hubers functions

The median and the MAD are not very efficient when the model is the Gaussian one, and a good compromise between robustness and efficiency can be obtained with M-estimates. If σ is known, an M-estimate of μ is implicitly defined as a solution of the estimating equation

$$\sum_{i=1}^{n} \psi_k \left(\frac{x_i - \mu}{\sigma} \right) = 0 , \qquad (2)$$

where $\psi_k(\cdot)$ is a suitable function. If, however, the scale parameter σ is unknown it is possible to estimate it by solving the equation

$$\frac{1}{(n-1)} \sum_{i=1}^{n} \chi\left(\frac{x_i - \mu}{\sigma}\right) = k_2 \tag{3}$$

for σ simultaneously with (2). In (3), $\chi(\cdot)$ is another suitable bounded function and k_2 a suitable constant, for consistency at the normal distribution. Alternatively, the scale parameter σ can be estimated with $\hat{\sigma}_{MAD}$ simultaneously with (2). Some simulation results have shown the superiority of M-estimators of location with initial scale estimate given by the MAD.

The huber function finds the Huber M-estimator of a location parameter with the scale parameter estimated with the MAD (see Huber, 1981; Venables and Ripley, 2002). In this case

$$\psi_k(x) = \max(-k, \min(k, x)) , \qquad (4)$$

where k is a constant the user specifies, taking into account the loss of efficiency he is prepared to accept at the Gaussian model in exchange to robustness. Its limit as $k \to 0$ is the median, and as $k \to \infty$ is the mean. The value k = 1.345 gives 95% efficiency at the Gaussian model. While the trimmed mean, the median and the MAD are estimators included in the base package of R, to compute the Huber M-estimator it is necessary to load to the library MASS (the main package of Venables and Ripley):

> library(MASS)

The usage of the huber function is:

$$huber(y, k = 1.5)$$

where the arguments are:

- y: the vector of data values;
- k: the truncation value of the Huber's estimator.

In case the scale parameter is known or if it is of interest to use the Huber's Proposal 2 scale estimator, the function hubers can be used. In particular, the command hubers finds the Huber M-estimator for location with scale specified, the scale with location specified, or both if neither is specified (see Huber, 1981; Venables and Ripley, 2002). The usage of the function hubers is:

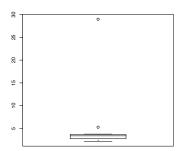


Figure 7: Chem data.

hubers(y, k = 1.5, mu, s, initmu = median(y))

The arguments of the function hubers are:

- y: the vector of data values;
- k: the truncation value of the Huber's estimator;
- mu: specified the value of the location parameter;
- s: specified the value of the scale parameter;
- initmu: an initial value for the location parameter.

The values of the functions huber and hubers are the list of the location and scale estimated parameters. In particular:

- mu: location estimate;
- s: MAD scale estimate or Huber's Proposal 2 scale estimate.

Example: The chem data

The chem data are a numeric vector of n=24 determinations of copper in wholemeal flour, in parts per million. Their boxplot is given in Figure 7 and we note how this plot is dominated by a single observation: the value 28.95 is clearly an outlier. The sample is clearly asymmetric with one value that appears to be out by a factor of 10. It was verified to be correct in the study.

```
> data(chem)
> summary(chem)
   Min. 1st Qu.
                  Median
                             Mean 3rd Qu.
                                              Max.
  2.200
          2.775
                   3.385
                            4.280
                                     3.700
                                            28.950
> huber(chem)
$mu
[1] 3.206724
$s
[1] 0.526323
> huber(chem, k=1.345)
```

```
$mu
[1] 3.216252
$s
[1] 0.526323
> huber(chem, k=5)
$mu
[1] 3.322244
$s
[1] 0.526323
> hubers(chem)
$mu
[1] 3.205498
$s
[1] 0.673652
> hubers(chem, k=1.345)
$mu
[1] 3.205
$s
[1] 0.6681223
> hubers(chem,mu=3)
$mu
[1] 3
$s
[1] 0.660182
> hubers(chem,s=1)
$mu
[1] 3.250001
$s
[1] 1
```

2.4 An introduction to the rlm function

The previous functions only allow to obtain point estimates of scale and location parameters. However, in many situations, it is preferable to derive a confidence interval for the parameter of interest or it may be of interest to test an hypothesis about the parameter. To this end we need an estimate of the asymptotic variance of the estimators. In these cases, it could be preferable to use the rlm function. This function, more generally, fits a linear model by robust regression using M-estimators (see Section 3). However, if only the intercept of the linear model is chosen, then a scale and location model is obtained.

The usage of the function rlm is:

```
rlm(formula, data, psi = psi.huber, scale.est, k2 = 1.345, ...)
```

Several additional arguments can be passed to rlm and fitting is done by iterated reweighted least squares (IWLS). The main arguments of the function rlm are:

• formula: a formula as in 1m (see Section 3 for more details);

- data: (optional) the data frame from which the variables specified in formula are taken;
- psi: the estimating function of the estimator of μ is specified by this argument;
- scale.est: the method used for scale estimation, i.e. re-scaled MAD of the residuals or Huber's Proposal 2;
- k2: the tuning constant used for Huber's Proposal.

Several ψ -functions are supplied for the Huber, Tukey's bisquare and Hampel proposals as psi.huber, psi.bisquare and psi.hampel. The well-known Huber proposal is given in (4). Remember that Huber's proposals have the drawback that large outliers are not down weighted to zero. This can be achieved with the Tukey's bisquare proposal, which is a redescending estimator such that $\psi(x) \to 0$ for $x \to \infty$; in particular, it has

$$\psi_k(x) = x(k - x^2)^2 \,\,\,(5)$$

for $-k \ge x \ge k$ and 0 otherwise, so that it gives extreme observations zero weights. The usual value of k is 4.685. In general, the standard error of these estimates are slightly smaller than in the Huber fit but the results are qualitatively similar. Also the Hampel's proposal is a redescending estimator defined by several pieces (see e.g. Huber, 1981, Sec. 4.8; Venables and Ripley, 2002, Sec. 5.5).

The function rlm gives an object of class lm. The additional components not in an lm object are:

- s: the robust scale estimate used;
- w: the weights used in the IWLS process (see Section 3);
- psi: the ψ -function with parameters substituted.

Example: The chem data

Consider again the chem data.

Residual standard error: 0.6792 on 23 degrees of freedom

On the contrary of hubers, using the rlm function one obtains also an estimate of the asymptotic standard error of the estimator of the location parameter (see Std.Error) and the value of the observed statistic Value/Std.Error for testing $H_0: \mu = 0$ vs $H_1: \mu \neq 0$ (see t value). To verify $H_0: \mu = 3$ vs $H_1: \mu \neq 3$ one can compute:

```
# Testing H0: mu=3 vs H1: mu!=3
> toss <- (fit$coef-3)/0.14
> p.value <- 2*min(1-pnorm(toss),pnorm(toss))
> p.value
[1] 0.1430456
```

An approximate $(1 - \alpha)$ confidence interval for μ can be computed as (Value $\pm z_{1-\alpha/2}$ Std.Error), where $z_{1-\alpha/2}$ is the $(1 - \alpha/2)$ -quantile of the standard normal distribution.

```
# 0.95% Confidence Interval
> ichub <- c(fit$coef-qnorm(0.975)*0.14,fit1$coef+qnorm(0.975)*0.14)
> ichub
(Intercept) (Intercept)
    2.930641    3.479431
```

A natural way to assess the stability of an estimator is to make a sensitivity analysis and a simple way to do this is to compute the sensitivity curve. It consists in replacing one observation of the sample by an arbitrary value y and plotting the value of $SC_n(y) = n\left(T_n(x_1,\ldots,x_{n-1},y)-T_{n-1}(x_1,\ldots,x_{n-1})\right)$, where $T_n(x)$ denotes the estimator of interest based on the sample x of size n. The sensitivity curve $SC_n(y)$ is a translated and rescaled version of the empirical influence function. In many situations, $SC_n(y)$ will converge to the influence function when $n \to \infty$. The supremum of the influence function is a measure of the maximum effect an observation can have on the estimator. It is called the gross error sensitivity.

In Figure 8 many examples of $SC_n(y)$ for estimators of the location parameter are plotted. Small changes to y do not change the estimates much, except for the arithmetic mean that can be made arbitrarily large by large changes to y. In fact, this estimator can break down in the sense of becoming infinite by moving a single observation to infinity. The *breakdown point* of an estimator is the largest fraction of the data that can be moved arbitrarily without perturbing the estimator to the boundary of the parameter space. Thus the higher the breakdown point, the more robust the estimator against extreme outliers.

```
> chem <- sort(chem)
> n <- length(chem)
> chem <- chem[-n]
> xmu <- seq(-10,10,length=100)
> mm <- hu2 <- ht <- rep(0,100)
> for(i in 1:100){
+ mm[i] <-n*( mean(c(chem,xmu[i])) - mean(chem) )
+ hu2[i] <- n*( hubers(c(chem,xmu[i]),k=1.345)$mu - hubers(chem,k=1.345)$mu)
+ ht[i] <- n*(rlm(c(chem,xmu[i])~1,psi=psi.bisquare)$coef-
    rlm(chem~1,psi=psi.bisquare)$coef) }
> plot(xmu,mm,ylim=c(-3,4),xlim=c(-3,10),type="l")
> lines(xmu,hu2,lty=5)
> lines(xmu,ht,lty=2)
> legend(-2,4,c("mean","hubers","tukey"),lty =c(1,5,2))
```

In Figure 8 several ways of treating deviant values can be observed: no treatment at all (mean), bounding its influence (Huber) and smooth rejection (Tukey).

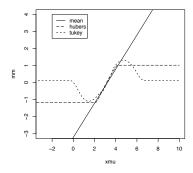


Figure 8: Chem data: Sensitivity analysis.

3 Estimation in scale and regression models

The aim of this Section is to describe the procedures given in R for computing robust solutions for scale and regression models. To this end both we extend the function rlm introduced in the simpler case of a scale and location model and we introduce several other R functions. The main references for the arguments discussed here are Huber (1981), Li (1985), Hampel et al. (1986) Marazzi (1993) and Venables and Ripley (2002).

A scale and regression model is given by

$$y_i = x_i^{\mathrm{T}} \beta + \sigma \epsilon_i , \quad i = 1, \dots, n ,$$
 (6)

where $y = (y_1, \ldots, y_n)$ is the response, x_i is a p-variate vector of regressors, $\beta \in \mathbb{R}^p$ is an unknown p-vector of regression coefficients, $\sigma > 0$ a scale parameter and ϵ_i are independent and identically distributed random variables according to a known density function $p_0(\cdot)$.

If $p_0(x) = \phi(x)$, i.e. the standard Gaussian distribution, the classical inferential procedures, based on the least squares (OLS) estimates, are the most efficient. In fact, in this case, the OLS estimates are the maximum likelihood estimates (MLE). However, it is well-known that a few atypical observations or small deviations from the assumed parametric model $p_0(\cdot)$ can have a large influence on the OLS estimates.

There are a number of ways to perform robust regression in R, and here the aim is to mention only the principal ones. In a regression problem there are two possible sources of errors: the observations y_i in the response and/or the p-variate vector x_i . Some robust methods in regression only consider the first source of outliers (outliers in y-direction), and in some situations of practical interest errors in the regressors can be ignored (such as in most bioassay experiments). It is well-known that outliers in y-direction have influence on classical estimates of β , but in particular on the classical estimates of the error variance. The presence of outliers in y-direction emerges typically in the graphical analysis of the residuals of the model. Outliers in x-direction, can be well aligned with the other points (the point is outlier also in the y-direction and in this case the outlier has a small influence on the fit) or can be a leverage point (not outlier in the y-direction, such as in Figure 2). Leverage points can be very dangerous since they are typically very influential. Moreover, their detection based on classical procedures can be very difficult, especially with high-dimensional data, since cases with high leverage may not stand out in the OLS residual plots.

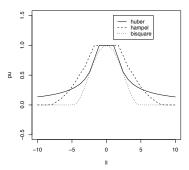


Figure 9: Huber, Hampel and bisquare weight functions in (7) and rlm.

In the scale and regression framework, three main classes of estimators can be identified. To deal with outliers in y-direction, the most commonly used robust methods are based on Huber-type estimators. Problems with a moderate percentage of multivariate outliers in the x-direction, or leverage points, can be treated with bounded influence estimators. Finally, to deal with problems in which the frequency of outliers in very high (up to 50%), we can use the high breakdown point estimators.

3.1 M-estimators

One important class of robust estimates are the M-estimates, such as Huber estimates, which have the advantage of combining robustness with efficiency under the regression model with normal errors. In general, an M-estimate of β is implicitly defined as a solution of the system of p equations

$$\sum_{i=1}^{n} w_i r_i x_{ij} = 0 , \quad j = 1, \dots, p ,$$
 (7)

where $r_i = y_i - x_i^{\mathrm{T}}\beta$ denotes the residual, $w_i = W(r_i/\sigma)$ is a weight, $i = 1, \ldots, n$, with W(u) suitable weight function. For example, for the Huber-type estimate $W(u) = \psi_k(u)/u$, with $\psi_k(\cdot)$ given in (4). The scale parameter σ can be estimated by using a simple and very resistant scale estimator, i.e. the MAD of the residuals. Alternatively, we can estimate σ by solving (7) with a supplementary equation for σ , given for example by Huber's Proposal 2. Equation (7) is the equation of a weighted OLS estimate. Of course, this cannot be used as a direct algorithm because the weights w_i depend on β and σ , but it can be the base of an iterative algorithm.

Huber-type estimates are robust when the outliers have low leverage, that is the values in the regressors are not outliers. To obtain estimates which are robust against any type of outliers, the bisquare function proposed by Tukey, or the Hampel's proposal, can be preferable. These estimates are M-estimates of the form (7), with redescending ψ -functions. However, these estimating equations may have multiple roots, and this may considerably complicate the computation of this estimate. In such cases it is usual to choose a good starting point and iterate carefully. Figure (9) gives the plots of the Huber, Hampel and bisquare weight functions in (7).

Robust M-estimation of scale and regression parameters can be performed using the rlm function, introduced in Section 2.4. The only difference is in the specification of the

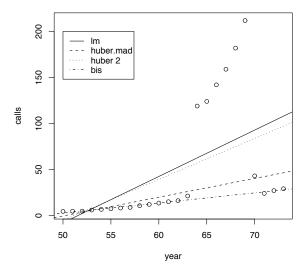


Figure 10: Phones data: several fits.

formula of the model. We remember that the syntax of rlm in general follows lm and its usage is:

```
rlm(formula, data, ..., weights, init, psi = psi.huber, scale.est,
    k2 = 1.345)
```

In rlm the model (6) is specified in a compact symbolic form. Remember that the \sim operator is basic in the formulation of such a model. An expression of the form $y\sim x1+x2+\ldots+xp$ is interpreted as a specification that the response y is modeled by a linear predictor specified as $\beta_1 + \beta_2 x_2 + \ldots + \beta_p x_p$. Moreover, the * operator denotes factor crossing and the - operator removes the specified terms.

The choice psi.huber with k = 1.345 for β and MAD of the residuals for σ represents the default in rlm. If it is of interest to use the Huber's Proposal 2 the option scale.est="proposal 2" must be specified. Other arguments of the function rlm are weights and init. Quantity weights gives (optional) prior weights for each case, while init specifies (optional) initial values for the coefficients. The default is 1s for an initial OLS fit, and a good starting point is necessary for Hampel and Tukey's proposals.

Example: phones data

This data set gives n=24 observations about the annual numbers of telephone calls made (calls, in millions of calls) in Belgium in the last two digits of the year (year); see Rousseeuw and Leroy (1987), and Venables and Ripley (2002). As it can be noted in Figure 10 there are several outliers in the y-direction in the late 1960s.

Let us start the analysis with the classical OLS fit.

- > data(phones)
 > attach(phones)
- > plot(year,calls)
- > fit.ols <- lm(calls~year)</pre>

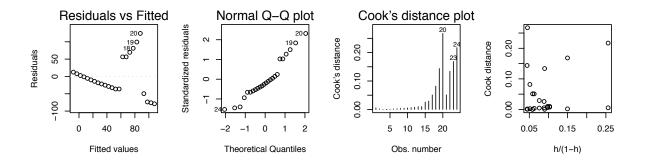


Figure 11: Phones data: Diagnostic plots for OLS estimates.

```
> summary(fit.ols,cor=F)
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -260.059
                                   -2.535
                         102.607
                                            0.0189 *
year
               5.041
                           1.658
                                    3.041
                                            0.0060 **
Residual standard error: 56.22 on 22 degrees of freedom
Multiple R-Squared: 0.2959,
                                 Adjusted R-squared: 0.2639
F-statistic: 9.247 on 1 and 22 DF, p-value: 0.005998
> abline(fit.ols$coef)
> par(mfrow=c(1,4))
> plot(fit.ols,1:2)
> plot(fit.ols,4)
> hmat.p <- hat(model.matrix(fit.ols))</pre>
> h.phone <- hat(hmat.p)</pre>
> cook.d <- cooks.distance(fit.ols)
> plot(h.phone/(1-h.phone),cook.d,xlab="h/(1-h)",ylab="Cook distance")
```

Figure 11 gives four possible diagnostic plots based on the OLS fit: the plot of the residuals versus the fitted values, the normal QQ-plot of the residuals, the Cook's distance plot and the Cook's distance statistic versus $h_{ii}/(1-h_{ii})$. It is important to remember that the plots give different information about the observations. In particular, there are some high leverage observations (such as the last two observations), which are not associated to large residuals, but originating influential points.

In order to take into account of observations related to high values of the residuals, i.e. the outliers in the late 1960s, consider a robust regression based on Huber-type estimates:

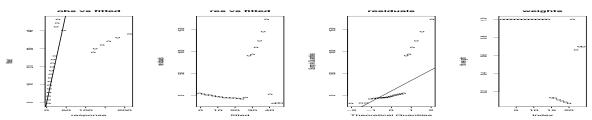


Figure 12: Phones data: Diagnostic plots for Huber's estimate with MAD.

```
> fit.hub <- rlm(calls~year,maxit=50)</pre>
> fit.hub2 <- rlm(calls~year,scale.est="proposal 2")</pre>
> summary(fit.hub,cor=F)
Coefficients:
            Value
                       Std. Error t value
(Intercept) -102.6222
                         26.6082
                                     -3.8568
                2.0414
                                      4.7480
year
                          0.4299
Residual standard error: 9.032 on 22 degrees of freedom
> summary(fit.hub2,cor=F)
Coefficients:
            Value
                       Std. Error t value
(Intercept) -227.9250
                        101.8740
                                     -2.2373
year
               4.4530
                          1.6461
                                      2.7052
Residual standard error: 57.25 on 22 degrees of freedom
> abline(fit.hub$coef,lty=2)
> abline(fit.hub2$coef,lty=3)
```

¿From these results and also from Figure 10, we note that there are some differences with the OLS estimates, in particular this is true for the Huber-type estimator with MAD. Consider again some classic diagnostic plots (see Figure 12 for the Huber-type estimator with MAD) about the robust fit: the plot of the observed values versus the fitted values, the plot of the residuals versus the fitted values, the normal QQ-plot of the residuals and the fit weights of the robust estimator. Note that there are some observations with low Huber-type weights which were not identified by the classical Cook's statistics. See McKean et al. (1993) for the use and the interpretability of the residual plots for a robust fit

```
> dia.check.rlm <- function(fit,fitols){
+ hmat.rlm <- hat(model.matrix(fitols))
+ h.rlm <- hat(hmat.rlm)
+ cook.d <- cooks.distance(fitols)
+ par(mfrow=c(1,4))
+ obs <- fit$fit+fit$res
+ plot(obs,fit$fit,xlab="response",ylab="fitted",main="obs vs fitted")
+ abline(0,1)
+ plot(fit$fit,fit$res,xlab="fitted",ylab="residuals",main="res vs fitted")
+ qqnorm(fit$res,main="residuals")
+ qqline(fit$res)</pre>
```

```
+ plot(fit$w,ylab="fit weight",main="weights")
+ par(mfrow=c(1,1))
+ invisible() }
> dia.check.rlm(fit.hub,fit.ols)
```

As it can be noted in Figure 10, Huber's Proposal 2 M-estimator does not reject the outliers completely. Let us try a redescending estimator:

It can be useful to compare the different weights in the robust estimations visualizing them. In this way the several ways of treating the data can be observed: bounding its influence and smooth rejection.

```
> tabweig.phones <- cbind(fit.hub$w,fit.hub2$w,fit.tuk$w)</pre>
> colnames(tabweig.phones) <- c("Huber MAD", "Huber 2", "Tukey")</pre>
> tabweig.phones
       Huber MAD
                   Huber 2
                                Tukey
 [1,] 1.00000000 1.0000000 0.8947891
 [2,] 1.00000000 1.0000000 0.9667133
 [3,] 1.00000000 1.0000000 0.9997063
 [4,] 1.00000000 1.0000000 0.9999979
 [5,] 1.00000000 1.0000000 0.9949381
 [6,] 1.00000000 1.0000000 0.9794196
 [7,] 1.00000000 1.0000000 0.9610927
 [8,] 1.00000000 1.0000000 0.9279780
 [9,] 1.00000000 1.0000000 0.9797105
[10,] 1.00000000 1.0000000 0.9923186
[11.] 1.00000000 1.0000000 0.9997925
[12,] 1.00000000 1.0000000 0.9983464
[13,] 1.00000000 1.0000000 0.9964913
[14,] 1.00000000 1.0000000 0.4739111
[15,] 0.13353494 1.0000000 0.0000000
[16,] 0.12932949 1.0000000 0.0000000
[17,] 0.11054769 1.0000000 0.0000000
[18,] 0.09730248 0.8694727 0.0000000
[19,] 0.08331587 0.7189231 0.0000000
[20,] 0.06991030 0.5804777 0.0000000
```

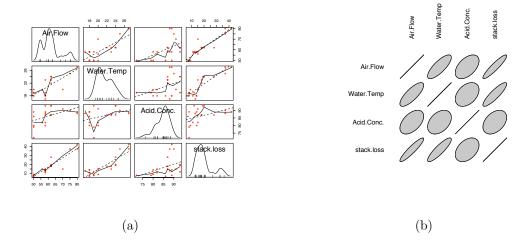


Figure 13: Stackloss data: (a) Scatterplots and (b) correlation plots.

```
[21,] 1.00000000 1.0000000 0.00000000
[22,] 0.66293888 1.0000000 0.9105473
[23,] 0.69951382 1.0000000 0.9980266
[24,] 0.69782955 1.0000000 0.9568027
```

Example: stackloss data

This data set, with n=21 observations on p=4 variables, are operational data of a plant for the oxidation of ammonia to nitric acid (see, e.g., Becker et al., 1988). In particular, the variables are: [,1] Air Flow, the rate of operation of the plant; [,2] Water Temp, temperature of cooling water circulated through coils in the absorption tower; [,3] Acid Conc., concentration of the acid circulating, minus 50, times 10: that is, 89 corresponds to 58.9 per cent acid; [,4] stack.loss, (the dependent variable) is 10 times the percentage of the ingoing ammonia to the plant that escapes from the absorption column unabsorbed: that is, an (inverse) measure of the over-all efficiency of the plant. An exploratory graphical analysis can be made using the scatterplots and the plot of the correlation matrix (see Figure 13). To use these plots it is necessary to load the two libraries car and ellipse. Note that, for this data set, it is not easy to identify the presence of outliers or leverage points in the observed data, looking at Figure 13.

```
> data(stackloss)
> library(car)
> library(ellipse)
> scatterplot.matrix(stackloss)
> plotcorr(cor(stackloss))
```

Consider a model of the form $y_i = \beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \sigma \epsilon_i$, i = 1, ..., 21, and let us start the analysis with the classical estimates given by lm and rlm.

```
> fit.ols <- lm(stack.loss ~ stackloss[,1]+stackloss[,2]+stackloss[,3])</pre>
```

```
> summary(fit.ols)
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)
              -39.9197
                          11.8960 -3.356 0.00375 **
stackloss[, 1]
                                    5.307 5.8e-05 ***
                0.7156
                           0.1349
stackloss[, 2] 1.2953
                           0.3680
                                    3.520 0.00263 **
stackloss[, 3] -0.1521
                           0.1563 -0.973 0.34405
Residual standard error: 3.243 on 17 degrees of freedom
Multiple R-Squared: 0.9136,
                              Adjusted R-squared: 0.8983
F-statistic: 59.9 on 3 and 17 DF, p-value: 3.016e-09
> fit.hub <- rlm(stack.loss ~ stackloss[,1]+stackloss[,2]+stackloss[,3],cor=F)</pre>
> summary(fit.hub)
Coefficients:
                       Std. Error t value
              Value
(Intercept)
              -41.0265
                         9.8073
                                   -4.1832
stackloss[, 1]
                0.8294
                         0.1112
                                    7.4597
stackloss[, 2]
                0.9261
                         0.3034
                                    3.0524
stackloss[, 3] -0.1278
                                   -0.9922
                         0.1289
Residual standard error: 2.441 on 17 degrees of freedom
> fit.ham <- rlm(stack.loss ~ stackloss[,1]+stackloss[,2]+stackloss[,3],</pre>
+ psi=psi.hampel,cor=F)
> summary(fit.ham)
Coefficients:
              Value
                       Std. Error t value
(Intercept)
              -40.4747 11.8932
                                   -3.4032
stackloss[, 1]
                0.7411
                         0.1348
                                    5.4966
stackloss[, 2] 1.2251 0.3679
                                    3.3296
stackloss[, 3] -0.1455
                         0.1563
                                   -0.9313
Residual standard error: 3.088 on 17 degrees of freedom
> fit.bis <- rlm(stack.loss ~ stackloss[,1]+stackloss[,2]+stackloss[,3],</pre>
+ psi=psi.bisquare,cor=F)
> summary(fit.bis)
Coefficients:
              Value
                       Std. Error t value
                         9.5316
(Intercept)
              -42.2853
                                   -4.4363
stackloss[, 1]
                                    8.5841
                0.9275
                         0.1081
```

2.2068

stackloss[, 2]

0.6507

0.2949

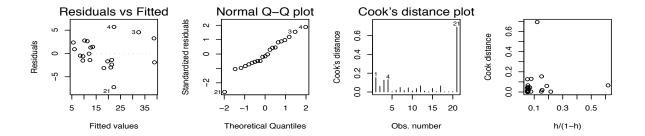


Figure 14: Stackloss data: Diagnostic plots for OLS fit.

```
stackloss[, 3] -0.1123 0.1252 -0.8970
```

Residual standard error: 2.282 on 17 degrees of freedom

In this case, the results of the different fits appear very similar. If it is of interest to test the null hypothesis $H_0: \beta_j = 0$ vs $H_1: \beta_j \neq 0$, a Wald-type test can be performed, using a consistent estimate of the asymptotic variance of the robust estimator. All these quantities are given in the output of the fit performed with rlm. In particular the function summary allows to derive the values of the estimates of the regression coefficients (Value), their estimated standard error (Std.Error) and the Wald-type statistic for $H_0: \beta_j = 0$ (t value). Choosing $z_{0.975} = 1.96$, in all the fits there is evidence against $H_0: \beta_4 = 0$.

Figure 14 gives several diagnostic plots based on the OLS fit. A leverage point and an influential point emerges.

```
> par(mfrow=c(1,4))
> plot(fit.ols,1:2)
> plot(fit.ols,4)
> hmat.p <- hat(model.matrix(fit.ols))
> h.st <- hat(hmat.p)
> cook.d <- cooks.distance(fit.ols)
> plot(h.st/(1-h.st),cook.d,xlab="h/(1-h)",ylab="Cook distance")
```

Using rlm the different weights in the robust estimates can be easily derived and a graphical inspection can be useful to identify those residuals which have a weight less than one (see Figure 15). In many applications, these weights are worth looking at because they automatically define the observations that have been considered by the robust estimator as more or less far from the bulk of data, and one can determine approximately the amount of contamination.

Diagnostic plots of the robust fitted models can be considered too (see, for example, Figure 16 for the Huber's estimate), in order to evaluate the fits. Similar plots can be obtained also for the other robust estimators and the results appears very similar.

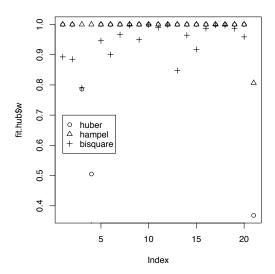


Figure 15: Stackloss data: Weights of different estimates.

```
> plot(fit.hub$w)
> points(fit.ham$w,pch=2)
> points(fit.bis$w,pch=3)
> legend(0.7, c("huber", "hampel", "bisquare",),lty = c(1,2,3))
> dia.check.rlm(fit.hub,fit.ols)
```

3.2 The weighted likelihood

Huber estimates are robust when the outliers have low leverage. Instead of the Tukey or Hampel's proposals, to derive robust estimates against any type of outliers, it is also possible to fit linear models using the weighted likelihood (Markatou et al., 1998; Agostinelli and Markatou, 1998). In particular, wle.lm (Agostinelli, 2001) allows to fit a linear model, when the errors are independent and identically distributed random variables from a Gaussian distribution. The resulting estimator is robust against the presence of bad leverage points too.

The weighted likelihood methodology consists in constructing a weight function $w(\cdot)$ that depends on the data y and on the distribution of the assumed parametric model. The estimators of the parameters are then obtained as solutions of a set of estimating functions of the form $\sum_{i=1}^{n} w(y_i)u_i = 0$, where u_i is the score function of observation y_i . There are several proposals for the weight function $w(\cdot)$, depending on a chosen distance. Note that the robust estimates can be interpreted as a redescending estimates with adaptive ψ -function, that is the shape of the ψ -function depends on the observed data.

The usage of wle.lm is:

```
wle.lm(formula,data,raf="HD",...)
where
```

• formula: is the symbolic description of the model to be fit;

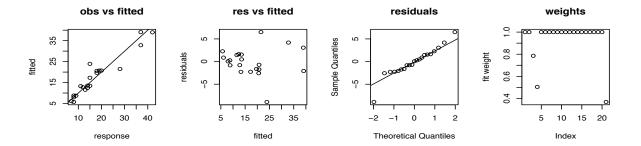


Figure 16: Stackloss data: Diagnostic plots for Huber estimates.

- data: (optional) data frame containing the variables in the model;
- raf: type of Residual adjustment function to be used to construct the weight function: raf="HD", Hellinger Distance RAF; raf="NED", Negative Exponential Disparity RAF; raf="SCHI2", Symmetric Chi-Squared Disparity RAF.

Function wle.lm returns an object of class lm, and thus the function summary can be used to obtain and print a summary of the results. Moreover, the usual functions coefficients, standard.error, scale, residuals, fitted.values and weights extract, respectively, coefficients, an estimation of the standard error of the parameters estimator, estimation of the error scale, residuals, fitted values and the weights associated to each observation.

Example: phones data

Let us consider again the **phones** data and let us complete the analysis by including also the weighted likelihood estimates.

Residual standard error: 55.62 on 21.12913 degrees of freedom Multiple R-Squared: 0.2978, Adjusted R-squared: 0.2646

F-statistic: 8.963 on 1 and 21.12913 degrees of freedom, p-value: 0.006888

```
> tabcoef.phones <- cbind(fit.hub$coef,fit.tuk$coef,fitr.wl$coef)</pre>
> colnames(tabcoef.phones) <- c("Huber", "Tukey", "WLE")</pre>
> tabcoef.phones
                  Huber
                              Tukey
                                             WLE
(Intercept) -102.622198 -52.302456 -257.441791
                           1.098041
year
               2.041350
                                       4.999245
> tabs.phones <- cbind(fit.hub$s,fit.tuk$s,fitr.wl$scale)</pre>
> colnames(tabs.phones) <- c("Huber","Tukey","WLE")</pre>
> tabs.phones
       Huber
                Tukey
                            WLE
[1,] 9.03168 1.654451 55.61679
> tabweig.phones <- cbind(fit.hub$w,fit.tuk$w,fitr.wl$w)</pre>
> colnames(tabweig.phones) <- c("Huber", "Tukey", "WLE")</pre>
> tabweig.phones
        Huber
                  Tukey
                               WLE
  1.00000000 0.8947891 0.9835997
  1.00000000 0.9667133 0.9999492
  1.00000000 0.9997063 0.9923673
  1.00000000 0.9999979 0.9848063
  1.00000000 0.9949381 0.9772509
  1.00000000 0.9794196 0.9698894
  1.00000000 0.9610927 0.9616714
  1.00000000 0.9279780 0.9521434
  1.00000000 0.9797105 0.9453642
10 1.00000000 0.9923186 0.9400354
11 1.00000000 0.9997925 0.9394768
12 1.00000000 0.9983464 0.9456869
13 1.00000000 0.9964913 0.9601966
14 1.00000000 0.4739111 0.9597216
15 0.13353494 0.0000000 0.9997955
16 0.12932949 0.0000000 0.9997960
17 0.11054769 0.0000000 0.9934905
18 0.09730248 0.0000000 0.9937017
19 0.08331587 0.0000000 0.9762205
20 0.06991030 0.0000000 0.8351528
21 1.00000000 0.0000000 0.9889019
22 0.66293888 0.9105473 0.9529798
23 0.69951382 0.9980266 0.9413971
24 0.69782955 0.9568027 0.9355390
```

The various fits are quite different and in view of this the estimated models can be different. Note also that the considered methods tend to downweight the observations in a different manner. Several plots can be considered in order to evaluate the fit using the plot.wle.lm function: the plot of the residuals versus the fitted values, the normal

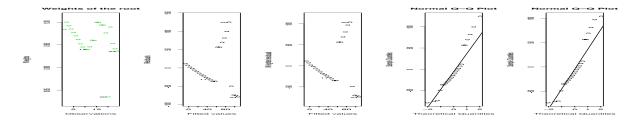


Figure 17: Diagnostic plots for WLE estimates for phones data.

QQ-plots of the residuals, the plot of the weighted residuals versus the weighted fitted values, the normal QQ-plots of the weighted residuals and a plot of the weights versus the position of the observations for each root.

> par(mfrow=c(1,5))
> plot.wle.lm(fitr.wl)

Note that the lower weight in the WLE fit corresponds to the observation with maximum value of the Cook's distance statistic (influential observation).

3.3 High breakdown regression

M-estimators are not very resistant to leverage points, unless they have redescending ψ -functions. In this case, they need a good starting point. Several robust estimators of regression have been proposed in order to remedy this shortcoming, and are high breakdown point estimators of regression. We remember that the breakdown point of the Huber-type and least residuals estimators is 0% (they cannot cope with leverage points), and in general it cannot exceed 1/p for other robust M-estimators (that is, it decreases with increasing dimension where there are more opportunities for outliers to occur).

The first estimator to become popular was the least median of squares (LMS) estimate, defined as the p-vector

$$\hat{\beta}_{lms} = \min med(y_i - x_i^{\mathrm{T}}\beta)^2 .$$

This fit is very resistant and needs no scale estimate. The breakdown point of the LMS estimator is 50%, but this estimator is highly inefficient we the central model is the Gaussian one.

Another proposal is the *least trimmed squares* (LTS) estimate, defined as the *p*-vector

$$\hat{\beta}_{lts} = \min \sum_{i=1}^k r_{[i]}^2 ,$$

where $r_{[1]}^2 \leq r_{[2]}^2 \leq \ldots \leq r_{[n]}^2$ are the ordered squared residuals $r_i^2 = (y_i - x_i^T \beta)^2$, $i = 1, \ldots, n$, and k is the largest integer such that $k \leq n/2+1$. This estimator is more efficient than LMS, having breakdown point 50%. Its main disadvantage is that it requires a heavy computational effort.

A further proposal is the S-estimator, in which the coefficients are chosen to find the solution of

$$\sum_{i=1}^{n} \chi\left(\frac{r_i}{c_o s}\right) = (n-p)k_2$$

with smallest scale s. Usually, $\chi(\cdot)$ is usually chosen to the integral of Tukey's bisquare function, $c_0 = 1.548$ and $k_2 = 0.5$ is chosen for consistency at the Gaussian distribution. S-estimates have breakdown point 50%, such as for the bisquare family. However, the asymptotic efficiency of an S-estimate under normal errors is 0.29, which is not very satisfactory but is better than LMS and LTS.

It is possible to combine the resistance of these high breakdown estimators with the efficiency of M-estimation. The MM-estimates (see Yohai, 1987, and Marazzi, 1993) have an asymptotic efficiency as close to one as desired, and simultaneously breakdown point 50%. Formally, the MM-estimate $\hat{\beta}_{MM}$ it consists in: (1) compute an S-estimate with breakdown point 1/2, denoted by $\hat{\beta}^*$; (2) compute the residuals $r_i^* = y_i - x_i^T \beta^*$ and find $\hat{\sigma}^*$ solution of $\sum_{i=1}^n \chi(r_i^*/\sigma) = k_2(n-p)$; (3) find the minimum $\hat{\beta}_{MM}$ of $\sum_{i=1}^n \rho((y_i - \beta^T x_i)/\hat{\sigma}^*)$, where $\rho(\cdot)$ is a suitable function. The function rlm has an option that allows to implement MM-estimation:

```
rlm(formula, data, ...,method="MM")
```

To use other breakdown point estimates, in R there exists the function lqs to fit a regression model using resistant procedures, that is achieving a regression estimator with a high breakdown point (see Rousseeuw and Leroy, 1987, Marazzi, 1993, and Venables and Ripley, 2002, Sec. 6.5). The usage of the function lqs is:

```
lqs(formula, data, method = c("lts", "lqs", "lms", "S"),...) where
```

- formula: is a formula of the form lm;
- data: (optional) is the data frame used in the analysis;
- method: the method to be used for resistant regression. The first three methods minimize some function of the sorted squared residuals. For methods lqs and lms is the quantile squared residual, and for lts it is the sum of the quantile smallest squared residuals.

Several other arguments are available for this function, such as the tuning constant k0 used for $\chi(\cdot)$ and $\psi(\cdot)$ functions when method = "S", currently corresponding to Tukey's biweight.

For summarizing the output of function lqs the function summary cannot be used. Function lqs gives a list with usual components, such as coefficients, scale residuals, fitted.values. In particular, scale gives the estimate(s) of the scale of the error. The first is based on the fit criterion. The second (not present for method == "S") is based on the variance of those residuals whose absolute value is less than 2.5 times the initial estimate. Finally, we remember that high breakdown procedures do not usually provide standard errors. However, these can be obtained by a data-based simulation, such as a bootstrap.

Example: stackloss data

Consider again the dataset with n = 21 observations on p = 4 variables about operational data of a plant for the oxidation of ammonia to nitric acid, and let us complete the analysis by including also high breakdown point estimators.

```
> data(stackloss)
> fit1 <- lqs(stack.loss ~ ., data = stackloss)</pre>
> fit2 <- lqs(stack.loss ~ ., data = stackloss, method = "S")</pre>
> fitmm <- rlm(stack.loss ~ ., data = stackloss, method = "MM")</pre>
> fit1$coefficients
 (Intercept)
                 Air.Flow
                             Water.Temp
                                          Acid.Conc.
-32.41826923
               0.75000000
                             0.32692308 -0.03846154
> fit2$coefficients
 (Intercept)
                 Air.Flow
                             Water.Temp
                                          Acid.Conc.
-35.37610619
                             0.44247788 -0.07964602
               0.82522124
> fitmm$coefficients
(Intercept)
               Air.Flow Water.Temp Acid.Conc.
-41.7072683
              0.9372710
                          0.5940631
                                     -0.1129477
> fit.hub$coefficients
   (Intercept) stackloss[, 1] stackloss[, 2] stackloss[, 3]
   -41.0265311
                    0.8293739
                                    0.9261082
                                                   -0.1278492
> fit.bis$coefficients
   (Intercept) stackloss[, 1] stackloss[, 2] stackloss[, 3]
   -42.2852537
                    0.9275471
                                    0.6507322
                                                   -0.1123310
> fit1$scale
[1] 0.9393087 1.0371971
> fit2$scale
[1] 1.911955
> fitmm$s
[1] 1.982660
> fit.hub$s
      11
2.440714
> fit.bis$s
      11
2.281886
```

Figure 18 compares the plots of the residuals versus fitted values for several fits. Figure 19 gives the normal QQ-plots of the residuals of several fits for the stackloss data: the OLS residuals and residuals from high breakdown regression.

```
> par(mfrow=c(1,3))
> plot(fit1$fit,fit1$res,main="LQS")
> plot(fit2$fit,fit2$res,main="S")
> plot(fitmm$fit,fitmm$res,main="MM")
> par(mfrow=c(1,4))
> fit <- lm(stack.loss ~ ., data = stackloss)
> qqnorm(residuals(fit),main="LS")
> qqline(residuals(fit1))
> qqnorm(residuals(fit1),main="LQS")
> qqline(residuals(fit1))
> qqnorm(residuals(fit1))
> qqnorm(residuals(fitmm),main="MM")
> qqline(residuals(fitmm))
```

- > qqnorm(residuals(fit2),main="S")
- > qqline(residuals(fit2))

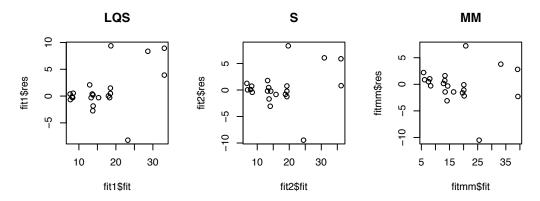


Figure 18: Residuals versus fitted values for several residuals for stackloss data.

In this data set bad leverage points are not present and, in general, all the results of the different robust fits are quite similar. Next Section will present an example in which the importance of high breakdown estimation emerges.

3.4 Bounded-influence estimation in linear regression models

The previous examples were based on some well-developed R libraries. We now present some further examples describing also some methods not implemented yet.

Huber type M-estimation of linear regression coefficients does not provide bounded-influence estimation, as the influence function of the estimators is bounded in the y space (direction) but not in the x space. A remedy to this is given by bounded-influence estimators, which use suitable weights on the design (x-weights). Here we consider both Mallows-type and Schweppe-type estimators, which can be obtained by suitable specification of the weights w_i in (7). Two commonly used methods are the Mallows estimator and the Hampel and Krasker estimator (see Hampel $et\ al.$, 1986, §6.3). They are both implemented by our simple function lm.BI, which uses the ψ function given by the Huber function (4). It implements an iterated weighted least squares algorithm following Jørgensen (1984), with σ updating and standard errors computed as in Street $et\ al.$ (1988). The function has the following usage

lm.BI(beta.in, sigma.in, X, y, method, k1, k2, maxiter, mytol)

The arguments of the function lm.BI are

- beta.in, sigma.in: initial values for β and σ ;
- X, y: design matrix and response vector;
- method: one of "huber", "mallows" or "hampel", implementing Huber, Mallows or Hampel-Krasker regression. For Mallows regression, the x-weights $w_i = (1 h_{ii})^{1/2}$ are used, where h_{ii} is the *i*-th diagonal value of the hat matrix; for Hampel and Krasker regression the x-weights are obtained according to the formulas given in

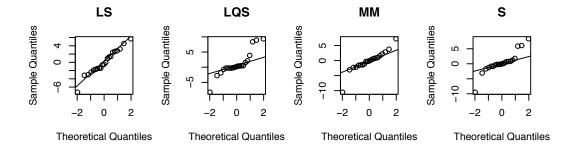


Figure 19: Normal QQ-plots for several residuals for stackloss data.

Krasker and Welsch (1982). For Huber regression, the scale is estimated by Huber Proposal 2, and for Mallows regression by a weighted version of the same method (Marazzi, 1993).

- k1, k2: tuning constants for regression and scale estimation. For Hampel and Krasker regression, k2 is not used. Default value for k1 is 1.345 (for Huber and Mallows method) or 4.2 (for Hampel method).
- maxiter, mytol: maximum number of iterations and tolerance for the algorithm.

The function returns a list with several components, including:

- coef, s: parameter estimates;
- se, V: estimated standard errors and asymptotic variance matrix for the regression coefficients;
- weights, fitted.values, residuals: vector of weights on the residuals, fitted values and (unstandardized) residuals.

The weights returned by the function are given by $\psi_k(r_i/v_i)/(r_i/v_i)$, $i=1,\ldots,n$, where r_i are the standardized residuals and the v_i s are given by the function $v(x_i)$ of Krasker and Welsch (1982) for the Hampel and Krasker estimator, and are 1 for the other methods. They can play an important role for diagnostic purposes, as shown in the following examples.

Example: U.S. Mortality Data

As an example, we consider the US mortality data, already analysed by several authors, including Krasker and Welsch (1982). The data consist of n=60 observations about age-adjusted mortality for a sample of U.S. cities, with several available covariates. The data are contained in the file mortality.txt.

```
> mort <- read.table("mortality.txt", T)
> mort$logSOD <- log(mort$SOD)</pre>
```

For the sake of simplicity, we consider the same subset of covariates already selected by Krasker and Welsch, namely percent nonwhite (NONW), average years of education (EDUC), population per square mile (DENS), precipitation (PREC) and a pollution variable (log(SOD)). The related scatterplots are shown in Figure 20.

> pairs(mort[,c(16,9,6,8,1,17)], panel = "panel.smooth")

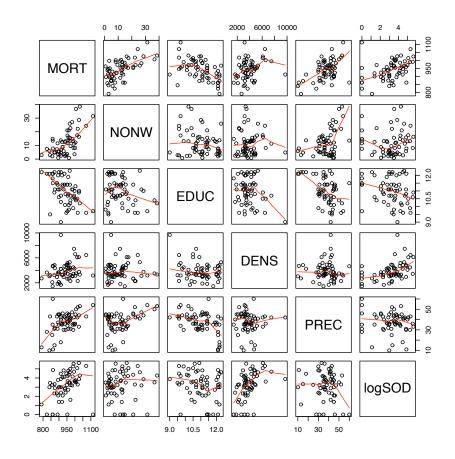


Figure 20: Mortality data: Scatterplots

We start the analysis with the OLS fit

```
> mort.ols <- lm(MORT ~ NONW + EDUC + DENS + PREC + log(SOD), data=mort)
> summary(mort.ols)
....
```

Coefficients:

```
Estimate Std. Error t value Pr(>|t|)
(Intercept) 930.282998
                                      9.675 2.17e-13
                         96.150153
NONW
              3.349968
                          0.588559
                                      5.692 5.29e-07
EDUC
            -13.296076
                          6.969107
                                    -1.908 0.061733
DENS
              0.002833
                          0.003758
                                      0.754 0.454249
PREC
              1.637312
                          0.615956
                                      2.658 0.010315
             13.778244
log(SOD)
                          3.815138
                                      3.611 0.000668
   . . . .
```

Residual standard error: 36.39 on 54 degrees of freedom Multiple R-Squared: 0.6868, Adjusted R-squared: 0.6578

Figure 21 show four diagnostic plots based on the OLS fit. In particular, the two upper panels show a plot of residuals $y_i - \mu_i^O$ versus fitted values μ_i^O , with $\mu_i^O = x_i^T \, \hat{\beta}_{OLS}$, and normal Q-Q plot of standardized residuals, respectively; these are two of the plots routinely provided by the plot.lm function. The two lower panels show a plot of Cook's statistics against $h_{ii}/(1-h_{ii})$ and case plot of Cook statistics. The two latter plots can be obtained, for example, by means of the glm.diag.plots in the library boot. We follow this latter function, and add to the plots the same lines usually drawn by glm.diag.plots to identify extreme values. More precisely, the threshold for Cook statistic is set at 8/(n-2p). Points above this line may be points with high influence on the model. For leverage points, the threshold is at 2p/(n-2p) and points beyond this value have high leverage compared to the variance of the raw residual at that point. From the plots, it is apparent that there are several high-leverage points, which in some cases are associated to large residuals, thus originating influential points.

```
> par(mfrow=c(2,2), pty = "s")
> plot.lm(mort.ols, which = 1:2)
> X.mort <- model.matrix(mort.ols)
> h.mort <- hat(X.mort)
> c.mort <- cooks.distance(mort.ols)
> plot(h.mort / (1 - h.mort), c.mort, xlab = "h/(1-h)", ylab = "Cook statistic")
> abline(h = 8 / (nrow(X.mort) - 2 * mort.ols$rank), lty = 2)
> abline(v = (2 * mort.ols$rank) / (nrow(X.mort) - 2 * mort.ols$rank), lty = 2)
> plot(c.mort,xlab = "Case", ylab = "Cook statistic")
> abline(h = 8 / (nrow(X.mort) - 2 * mort.ols$rank), lty = 2)
```

We start the robust analysis by getting Huber-regression estimates. Note that the Huber estimates provided lm.BI are quite similar to those returned by rlm using Huber Proposal 2 for the scale, although there are some slight differences for standard errors.

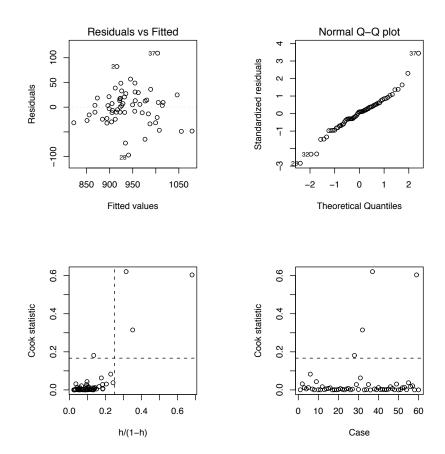


Figure 21: Mortality data: Diagnostic plots for OLS estimates

(Intercept)	930.28300	915.74868	96.15015	82.41696
NONW	3.34997	2.83928	0.58856	0.50450
EDUC	-13.29608	-12.94116	6.96911	5.97370
DENS	0.00283	0.00396	0.00376	0.00322
PREC	1.63731	1.86757	0.61596	0.52798
log(SOD)	13.77824	14.89441	3.81514	3.27022

One of the main use of robust regression is for diagnostic purposes. To this end, we can compare the classical OLS-based diagnostics with the Huber weights. In particular, we compare the Huber weights with $h_{ii}/(1-h_{ii})$, the Cook's statistics and the DFFIT statistic (Belsley et al., 1980), defined as DFFIT= $(y_i - \hat{\mu}_i^O) \sqrt{h_{ii}}/\{s_{(i)} (1-h_{ii})\}$, with $s_{(i)}$ is the estimate of σ after dropping the *i*-th observation. See Figure 22. Although all the points associated with high values of the classical statistics have a Huber weight less then 1, there are also some observations with a low Huber weight which were not identified by the classical diagnostics.

```
> abline(v = 8 / (nrow(X.mort) - 2 * mort.ols$rank), lty = 2)
> df.mort <- dffits(mort.ols)
> plot(df.mort, mort.hub$weights, xlab = "DFFIT", ylab = "Huber weight")
```

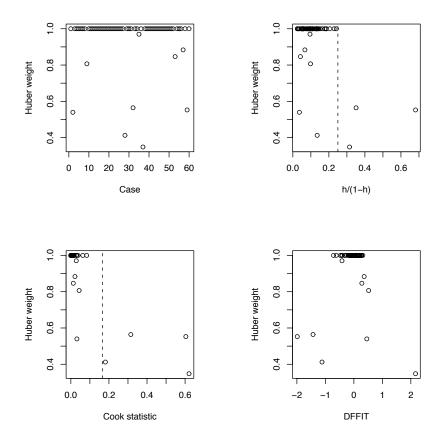


Figure 22: Mortality data: Comparison between OLS-based and Huber-based diagnostics

It is also interesting to look at some residual plots based on the Huber estimates. After having defined the fitted values $\mu_i^H = x_i^T \hat{\beta}_{Huber}$ and the residuals $y_i - \mu_i^H$, we obtain the plot of residuals versus fitted values and a normal Q-Q plot of standardized residuals. They are reported in Figure 23.

We now turn to bounded-influence estimation, and fit both the Mallows and the Hampel and Krasker estimator. We use the same values of the tuning constants selected by Krasker and Welsch (1982), hence setting k1=1.345 and k1=4.2 respectively, and achieving roughly the same amount of weighting in both cases.

mort.mal<- lm.BI(mort.ols\$coef, s.est, X.mort, mort\$MORT, "mallows", 1.345,

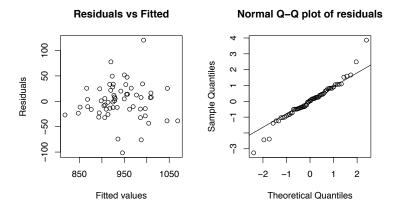


Figure 23: Mortality data: Diagnostic plots for Huber estimates

```
1.5)
mort.hk<- lm.BI(mort.ols$coef, s.est, X.mort, mort$MORT, "hampel", 4.2)
Let us have a look at the different estimates.
> tab.bi <- cbind(mort.ols$coef, mort.mal$coef, mort.hk$coef,
                sqrt(diag(vcov(mort.ols))), mort.mal$se, mort.hk$se)
> colnames(tab.bi) <- c("OLS coef", "MAL coef", "H-K coef", "OLS se",
                        "MAL se", "H-K se")
> print(tab.bi, digits=3)
                      MAL coef
             OLS coef
                                  H-K coef
                                              OLS se
                                                       MAL se
                                                                 H-K se
(Intercept) 930.28300 915.63660 915.40807 96.15015 81.39012 85.35153
NONW
              3.34997
                         2.80715
                                    2.59896
                                             0.58856
                                                      0.49797
                                                                0.51438
EDUC
            -13.29608 -13.17073 -13.68873
                                             6.96911
                                                      5.90093
                                                                6.18970
DENS
              0.00283
                         0.00509
                                   0.00716
                                             0.00376
                                                      0.00319
                                                                0.00341
PREC
              1.63731
                         1.89309
                                   2.01018
                                             0.61596
                                                      0.52120
                                                                0.54165
                        14.35093
                                  13.59010
                                             3.81514
                                                      3.23012
log(SOD)
             13.77824
                                                                3.39482
```

Both the Mallows estimates and the Hampel and Krasker ones seem to deviate from the OLS results, but the direction of the adjustment is different for some coefficients. Standard errors are generally smaller for robust methods, due to smaller estimate of the scale parameter σ . More precisely, the different estimated scales are given by

```
> tab.sigma <- c(s.est, mort.hub$s, mort.mal$s, mort.hk$s)
> names(tab.sigma) <- c("OLS", "HUB", "MAL", "H-K")
> print(tab.sigma, digits=4)
   OLS   HUB   MAL   H-K
34.52   31.17   30.50   29.90
```

It may be useful to compare the weighting action performed by the various methods. To this end, we can compare the weights for those observations where one the method gave a weight smaller than 1.

```
> w.mort <- cbind(mort.hub$weights, mort.mal$weights, mort.hk$weights)
> cond <- apply(w.mort, 1, "<",1)</pre>
> cond <- apply(cond, 2, sum)</pre>
> w.mort[(cond>0),]
        [,1]
                   [,2]
                             [,3]
2 0.5398001 0.5349548 1.0000000
6 1.0000000 1.0000000 0.8925994
9 0.8067073 0.8480886 0.9923542
28 0.4124823 0.4018182 0.3830221
31 1.0000000 1.0000000 0.9504858
32 0.5642053 0.5265649 0.2930613
35 0.9703016 0.9788623 1.0000000
37 0.3482611 0.3453883 0.2206260
53 0.8466948 0.8257080 1.0000000
57 0.8836090 0.8569866 1.0000000
59 0.5524462 0.4915569 0.1865103
```

All the three methods tend to downweight the observations in a similar fashion, but there are some differences.

We now turn to some of the high-breakdown methods introduced in the previous sections. First we compute the MM-estimate using the function rlm

```
> mort.MM<- rlm(MORT ~ NONW + EDUC + DENS + PREC + log(SOD), data=mort,
                method="MM")
> summary(mort.MM, corr=F)
   . . . .
Coefficients:
            Value
                     Std. Error t value
(Intercept) 904.1765 85.6275
                                  10.5594
NONW
              2.5952
                        0.5241
                                   4.9513
EDUC
            -11.9896
                        6.2064
                                  -1.9318
DENS
              0.0025
                        0.0033
                                   0.7337
PREC
              1.8681
                        0.5485
                                   3.4055
```

Another possibility is to use the weighted-likelihood estimating equations approach implemented by the library wle.

5.1923

log(SOD)

17.6414

3.3976

Residual standard error: 29.47 on 54 degrees of freedom

```
(Intercept) 891.369970
                       85.921397
                                   10.374 2.98e-14
NONW
              2.651674
                         0.530454
                                    4.999 6.95e-06
EDUC
            -10.425735
                         6.251666
                                   -1.668 0.10141
DENS
              0.001109
                         0.003260
                                    0.340 0.73513
PREC
              1.781121
                         0.531708
                                    3.350 0.00151
log(SOD)
             18.691913
                         3.500043
                                    5.340 2.08e-06
Residual standard error: 31.18 on 51.86464 degrees of freedom
```

Both the two high-breakdown methods give similar results. A more thorough summary of all the results for this example can be obtained by plotting the Wald statistics $\hat{\beta}_k/\text{se}(\beta_k)$ for the various coefficients, as shown in Figure 24.

Example: Artificial Data

This data set was generated by Hawkins *et al.* (1984) for illustrating some of the merits of a robust technique. The data set consists of n = 75 observations in four dimensions (one response and three explanatory variables). The first 10 observations are bad leverage points, and the next four points are good leverage points (see also Rousseeuw and Leroy, 1987).

An exploratory graphical analysis can be made using the fancy scatterplots provided by the function scatterplot.matrix in the library car (see Figure 25). In this case, for all the variables considered, the presence of the bad and good leverage points is clearly noticeable.

```
> library(wle)
> data(artificial)
> scatterplot.matrix(artificial)
```

We get some useful indications from some plots of residuals versus fitted values, shown in Figure 26.

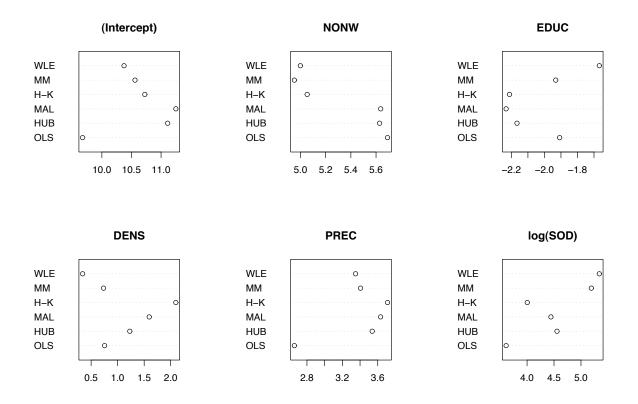


Figure 24: Mortality data: Comparison of Wald statistics

```
(Intercept)
             -0.3934
                          0.4106
                                  -0.958
                                          0.34133
              0.2492
                          0.2580
x1
                                   0.966
                                          0.33731
             -0.3354
x2
                          0.1550
                                  -2.164
                                          0.03380
              0.3808
                                   2.974
хЗ
                          0.1281
                                          0.00402
Residual standard error: 2.249 on 71 degrees of freedom
Multiple R-Squared: 0.6024,
                                 Adjusted R-squared: 0.5856
> par(mfrow=c(1,2), pty="s")
> plot(art.ols$fit, art.ols$res, xlab = "Fitted values", ylab = "Residuals",
       main = "OLS fit")
> art.hub <- lm.BI(art.ols$coef, mean(art.ols$res^2), model.matrix(art.ols),</pre>
                 artificial$y, "huber", 1.345, 1.5)
> art.mal <- lm.BI(art.ols$coef, mean(art.ols$res^2), model.matrix(art.ols),
                 artificial$y, "mallows", 1.345, 1.5)
> plot(art.mal$fit, art.mal$res, xlab = "Fitted values", ylab = "Residuals",
                 main= "Mallows fit")
```

The 14 high-leverage points are clearly noticeable with both OLS and robust estimation, as they form two rather distinct clusters. However, due to the effect of influential observations on the fit, now the role of good and bad leverage points has been totally reversed. This fact is even more apparent for the Mallows estimate. Here only high-breakdown estimation is capable of correctly identify the bad leverage points. For example, let us try the weighted likelihood approach. The summary reveals that wle.lm has found two

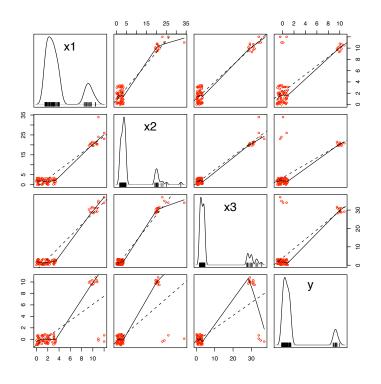


Figure 25: Artificial data: Scatterplots

roots of the estimating equations.

```
> art.wle <- wle.lm(y.artificial ~ x.artificial, boot = 40, num.sol = 3)
Root 1
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)
              -0.94351
                          0.12792 -7.376 3.46e-10
x.artificial1 0.15653
                          0.07809
                                    2.005 0.049112
                          0.07168
x.artificial2 0.18912
                                    2.638 0.010382
                                    3.615 0.000581
x.artificial3
              0.18152
                          0.05021
Residual standard error: 0.6688 on 66.03095 degrees of freedom
Root 2
Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)
              -0.19670
                          0.10419 -1.888
                                             0.064 .
x.artificial1 0.08969
                          0.06655
                                    1.348
                                             0.183
x.artificial2 0.03875
                          0.04076
                                    0.951
                                             0.346
x.artificial3 -0.05298
                          0.03549
                                  -1.493
                                             0.141
```

The residual versus fitted values plots corresponding to the two roots are readily obtained

Residual standard error: 0.5561 on 58.6243 degrees of freedom

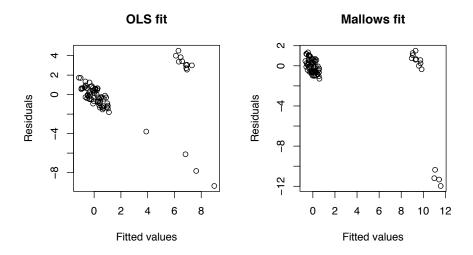


Figure 26: Artificial data: Residuals vs Fitted values

(Figure 27).

```
plot(art.wle$fit[1,], art.wle$res[1,], xlab = "Fitted values",
    ylab = "Residuals", main = "First root")
plot(art.wle$fit[2,], art.wle$res[2,], xlab = "Fitted values",
    ylab = "Residuals", main = "Second root")
```

The two plots are rather different. While the one related to the first root looks quite similar to the one based on Mallows estimate, the second root gives a rather different picture. In particular, it correctly identifies the bad leverage points, and the fitted values are all around 0, as it should be due to the way the data were generated. The same happens also with the MM-estimator. In fact, the MM-estimates obtained with rlm are very close to the second wle.lm root, while the bounded-influence estimates are close to the first one.

```
> art.MM <- rlm(y ~ x1 + x2 + x3, artificial, method="MM")
> tab.coef <- cbind(art.ols$coef, art.mal$coef, art.hk$coef, art.MM$coef,
                    art.wle$coef[1,], art.wle$coef[2,])
> colnames(tab.coef) <- c("OLS", "MAL", "H-K", "MM", "WLE-1", "WLE-2")</pre>
> print(tab.coef, digits=3)
                OLS
                        MAL
                               H-K
                                         MM
                                             WLE-1
                                                      WLE-2
(Intercept) -0.393 -0.8293 -0.877 -0.1994 -0.944 -0.1967
             0.249
                     0.1714
                             0.163
                                     0.0960
                                             0.157
x1
                                                     0.0897
x2
            -0.335
                     0.0674
                             0.133
                                     0.0405
                                             0.189
                                                     0.0387
хЗ
             0.381
                     0.2377
                             0.204 - 0.0565
                                             0.182 - 0.0530
```

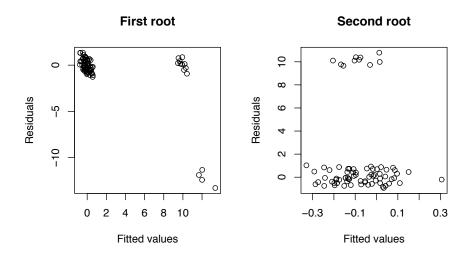


Figure 27: Artificial data: Residuals vs Fitted values for weighted likelihood estimates

```
> tab.se <- cbind(sqrt(diag(vcov(art.ols))), art.mal$se, art.hk$se,</pre>
                 sqrt(diag(vcov(art.MM))), art.wle$sta[1,],art.wle$sta[2,])
> colnames(tab.se) <- c("OLS", "MAL", "H-K", "MM", "WLE-1", "WLE-2")</pre>
> print(tab.se, digits=3)
               OLS
                        MAL
                                H-K
                                         MM
                                               WLE-1
                                                         WLE-2
(Intercept) 0.411
                    0.1526
                             0.1528
                                      0.1154
                                               0.1279
                                                       0.1042
             0.258
                    0.0959
                             0.0952
                                      0.0725
                                               0.0781
x1
                                                        0.0666
x2
             0.155
                    0.0585
                             0.0680
                                      0.0436
                                               0.0717
                                                        0.0408
             0.128
хЗ
                    0.0479
                             0.0518
                                      0.0360
                                               0.0502
                                                       0.0355
```

To wind up, this example show that sometimes bounded-influence estimation can give rather misleading results. Although this is an artificially extreme example, it suggests the important role played by high-breakdown estimation.

4 Bounded-influence estimation in logistic regression

There are several methods developed for logistic regression, like the Optimal Bias-Robust Estimator (OBRE) of Künsch *et al.* (1989), the Bianco and Yohai estimator (1996) or the Mallows-type estimator of Cantoni and Ronchetti (2001). Here we focus in particular on the latter two proposals, noticing however that the ROBETH software (Marazzi, 1993) includes also several FORTRAN routines for the computation of the OBRE, some of which have been (partially) ported to R.

4.1 Mallows-type estimation

The Mallows-type estimator of Cantoni and Ronchetti (2001) is defined for the class of generalized linear models. They defined some estimating equations which nicely extend the likelihood equations. Such estimating equations can be written as

$$g(\beta; y) = \sum_{i=1}^{n} w(x_i) \frac{\{\psi_k(r_i) - a(\mu_i)\}}{V_i(\mu_i)^{1/2}} \frac{\partial \mu_i}{\partial \beta}^T = 0,$$
 (8)

where $V(\mu_i)$ is the variance function, $r_i = (y_i - \mu_i)/\sqrt{V_i}$ the Pearson residuals and ψ_k the Huber function introduced in section 2.3. The non-random values $a(\mu_i)$ are defined as $a(\mu_i) = E[\psi_k(R_i)|x_i]$, and ensure the conditional Fisher-consistency of the estimating equations. For binomial or Poisson response the computation of $a(\mu_i)$ is not difficult, as reported in Cantoni and Ronchetti (2001). From general theory of M-estimation it follows that the estimator $\hat{\beta}_M$ defined as the solution of the equations $g(\beta;Y) = 0$ has bounded influence function, as the effect of outlying values in the response is bounded by a finite value of the tuning constant k and the effect of outlying values in the covariates is bounded by a suitable choice of the weights $w(x_i)$ (Cantoni and Ronchetti, 2001). Note that when $k \to \infty$ and $w(x_i) = 1$, then $a(\mu_i) = 0$ and $g(\beta; y)$ becomes the score function, hence the Maximum Likelihood Estimator (MLE) is a special case of $\hat{\beta}_M$.

An important special case of (8) is obtained with normal homoscedastic data and identity link function, for which $V(\mu_i) = \sigma^2$. The resulting model belong to the GLM class for a fixed value of the scale parameter σ . In this case, $\hat{\beta}_M$ is a Mallows estimate for linear regression, becoming the Huber estimate for $w(x_i) = 1$.

Some S-PLUS functions for the solution of (8) are available (Cantoni 2004), which can be used in R with some minor changes. A simple, direct implementation of the method is actually not difficult, and we propose it in the following just for illustrative purposes.

The first step is to write a function for the computation of the estimating function $g(\beta; y)$. For the particular case of logistic regression this can be done by considering that $\mu_i = F(x_i^T \beta)$, with $F(u) = \exp(u)/(1 + \exp(u))$, $V_i(\mu_i) = \mu_i (1 - \mu_i) = V_i$ and

$$a(\mu_i) = \psi_k \left((1 - \mu_i) / \sqrt{V_i} \right) \mu_i + \psi_k \left(-\mu_i / \sqrt{V_i} \right) (1 - \mu_i).$$

A simple function for computing $g(\beta; y)$ is readily written

```
g.fun <- function(beta, X, y, offset, w.x, k1)
    {
        mu<- plogis(X %*% beta + offset)
        V <- mu * (1 - mu)
        r <- (y - mu) / sqrt(V)
        a <- psiHub((1 - mu) / sqrt(V), k1) * mu + psiHub(-mu / sqrt(V), k1)
            * ( 1 - mu)
        colSums(X * as.vector(1 / sqrt(V) * w.x * (psiHub(r.stand, k1) - a) * V))
    }</pre>
```

where the function psiHub(x, k) = psi.huber(x, k) * x and k1 is the k constant. The solution of the equation $g(\beta; y) = 0$ can be obtained in several ways, but the simplest possibility is to implement a Newton-Rapshon algorithm, obtaining the Jacobian of $g(\beta; y)$

by numerical differentiation. In our function logit.BI we use the simple numerical routine num.deriv from the sn library. Hence, the updating of the beta coefficients is essentially performed by the commands

The logit.BI function has the following usage

logit.BI(beta.in, X, y, k1, offset, w.x, maxiter, mytol)

and the various arguments are:

- beta.in: initial value for β ;
- X, y: design matrix, response vector;
- k1: tuning constant, default is 1.2.
- offset: offset (default is a vector of 0s);
- w.x: x-based prior weights for Mallows estimation (default is a vector of 1s);
- maxiter, mytol: maximum number of iterations and tolerance for the algorithm.

The function returns a list with several components, including:

- coef: parameter estimates;
- se, V: estimated standard errors and asymptotic variance matrix for the regression coefficients;
- weights: vector of weights on the residuals.

4.2 The Bianco and Yohai estimator

An alternative method is given by the Bianco and Yohai estimator (Bianco and Yohai, 1996), defined as

$$\hat{\beta}_{BY} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} \left\{ \rho_k(d(x_i^T \beta; y_i)) + C(x_i^T \beta) \right\}$$
(9)

where $d(u; y) = -y \log F(u) - (1 - y) \log\{(1 - u)\}$, ρ_k is a bounded function and $C(x_i^T \beta)$ is a bias correction term. Bianco and Yohai (1996) proposed the following ρ function,

$$\rho_k(x) = \begin{cases} x - \frac{x^2}{2k} & \text{if } x \le k \\ \frac{k}{2} & \text{otherwise} \end{cases}$$

but stressed that other choices are possible. Croux and Haesbroeck (2003) extend the Bianco and Yohai estimator by including weights for downweighting high-leverage points, thus defining a bounded-influence estimator

$$\hat{\beta}_{WBY} = \underset{\beta}{\operatorname{argmin}} \sum_{i=1}^{n} w(x_i) \left\{ \rho_k(d(x_i^T \beta; y_i)) + C(x_i^T \beta) \right\}. \tag{10}$$

They suggested a decreasing function of robust Mahalanobis distances for the weights $w(x_i)$, where the distances are computed using the Minimum Covariance Determinant (MCD) estimator (see Rousseeuw and Leroy, 1987). More precisely, $w(x_i)$ are obtained as follows. The MCD method seeks h points whose covariance has minimum determinant, and Croux and Haesbroeck (2003) suggest h = 3/4 n, giving a 25% breakdown point estimator. The method is implemented by the function cov.rob (or cov.mcd, which is a convenient wrapper) in the MASS library. If X is the design matrix, the robust estimate of multivariate location and scale are obtained by

```
> hp <- floor(nrow(X) * 0.75) + 1
> mcdx <- cov.rob(X, quan = hp, method = "mcd")
```

Once the robust estimate of location and scale have been computed, we can obtain the robust distances RD_i . Finally the weights are defined as $w(x_i) = W(RD_i)$, where W is the weight function $W(t) = I_{\{t^2 \leq \chi^2_{p,0.975}\}}$, with I_A denoting the indicator function of the set A.

```
> rdx <- sqrt(mahalanobis(X, center = mcdx$center, cov = mcdx$cov))
> vc <- sqrt(qchisq(0.975, ncol(X)))
> wx <- as.numeric(rdx <= vc)</pre>
```

Notice that the same weights could also be used in (8). Croux and Haesbroeck (2003) have implemented both the Bianco and Yohai estimator and their weighted version in some public-domain S-PLUS functions, which can be also used in R with a few changes. The two functions are BYlogreg and WBYlogreg, respectively, which we slightly modified in order to deal with dummy covariates in the design matrix. The arguments of the function BYlogreg are

- x0, y: design matrix (not including the intercept), response vector;
- x0cont: design matrix to use for computing the weighted MLE (if initwml=T)
- initwml: logical value for selecting one of the two possible methods for computing the initial value: if initwml=T a weighted MLE, otherwise the classical MLE.
- const: tuning constant, default is 0.5.
- kmax, maxhalf: maximum number of iterations and max number of step-halving. the algorithm.

The functions returns a list, including the components coef and sterror for parameter estimates and standard errors. The function WBYlogreg has exactly the same arguments, with the exception of initwml as the weighted MLE is always used as starting point.

Example: Food Stamp Data

This is a classical example of robust statistics, see for example Künsch et al. (1989). The food stamp data set, of sample size 150, consists of a binary response variable participation in the US Food Stamp Program. The covariates included in the model are tenancy (Tenancy), supplemental income (SupInc), and log(monthly income + 1) (log(Inc+1)). The data are contained in the file foodstamp.txt. Let us start the analysis by getting the MLE.

```
> food <- read.table("foodstamp.txt", T)</pre>
> food.glm <- glm(y ~ Tenancy + SupInc + log(Inc+1), binomial, food)</pre>
> summary(food.glm)
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept)
                0.9264
                            1.6229
                                     0.571
                                             0.56813
Tenancy
               -1.8502
                            0.5347
                                    -3.460
                                             0.00054
SupInc
                0.8961
                            0.5009
                                     1.789
                                             0.07365
log(Inc + 1)
              -0.3328
                            0.2729
                                    -1.219
                                             0.22280
```

The only significant coefficient seems to be that of the variable tenancy. A look at some diagnostic plots is quite useful (see Figure 28).

```
> glm.diag.plots(food.glm)
```

It is clear that there is an observation with totally anomalous covariate values, which has a very strong effect on the fit. In fact, observation 5 is the only one with a zero value for the monthly income.

```
> food$Inc
[1] 271 287 714 521 0 518 458 1266 350 168 235 450 683 519
...
```

Any kind of robust method suitable for this data set must clearly bound the influence of the design points. We get both the weights based on the hat matrix (used in their examples by Cantoni and Ronchetti, 2001), and those based on the robust estimation of location and scale. Following the suggestions in the code by Croux and Haesbroeck, in the latter case we compute the weights using only the continuous covariate.

The two sets of weights present some differences, and the hat matrix-based ones provide a smaller degree of weighting

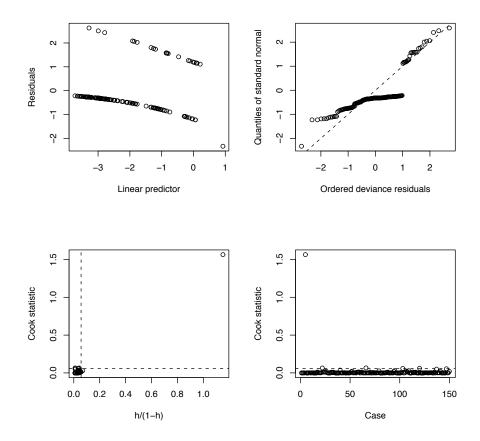


Figure 28: Foodstamp data: diagnostic plots for maximum likelihood estimates

```
> mean(w.rob.food)
[1] 0.94
> mean(w.hat.food)
[1] 0.9864798
```

log(Inc + 1) -0.333

However, both types of weight reach their minimum value at the observation 5. We now compute the robust estimates $\hat{\beta}_M$, including a Huber-type version without any prior x-weights. We start the algorithm from the MLE and, following Cantoni and Ronchetti (2001), we set k = 1.2.

```
> food.hub <- logit.BI(food.glm$coef, X.food, food$y, 1.2,)</pre>
> food.mal <- logit.BI(food.glm$coef, X.food, food$y, 1.2, w.x = w.hat.food)</pre>
> food.mal.wrd <- logit.BI(food.glm$coef, X.food, food$y, 1.2, w.x = w.rob.food)
> tab.coef <- (cbind(food.glm$coef, food.hub$coef, food.mal$coef, food.mal.wrd$coef))
> colnames(tab.coef)<- c("MLE", "HUB", "MAL-HAT", "MAL-ROB")</pre>
> print(tab.coef, digits = 3)
                 MLE
                          HUB
                                  MAL-HAT
                                             MAL-ROB
(Intercept)
              0.926
                                   6.687
                                              8.065
                        0.710
Tenancy
             -1.850
                       -1.778
                                  -1.855
                                             -1.784
SupInc
               0.896
                        0.802
                                   0.606
                                              0.586
```

-1.540

-1.298

-0.287

The standard errors are as follows.

```
> tab.se <- cbind(sqrt(diag(vcov(food.glm))), food.hub$se, food.mal$se,
                  food.mal.wrd$se)
> colnames(tab.se) <- c("MLE", "HUB", "MAL-HAT", "MAL-ROB")</pre>
> print(tab.se, digits = 3)
              MLE
                       HUB
                              MAL-HAT
                                         MAL-ROB
(Intercept)
             1.623
                      1.636
                                3.039
                                          3.328
Tenancy
             0.535
                      0.527
                                0.581
                                          0.588
SupInc
             0.501
                      0.516
                                0.553
                                          0.561
log(Inc + 1) 0.273
                      0.276
                                0.519
                                          0.572
```

We notice that the Mallows estimates are quite different from both the MLE and the Huber estimates. The estimated weights for the residual $\psi_c(r_i)/r_i$, where r_i is the Pearson residual, provide a explanation for this fact.

```
> wei.food <- cbind(food.hub$weights, food.mal$weights, food.mal.wrob$weights)
> cond <- apply(wei.food, 1, "<", 1)</pre>
> cond <- apply(cond, 2, sum)</pre>
> wei.food[(cond>0),]
       [,1]
                  [,2]
                             [,3]
    0.8412010 0.04237215 0.02127919
5
22 0.4953700 0.60685048 0.65761723
   1.0000000 0.97042523 0.93395722
26 0.8020679 1.00000000 1.00000000
40 0.6464152 0.41587812 0.36433034
   1.0000000 0.96380099 0.92400623
51
52 0.8144845 1.00000000 1.00000000
59 1.0000000 0.97674194 0.94117456
66 0.2543750 0.13502255 0.11816794
79 0.6857541 0.54321273 0.50018522
94 0.7980593 1.00000000 1.00000000
95 0.6679639 0.48234377 0.43440327
103 0.4653931 0.45762357 0.47048220
107 0.8014854 1.00000000 1.00000000
109 0.9518519 0.52815274 0.45262133
120 0.4756079 0.50482509 0.52859808
137 0.2884602 0.23841016 0.23198605
141 0.7969428 1.00000000 1.00000000
147 0.3144637 0.35221333 0.36859260
150 0.7920675 1.00000000 1.00000000
```

The weights based on the Huber-type estimates are quite different from the Mallowstype ones. In particular, Huber-type regression does not downweight enough observation 5. Things are different if we choose another starting point for the algorithm. A sensible choice could be to start from a weighted MLE, obtained by selecting only the observations for which the robust distance weights $W(RD_i)$ are equal to 1.

```
> food.glm.wml <- glm(y ~ Tenancy + SupInc + log(Inc+1), binomial, food,
```

```
subset = (w.rob.food==1))
```

Coefficients:

```
Estimate Std. Error z value Pr(>|z|)
(Intercept) 5.6408 2.7665 2.039 0.041452
Tenancy -1.7749 0.5352 -3.317 0.000911
SupInc 0.6491 0.5181 1.253 0.210238
log(Inc + 1) -1.1123 0.4685 -2.374 0.017589
```

If we recompute the algorithm form the weighted MLE, the Huber-type estimates are close to the Mallows one, and the weight given to observation 5 is now much smaller.

A similar result is obtained with the Bianco and Yohai estimator. If we call the BYlogreg with the argument initwml = F, the MLE is used as starting point.

The results are not much different from the MLE. A better option is to use the weighted MLE as starting point. This requires as a further argument the matrix used to compute the weights.

The results are similar to the weighted version of the Bianco and Yohai estimator.

```
> food.WBY <- WBYlogreg(X.food[,-1], food$y, as.matrix(X.food[,-(1:3)]) )
>food.WBY
```

\$coef (Intercept) subx01 subx02 subx03 [1,] 5.824949 -1.832782 0.6703187 -1.148582 \$sterror [1] 3.3923786 0.5822091 0.5220386 0.5906120

In order to compare all the various estimates, we follow the approach of Kordzakhia et al. (2001). They proposed to compare the various estimates using a goodness-of-fit discrepancy, the chi-square statistic based on the arcsin transformation

$$X_{arc}^2 = \sum_{i=1}^n 4 \left(\arcsin \sqrt{y_i} - \arcsin \sqrt{\hat{\pi}_i} \right) ,$$

where $\sqrt{\hat{\pi}_i}$ are the fitted probabilities. The values of the statistic for the various estimates show again the importance of using x-weights for this data set.

```
> X2.arc <- function(y, mu) 4 * sum((asin(sqrt(y)) - asin(sqrt(mu)))^2)</pre>
> X2.arc(food$y, plogis(X.food %*% food.glm$coef))
[1] 173.5109
> X2.arc(food$y, plogis(X.food %*% food.glm.wml$coef))
[1] 172.3801
> X2.arc(food$y, plogis(X.food %*% food.hub$coef))
[1] 175.4812
> X2.arc(food$y, plogis(X.food %*% food.hub.wml$coef))
[1] 170.2295
> X2.arc(food$y, plogis(X.food %*% food.mal$coef))
[1] 170.0075
> X2.arc(food$y, plogis(X.food %*% food.mal.wrob$coef))
[1] 169.8280
> X2.arc(food$y, plogis(X.food %*% t(food.BY$coef)))
[1] 174.8348
> X2.arc(food$y, plogis(X.food %*% t(food.BY.wml$coef)))
[1] 173.0532
> X2.arc(food$y, plogis(X.food %*% t(food.WBY$coef)))
[1] 171.0866
Finally, the S-PLUS code of Cantoni (2004) gives the following results for the Mallows
estimator using the x-weights (1-h_{ii})^{1/2} (here we used our own port of the code)
> food.can <- glm.rob(X.food[,-1], food$y, chuber = 1.2,</pre>
                     weights.on.x = T, ni = rep(1,nrow(X.food)))
```

Tenancy SupInc log(Inc + 1) 3.0756946 0.5946090 0.5592972 0.5264943

The coefficients and standard erros are essentially the same as those obtained with our function and stored in food.mal. The code by Cantoni (2004), however, is more reliable and has a broad range of functions, including some functions for testing based on quasi deviances (Cantoni and Ronchetti, 2004).

Example: Vaso-constriction Data

We consider an example from Finney (1947), already analysed in Künsch *et al.* (1989). These data consist of 39 observations on three variables: the occurrence of vaso-constriction in the skin of the digits, and the rate and volume of air inspired. The model considered by Künsch *et al.* (1989) regresses the occurrence of vaso-constriction on the logarithm of air rate and volume. The data are in the file vaso.txt.

```
vaso <- read.table("vaso.txt", T)
vaso$lVol <- log(vaso$Vol)
vaso$lRate <- log(vaso$Rate)
vaso$Resp <- 1 - (as.numeric(vaso$Resp) - 1)
vaso$y <- vaso$Resp</pre>
```

A plot of the data show some difference in the covariates for the two groups of patients with different response values.

```
> plot(vaso$Vol,vaso$Rate,type = "n", xlab = "Volume", ylab = "Rate")
> points(vaso$Vol[vaso$y==0], vaso$Rate[vaso$y==0], col = 1, pch = 16)
> points(vaso$Vol[vaso$y==1], vaso$Rate[vaso$y==1], col = 2, pch = 16)
> legend(2.5, 3.0, c("y=0 ", "y=1 "), fill = c(1, 2), text.col = c("black", "red"))
```

Standard diagnostic plots based on the maximum likelihood fit show that there two quite influential observations (4 and 18):

```
> vaso.glm <- glm(Resp ~ 1Vol + 1Rate,family = binomial, data = vaso)
> summary(vaso.glm)
....
```

Coefficients:

If we re-estimate the model after removing these two observations, we can observe that their effect on the model estimate is huge.

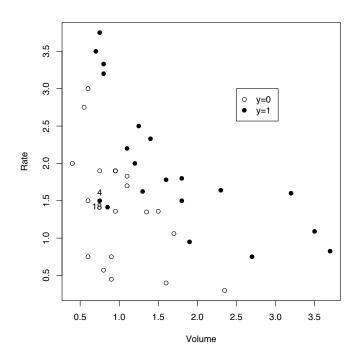


Figure 29: Vaso-constriction data: covariate scatterplot

lRate 31.94 17.76 1.798 0.0721

There is a dramatic increase in both coefficient values and standard errors. Actually, without the two observations we are in situation of quasi-complete separation (Albert and Anderson, 1984), with little overlap between observations with $y_i = 0$ and $y_i = 1$. The model is nearly undeterminated. This is readily confirmed by Mallows (or Huber) estimation, which assigns low weight to both observations 4 and 18, and provides results similar to those obtained with MLE after removing the influential points.

The same happens with the both versions of the Bianco and Yohai estimator. Once again, the near-indeterminacy is reflected by large increases of coefficients and standard errors.

```
> vaso.WBY<- WBYlogreg(X.vaso[,-1], vaso$y)
> vaso.WBY
```

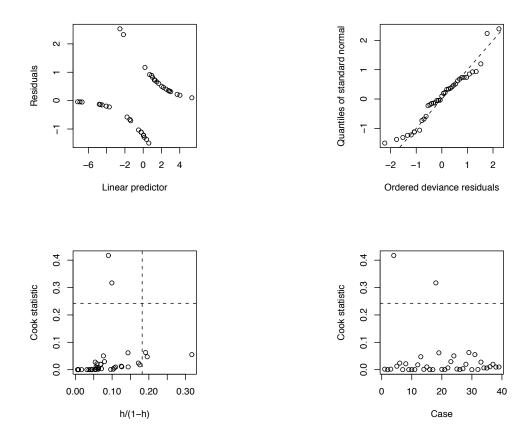


Figure 30: Vaso-constriction data: diagnostic plots for maximum likelihood estimates

\$coef (Intercept) subx01 subx02 [1,] -6.859868 10.74855 9.3733 \$sterror [1] 10.07252 15.34863 12.80866

Notice, however, that alternative methods may give different results, like in the case of the OBRE (see Künsch *et al.*, 1989).

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