# Robust Regression

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## Motivation

- Least squares regression is sensitive to violation of assumptions
- Individual high-leverage points can substantially influence inference
- Specifically, least squares is vulnerable when error distribution is heavy-tailed
- We have considered one possible remedy: detect influential observations
- This has several drawbacks:
  - We cannot realistically expect users to always screen the data
  - The binary decision to keep/reject suspicious observations seems extreme; we may instead prefer to downweight such observations
  - Finding outliers may be difficult in multivariate or structured data
  - Rejecting outliers changes the sampling distribution of estimates; we should but usually do not make adjustments.
- Another alternative is to consider procedures that systematically guard against outliers

#### Motivation: Location and scale

• A more familiar example before considering the regression problem:

$$X_1,\ldots,X_n \sim N(\mu,\sigma^2)$$

(x <- morm(10, mean = 5, sd = 3))

- [1] 4.2967261 0.8741864 7.7031483 -0.0853126 2.5003953 5.6141429 8.6149780 11.0482167 -1.9215526
  - Want to estimate location  $\mu$  (as well as scale  $\sigma$ )
  - Common estimators of location  $\mu$ :

Mean	mean(x)	3.8344398
Median	median(x)	3.3985607
Trimmed mean	mean(x, trim = 0.25)	3.4838811

## Robust estimation of location

- How do these behave when data is "contaminated"?
- We know that
  - Mean can be changed by an arbitrary amount by changing a single observation
  - Median can be changed arbitrarily only by changing more than 50% observations

- But there is a cost: median is less "efficient"!

• Let us try to make these ideas formal

#### **Relative efficiency**

- Consider two estimators  $T_1$  and  $T_2$
- Define the relative efficiency of  $T_1$  w.r.t.  $T_2$  (for a given underlying distribution) as

$$RE(T_1; T_2) = \frac{V(T_2)}{V(T_1)}$$

- For biased estimators, variance could be replaced by MSE
- $T_2$  is usually taken to be the optimal estimator, if one is available
- What are relative efficiencies of median and trimmed mean?
- Instead of trying to obtain variances theoretically (which is often difficult), we could use simulation to get a rough idea

```
sampling.variance <- function(estimator, rfun, n, NREP = 10000)
{
    var(replicate(NREP, estimator(rfun(n))))
}
trim.mean <- function(x) mean(x, trim = 0.25)
rdist <- function(n) rnorm(n, mean = 5, sd = 3)
var.mean <- sampling.variance(mean, rdist, n = 10)
var.median <- sampling.variance(median, rdist, n = 10)
var.tmean <- sampling.variance(trim.mean, rdist, n = 10)
round(100 * var.mean / var.median)
[1] 74
round(100 * var.mean / var.tmean)
[1] 91</pre>
```

## Asymptotic relative efficiency

 $ARE(T_1;T_2)$  is the limiting value of relative efficiency as  $n \to \infty$ 

```
rdist <- function(n) rnorm(n, mean = 5, sd = 3)
var.mean <- sampling.variance(mean, rdist, n = 5000)
var.median <- sampling.variance(median, rdist, n = 5000)
var.tmean <- sampling.variance(trim.mean, rdist, n = 5000)
round(100 * var.mean / var.median)
[1] 63</pre>
```

round(100 \* var.mean / var.tmean)

[1] 84

- For comparison, the exact ARE of the median is  $\frac{2}{\pi} = 63.6\%$
- This is when the data comes from a normal distribution

#### Relative efficiency for heavier tails

• Suppose errors are instead from t with 5 degrees of freedom

```
rdist <- function(n) 5 + 3 * rt(n, df = 5)
var.mean <- sampling.variance(mean, rdist, n = 5000)
var.median <- sampling.variance(median, rdist, n = 5000)
var.tmean <- sampling.variance(trim.mean, rdist, n = 5000)
round(100 * var.mean / var.median)
[1] 96
round(100 * var.mean / var.tmean)
[1] 121
```

#### Winsorized trimmed mean

• Similar to trimmed mean, but replaces trimmed observations by nearest untrimmed observation

```
win.mean <- function(x, trim = 0.25)
{
    q <- quantile(x, c(trim, 1-trim))</pre>
    x[x < q[1]] <- q[1]
    x[x > q[2]] <- q[2]
    mean(x)
}
rdist <- function(n) rnorm(n, mean = 5, sd = 3) # normal</pre>
var.mean <- sampling.variance(mean, rdist, n = 5000)</pre>
var.win.mean <- sampling.variance(win.mean, rdist, n = 5000)</pre>
round(100 * var.mean / var.win.mean)
[1] 91
rdist <- function(n) 5 + 3 * rt(n, df = 5) # t_{-5}
var.mean <- sampling.variance(mean, rdist, n = 5000)</pre>
var.win.mean <- sampling.variance(win.mean, rdist, n = 5000)</pre>
round(100 * var.mean / var.win.mean)
[1] 117
```

#### Relative efficiency for contamination

- Another "departure" model: contamination
- Suppose data is a mixture of  $N(\mu, \sigma^2)$  with probability  $1 \epsilon$  and  $N(\mu, 9\sigma^2)$  with probability  $\epsilon$

## Sensitivity / influence function

- How much does changing one observation change the estimate T?
- This is measured by the empirical influence function or sensitivity curve

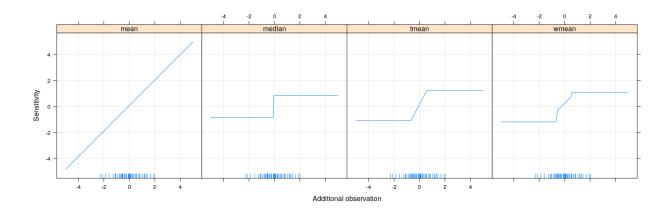
$$SC(x; x_1, \dots, x_{n-1}, T) = \frac{T(x_1, \dots, x_{n-1}, x) - T(x_1, \dots, x_{n-1})}{1/n}$$

- We are usually interested in limiting behaviour as  $n \to \infty$
- The population version, independent of the sample  $x_1, \ldots, x_{n-1}$ , is known as the *influence function*

$$IF(x; F, T) = \lim_{\epsilon \to 0} \frac{T((1 - \epsilon)F + \epsilon \delta_x) - T(F)}{\epsilon}$$

- Here  $\delta_x$  is a point mass at x
- How does mean(c(x, xnew)) change as function of xnew?
- How do other estimates change?

```
n <- 50
x \leftarrow rnorm(n, mean = 0, sd = 1)
summary(x)
   Min. 1st Qu. Median
                               Mean 3rd Qu.
                                                 Max.
-2.28099 -0.61800 -0.06070 -0.06727 0.51522 2.01596
xx <- seq(-5, 5, 0.01)
sensitivity <-
   data.frame(xx = xx,
               mean = n * (sapply(xx, function(xnew) mean(c(x, xnew))) - mean(x)),
               median = n * (sapply(xx, function(xnew) median(c(x, xnew))) - median(x)),
               tmean = n * (sapply(xx, function(xnew) trim.mean(c(x, xnew))) - trim.mean(x)),
               wmean = n * (sapply(xx, function(xnew) win.mean(c(x, xnew))) - win.mean(x)))
xyplot(mean + median + tmean + wmean ~ xx, sensitivity, type = "1", outer = TRUE,
       xlab = "Additional observation", ylab = "Sensitivity", grid = TRUE) +
   layer(panel.rug(x = .GlobalEnv$x))
```



#### Breakdown point

- Defined as the proportion of the sample size that must be perturbed to make the estimate unbounded
- 50% is the best we can hope for
- For location, mean has 0% breakdown point (one out of n), median has 50%.

## Estimators of scale

- We can similarly consider estimators of scale  $\sigma$
- Common estimators:
  - Sample standard deviation (sd in R)
  - Mean absolute deviation from mean
  - Median absolute deviation (MAD) from median (mad in R)
  - Inter-quartile range (IQR in R)
- May need scaling for normal distribution:

```
T1 <- sd
T2 <- function(x, ...) mean(abs(x - mean(x))) / sqrt(2/pi)
T3 <- function(x, ...) median(abs(x - median(x))) / sqrt(qchisq(0.5, df = 1))
T4 <- function(x, ...) IQR(x) / diff(qnorm(c(0.25, 0.75)))</pre>
```

#### Relative efficiency for estimators of scale

```
rdist <- function(n) rnorm(n, mean = 5, sd = ifelse(runif(n) < 0.01, 3, 1)) # 1% Contamination
var.T1 <- sampling.variance(T1, rdist, n = 5000)</pre>
```

```
var.T2 <- sampling.variance(T2, rdist, n = 5000)
var.T3 <- sampling.variance(T3, rdist, n = 5000)
var.T4 <- sampling.variance(T4, rdist, n = 5000)
round(100 * var.T1 / c(mean.abs.dev = var.T2, median.abs.dev = var.T3, iqr = var.T4))
mean.abs.dev median.abs.dev iqr
152 70 70</pre>
```

#### **M**-estimators

• Most common location estimators can be expressed as M-estimators (MLE-like)

$$T(x_1, \dots, x_n) = \arg\min_{\theta} \sum_{i=1}^n \rho(x_i, \theta)$$

- For MLE,  $\rho(x_i, \theta)$  is the negative log-density, but  $\rho$  need not correspond to a likelihood
- If  $\psi(x_i, \theta) = \frac{d}{d\theta} \rho(x_i, \theta)$  exists, then T is the solution to the score equation

$$\sum_{i=1}^{n} \psi(x_i, \theta) = 0$$

- We usually consider loss functions of the form  $\rho(x-\theta)$
- Corresponding  $\psi$  function is  $\psi(x \theta) = \rho'(x \theta)$  (disregarding change in sign)
- This easily generalizes to vector parameters
- Mean

$$\rho(x-\theta) = (x-\theta)^2, \quad \psi(x-\theta) = 2(x-\theta)$$

• Median (ignoring non-differentiability of |x| at 0)

$$\rho(x-\theta) = |x-\theta|, \quad \psi(x-\theta) = \operatorname{sign}(x-\theta)$$

• Trimmed mean (for some c, ignoring dependence of c on the data)

$$\rho(x-\theta) = \begin{cases} (x-\theta)^2 & |x-\theta| \le c\\ c^2 & \text{otherwise} \end{cases}$$
$$\psi(x-\theta) = \begin{cases} 2(x-\theta) & |x-\theta| \le c\\ 0 & \text{otherwise} \end{cases}$$

• Huber loss (similar to Winsorized trimmed mean)

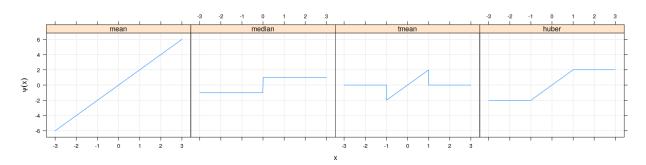
$$\rho(x-\theta) = \begin{cases} (x-\theta)^2 & |x-\theta| \le c\\ c(2|x-\theta|-c) & \text{otherwise} \end{cases}$$
$$\begin{pmatrix} -2c & x-\theta < -c \end{cases}$$

$$\psi(x-\theta) = \begin{cases} 2(x-\theta) & |x-\theta| \le c\\ 2c & x-\theta > c \end{cases}$$

- Can be thought of compromise between mean (squared error) and median (absolute error)
- Estimator reduces to mean as  $c \to \infty$ , median as  $c \to 0$
- $\rho$  is differentiable everywhere
- Exercise: What do plots of  $\rho$  and  $\psi$  look like?

#### Influence function revisited

```
xx <- seq(-3, 3, 0.01)
sensitivity <-
    data.frame(xx = xx,
        mean = 2 * xx,
        median = sign(xx),
        tmean = ifelse(abs(xx) < 1, 2 * xx, 0),
        huber = ifelse(abs(xx) < 1, 2 * xx, 2 * sign(xx)))
xyplot(mean + median + tmean + huber ~ xx, sensitivity, type = "1", outer = TRUE,
        xlab = "x", ylab = expression(psi(x)), grid = TRUE)</pre>
```



• Turns out that the corresponding influence functions have the same shape (but will not discuss why)

## M-estimation: general approach for location

- Choose function  $\psi(x-\theta)$
- Find T by solving (for  $\theta$ )

$$\sum_{i=1}^{n} \psi(x_i - \theta) = 0$$

• We can rewrite this as

$$\sum_{i=1}^{n} \frac{\psi(x_i - \theta)}{(x_i - \theta)} (x_i - \theta) = 0$$

- This suggests an iterative approach using weighted least squares in each step:
  - 1. Start with initial estimate  $\hat{\theta}$
  - 2. Obtain current weights  $w_i = \frac{\psi(x_i \hat{\theta})}{(x_i \hat{\theta})}$
  - 3. Obtain new estimate of  $\theta$  by solving  $\sum_i w_i(x_i \theta) = 0 \implies \hat{\theta} = \sum_i w_i x_i / \sum_i w_i$
- Of course, a black-box numerical optimizer (e.g., optim()) can also be used instead

## Common robust loss function derivatives

- Absolute deviation  $\psi(x) = \operatorname{sign}(x)$
- Huber (same as Winsorized trimmed mean)

$$\psi(x) = \begin{cases} -c & x < c \\ x & |x| \le c \\ c & x > c \end{cases}$$

• Trimmed mean

$$\psi(x) = \begin{cases} x & |x| \le c \\ 0 & \text{otherwise} \end{cases}$$

• Tukey bisquare

$$\psi(x) = x \left[ 1 - (x/R)^2 \right]_+^2 \quad \text{for } \rho(x) = \begin{cases} R^2 \left[ 1 - (1 - (x/R)^2) \right]^3 & |x| \le R \\ R^2 & \text{otherwise} \end{cases}$$

• For the last three, choice of scale (c, R) is a tuning parameter

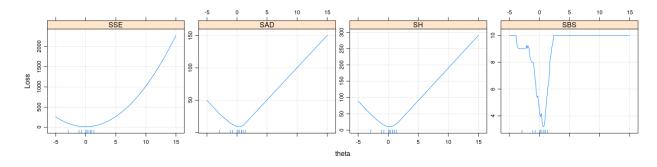
```
xx <- seq(-2, 2, 0.01)
c <- 1; R <- 1
psi <-
    data.frame(xx = xx,
                median = sign(xx),
                huber = ifelse(abs(xx) <= c, xx, c * sign(xx)),</pre>
                 tmean = ifelse(abs(xx) <= c, xx, 0),</pre>
                bisquare = xx * pmax(0, (1 - (xx/R)^2))^2)
xyplot(median + huber + tmean + bisquare ~ xx, psi, type = "l", outer = TRUE,
        ylab = expression(psi(x)), xlab = "x", grid = TRUE)
               mediar
                                       hube
                                                              tmean
   0.5
ψ(x)
   0.0
   -0.5
   -1.0
                                                     -2
                                                                ò
                                                    х
```

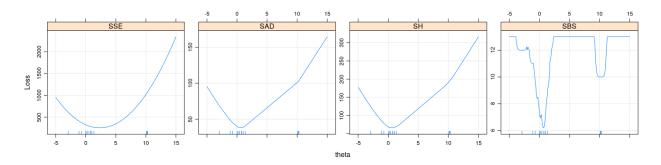
- The last two functions are examples of "redescending" influence functions
- Corresponding loss function  $\rho$  becomes flat beyond a threshold
- In effect, beyond this threshold, extreme observations are *completely discounted*
- In other words, they have zero/constant contribution to the total loss
- However, this does make the objective function (to be minimized) non-convex

• Let us see what the objective function looks like for various loss functions

```
huber.loss <- function(x, c = 1) ifelse(abs(x) < c, x<sup>2</sup>, c * (2 * abs(x) - c))
bisquare.loss <- function(x, R = 1) ifelse(abs(x) < R, R<sup>2</sup> * (1 - (1 - (x/R)<sup>2</sup>))<sup>3</sup>, R<sup>2</sup>)
x <- rnorm(10)
y <- c(x, 10.1, 10.2, 10.3) # add three extreme observations to x
t <- seq(-5, 15, 0.01)</pre>
```

#### Example: loss functions





• For non-convex loss functions, important to have good starting estimates

## Other practical considerations

- Tuning parameters are arbitrary
- Natural to express tuning parameter in terms of scale  $\sigma$  (unknown) scale invariance
- Common to take  $\hat{\sigma}$  to be a multiple of the median absolute deviation (MAD) from the median
- Tuning parameter can then be chosen to achieve some target asymptotic relative efficiency under normality
- For example, Huber loss function with  $c = 1.345\sigma$  would give 95% ARE if  $\sigma$  was known

## Standard errors

• M-estimators are consistent and asymptotically normal with variance  $\tau \sigma^2/n$ , where

$$\tau = \frac{E(\psi^2(X))}{[E(\psi'(X))]^2}$$

• Could be estimated by replacing X by fitted (standardized) residuals

$$\hat{\tau} = \frac{\frac{1}{n} \sum_{i} \psi^2(e_i/\hat{\sigma})}{[\frac{1}{n} \sum_{i} \psi'(e_i/\hat{\sigma})]^2}$$

• Not necessarily reliable in small samples

#### M-estimation for regression

- The ideas described above translate directly to linear regression
- Instead of minimizing least squared errors, minimize

$$\sum_{i=1}^{n} \rho(y_i - \mathbf{x}_i^T \beta)$$

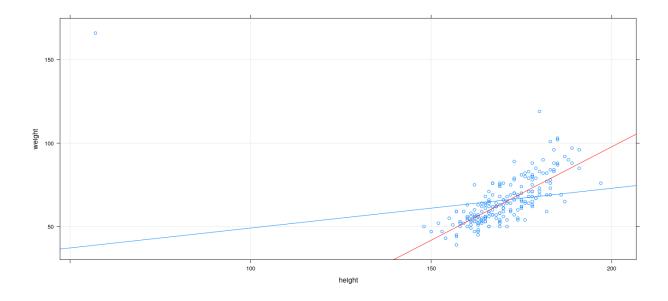
• Simple estimation approach: Iteratively (Re)Weighted Least Squares (IWLS / IRLS) with weights

$$w_i^{(t+1)} = \frac{\psi\left(y_i - \mathbf{x}_i^T \hat{\beta}^{(t)}\right)}{y_i - \mathbf{x}_i^T \hat{\beta}^{(t)}} = \frac{\psi(e_i^{(t)})}{e_i^{(t)}} > 0$$

- Implemented in the rlm() function (in the MASS package) among others
- By default, scale is estimated using MAD of residuals (updated for each iteration)

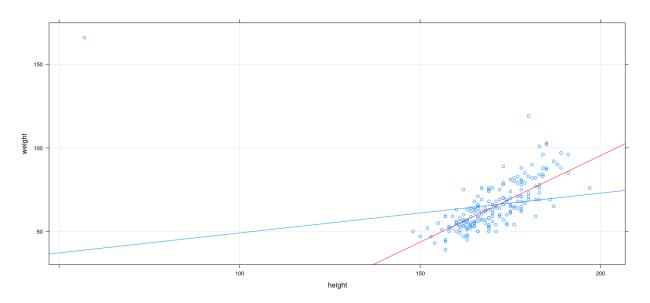
#### M-estimation example: Bisquare

library(MASS)
fm <- rlm(weight ~ height, data = Davis, psi = psi.bisquare)
xyplot(weight ~ height, Davis, type = c("p", "r"), grid = TRUE) + layer(panel.abline(fm, col = "red"))</pre>



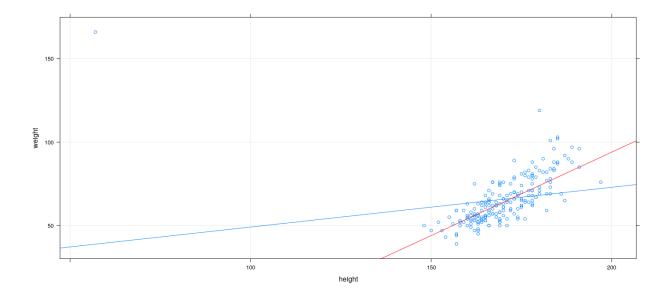
## M-estimation example: Huber

```
library(MASS)
fm <- rlm(weight ~ height, data = Davis, psi = psi.huber)
xyplot(weight ~ height, Davis, type = c("p", "r"), grid = TRUE) + layer(panel.abline(fm, col = "red"))</pre>
```



M-estimation example: Least absolute deviation (using optim())

```
L <- function(p) with(Davis, sum(abs(weight - p[1] - p[2] * height)))
bhat <- optim(coef(fm), L)$par
xyplot(weight ~ height, Davis, type = c("p", "r"), grid = TRUE) + layer(panel.abline(bhat, col = "red")</pre>
```



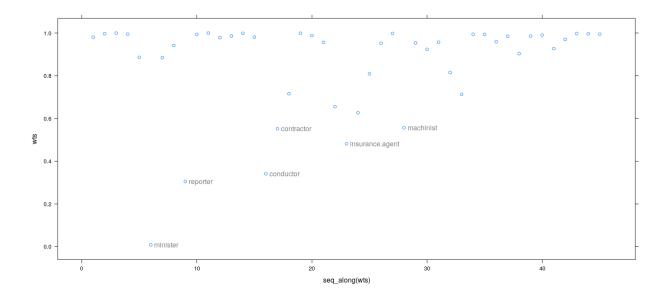
#### M-estimation example: multiple regression

```
fm1 <- lm(prestige ~ income + education, data = Duncan, na.action = na.exclude)</pre>
fm2 <- rlm(prestige ~ income + education, data = Duncan, psi = psi.bisquare, na.action = na.exclude)
fm3 <- rlm(prestige ~ income + education, data = Duncan, psi = psi.huber, na.action = na.exclude)
coefficients(summary(fm1))
              Estimate Std. Error
                                    t value
                                                Pr(>|t|)
(Intercept) -6.0646629 4.27194117 -1.419650 1.630896e-01
income
             0.5987328 0.11966735 5.003310 1.053184e-05
education
             0.5458339 0.09825264 5.555412 1.727192e-06
coefficients(summary(fm2))
                 Value Std. Error
                                    t value
(Intercept) -7.4121192 3.87702087 -1.911808
income
             0.7902166 0.10860468 7.276082
education
             0.4185775 0.08916966 4.694169
coefficients(summary(fm3))
                 Value Std. Error
                                    t value
(Intercept) -7.1107028 3.88131509 -1.832034
             0.7014493 0.10872497 6.451593
income
             0.4854390 0.08926842 5.437970
education
```

## M-estimation example: weights as diagnostics

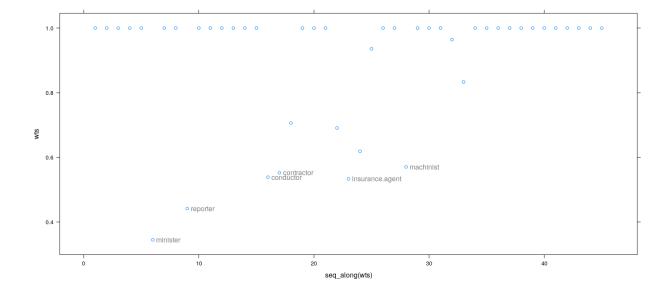
• IWLS weights give an alternative measure of influence

```
wts <- fm2$w # bisquare
id <- which(wts < 0.6)
xyplot(wts ~ seq_along(wts)) +
    layer(panel.text(x[id], y[id], labels = rownames(Duncan)[id], pos = 4, col = "grey50"))
```



• IWLS weights give an alternative measure of influence

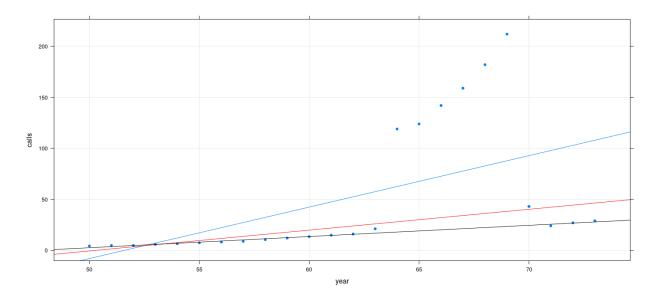
```
wts <- fm3$w # Huber
id <- which(wts < 0.6)
xyplot(wts ~ seq_along(wts)) +
    layer(panel.text(x[id], y[id], labels = rownames(Duncan)[id], pos = 4, col = "grey50"))
```



## Does M-estimation ensure high breakdown point?

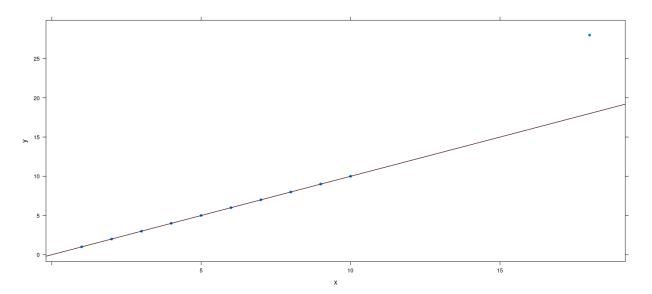
- Example: Number of phone calls (in millions) in Belgium
- Data available in the MASS package
- For 1964–1969, length of calls (in minutes) had been recorded instead of number

```
data(phones, package = "MASS")
fm2 <- rlm(calls ~ year, data = phones, psi = psi.huber, maxit = 100)
fm3 <- rlm(calls ~ year, data = phones, psi = psi.bisquare)
xyplot(calls ~ year, data = phones, grid = TRUE, type = c("p", "r"), pch = 16) +
layer(panel.abline(fm2, col = "red")) + layer(panel.abline(fm3, col = "black"))</pre>
```

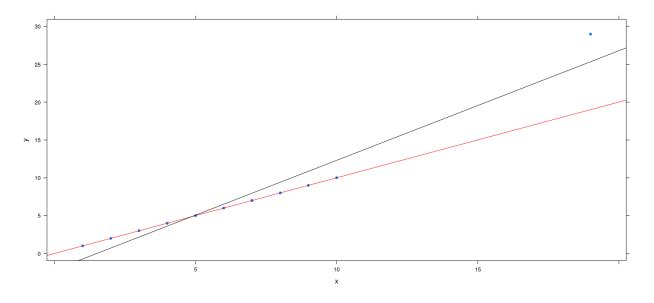


An artificial example

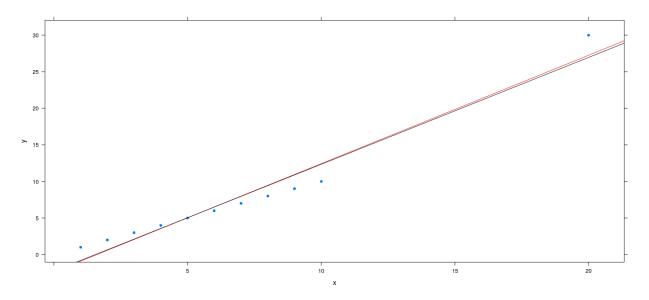
```
x <- c(1:10, 18)
y <- c(1:10, 18 + 10)
fm.h <- rlm(y ~ x, psi = psi.huber, maxit = 100)
fm.bs <- rlm(y ~ x, psi = psi.bisquare)
xyplot(y ~ x, pch = 16) + layer(panel.abline(fm.h, col = "red")) + layer(panel.abline(fm.bs, col = "bla
```



```
x <- c(1:10, 19)
y <- c(1:10, 19 + 10)
fm.h <- rlm(y ~ x, psi = psi.huber, maxit = 200)
fm.bs <- rlm(y ~ x, psi = psi.bisquare, maxit = 200)
xyplot(y ~ x, pch = 16) + layer(panel.abline(fm.h, col = "red")) + layer(panel.abline(fm.bs, col = "bla
```



x <- c(1:10, 20) y <- c(1:10, 20 + 10) fm.h <- rlm(y ~ x, psi = psi.huber, maxit = 100) fm.bs <- rlm(y ~ x, psi = psi.bisquare) xyplot(y ~ x, pch = 16) + layer(panel.abline(fm.h, col = "red")) + layer(panel.abline(fm.bs, col = "bla



## Why does this happen?

- M-estimation approach can ensure high breakdown point for univariate location estimation
- This is not automatically true for regression
- Increasing loss function (LAD, Huber): sufficiently high-leverage outlier can always attract optimum line
- Loss functions that flatten out (Bisquare): result depends on choice of c (which is estimated)
- In general, no guarantee that M-estimation approach has bounded influence in regression

#### **Resistant regression**

- Resistant alternatives exist, but are much more difficult to fit computationally
- We will mention two examples: LMS and LTS regression
- Least Median of Squares (LMS) regression: Find  $\hat{\beta}$  as

$$\arg\min_{\beta} \operatorname{median} \left\{ (y_i - \mathbf{x}_i^T \beta)^2; i = 1, \dots, n \right\}$$

- More generally, LQS minimizes some quantile of the squared errors
- Least Trimmed Squares (LTS) regression: Find  $\hat{\beta}$  as

$$\arg\min_{\beta} \sum_{i=1}^{q} (y_i - \mathbf{x}_i^T \beta)_{(i)}^2$$

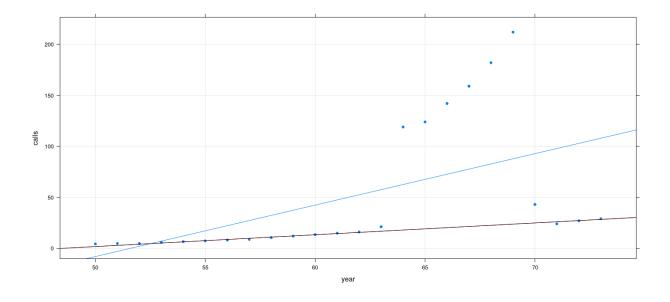
- Here the objective is the sum of the q smallest error terms
- The recommended value of q is  $\lfloor (n+p+1)/2 \rfloor$

#### Resistant regression: LMS and LTS

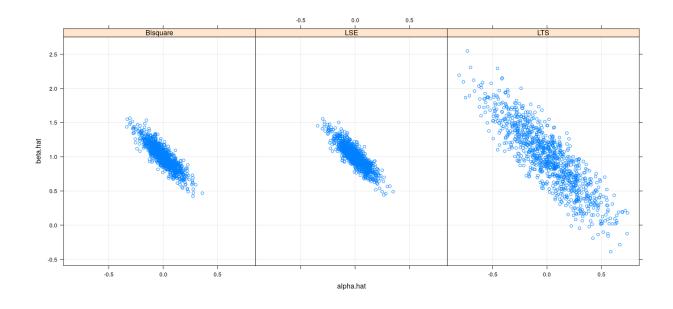
- Both LMS/LQS and LTS have high resistance (breakdown point) but low efficiency
- LMS/LQS has lower efficiency than LTS, and there is no reason to prefer LMS over LTS
- Computation of both are difficult
- The MASS package provides one implementation in lmsreg() and ltsreg()

## Example: Number of phone calls (in millions) in Belgium

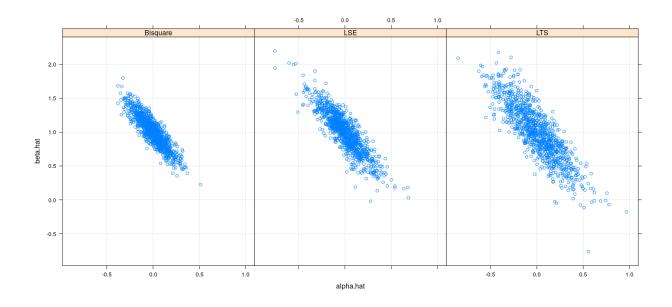
```
data(phones, package = "MASS")
fm2 <- lmsreg(calls ~ year, data = phones)
fm3 <- ltsreg(calls ~ year, data = phones)
xyplot(calls ~ year, data = phones, grid = TRUE, type = c("p", "r"), pch = 16) +
layer(panel.abline(fm2, col = "red")) + layer(panel.abline(fm3, col = "black"))</pre>
```



Efficiency comparison: simulation study (normal)



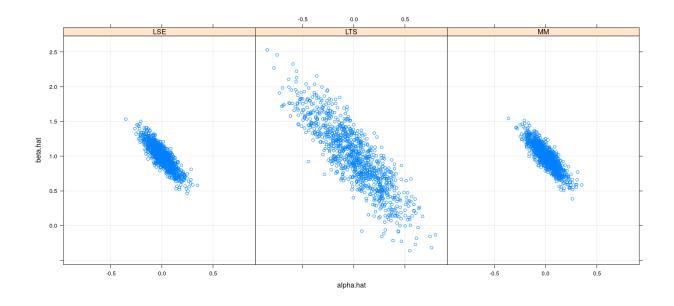
Efficiency comparison: simulation study  $(t_3)$ 



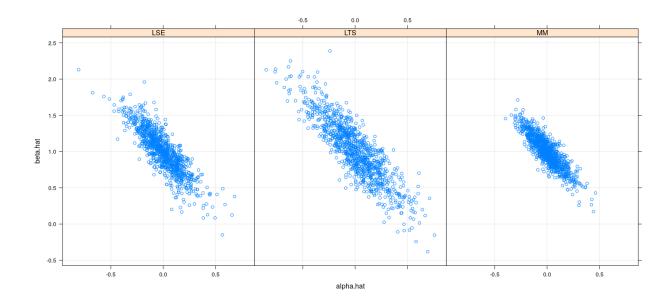
## **MM-estimation**

- M-estimation with Bisquare error has reasonable efficiency
- Should have high breakdown point if scale is "correctly" estimated
- High breakdown potentially fails if initial scale estimate is too high
- MM-estimation tries to ensure high breakdown point with high efficiency of Bisquare loss
- First step is to obtain a better scale estimate using S-estimation (will not discuss)
- This is followed by M-estimation with Bisquare loss function calibrated by estimated scale
- Implemented in rlm() with method = "MM"

#### Efficiency comparison: simulation study (normal)

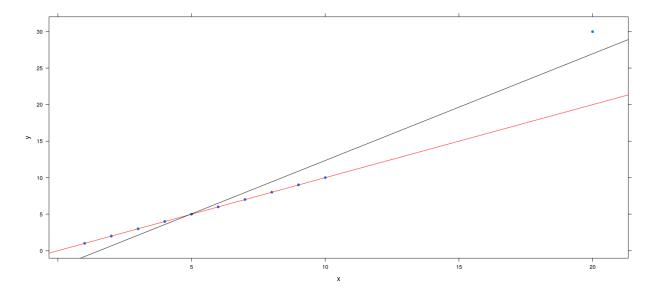


Efficiency comparison: simulation study  $(t_3)$ 



# Artificial example revisited

```
x <- c(1:10, 20)
y <- c(1:10 + rnorm(10, sd = 0.00001), 20 + 10)
fm.mm <- rlm(y ~ x, method = "MM")
fm.bs <- rlm(y ~ x, psi = psi.bisquare)
xyplot(y ~ x, pch = 16) + layer(panel.abline(fm.mm, col = "red")) + layer(panel.abline(fm.bs, col = "bl
```



# Software implementations in R

- The  ${\tt MASS}$  package implements basic robust regression approaches

• For more comprehensive implementations, see the Robust Statistical Methods Task View on CRAN