

STAT 593

Robustness and Linear Models

Joseph Salmon

<http://josephsalmon.eu>

Télécom Paristech, Institut Mines-Télécom
&
University of Washington, Department of Statistics
(Visiting Assistant Professor)

Outline

Least Absolute Deviation

Equivariance

Least Trimmed Squares (LTS)

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Least Absolute Deviation

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Reminder on (Ordinary) Least squares, (O)LS

Model:

$\mathbf{y} \approx X\boldsymbol{\beta}^*$ where $\mathbf{y} \in \mathbb{R}^n$, $X \in \mathbb{R}^{n \times p}$, $\boldsymbol{\beta}^* \in \mathbb{R}^p$ (true coefficient)

A least square estimator is any solution of the following problem:

$$\hat{\boldsymbol{\beta}} \in \arg \min_{\boldsymbol{\beta} \in \mathbb{R}^p} \frac{1}{2} \|\mathbf{y} - X\boldsymbol{\beta}\|_2^2 := f(\boldsymbol{\beta})$$

$$\hat{\boldsymbol{\beta}} \in \arg \min_{\boldsymbol{\beta} \in \mathbb{R}^p} \frac{1}{2} \sum_{i=1}^n [y_i - \langle x_i, \boldsymbol{\beta} \rangle]^2$$

Rem: Gaussian (-log)-likelihood leads to square formulation

Least Absolute Deviation (LAD)

$$\hat{\beta} \in \arg \min_{\beta \in \mathbb{R}^p} \|\mathbf{y} - X\beta\|_1 := f(\beta)$$

$$\hat{\beta} \in \arg \min_{\beta \in \mathbb{R}^p} \sum_{i=1}^n |y_i - \langle x_i, \beta \rangle|$$

Many properties, see [Bloomfield and Steiger \(1983\)](#) for instance for historical purpose

When $p = 1$, the estimator is

$$\hat{\beta} \in \arg \min_{\beta \in \mathbb{R}} \sum_{i=1}^n |y_i - x_i \beta|$$

and one can find a solution with zero residuals, i.e., $y_{i_0} = x_{i_0} \beta$

Proof

First, one can simplify the problems to cases without any $x_i = 0$ by noticing that

$$\sum_{i=1}^n |y_i - x_i \beta| \geq \sum_{i: x_i \neq 0} |y_i - x_i \beta| + \sum_{i: x_i = 0} |y_i|$$

Second, we assume “ab absurdum” that no solution achieves zero residuals. Ordering the slopes $\frac{y_1}{x_1} \leq \dots \leq \frac{y_n}{x_n}$ one can assume that

$\hat{\beta}$, a LAD solution satisfies: $\hat{i} \in [n]$ s.t. $\hat{\beta} \in \left(\frac{y_{\hat{i}}}{x_{\hat{i}}}, \frac{y_{\hat{i}+1}}{x_{\hat{i}+1}} \right)$

By Fermat's rule and hypothesis: $\sum_{i: \hat{\beta} > \frac{y_i}{x_i}} |x_i| = \sum_{i: \hat{\beta} < \frac{y_i}{x_i}} |x_i|$

One can check that $\tilde{\beta} = \frac{y_{\hat{i}}}{x_{\hat{i}}}$, also satisfies the first order condition:

$$\sum_{i: \tilde{\beta} > \frac{y_i}{x_i}} |x_i| - \sum_{i: \tilde{\beta} < \frac{y_i}{x_i}} |x_i| + |x_{\hat{i}}| = \sum_{i: \hat{\beta} > \frac{y_i}{x_i}} |x_i| - \sum_{i: \hat{\beta} < \frac{y_i}{x_i}} |x_i| = 0$$



LAD in any dimension

Theorem

There exist at least one solution $\hat{\beta}$ of the LAD for which $y_i = \langle x_i, \beta \rangle$ for at least $\text{rank}(X)$ indices.

LAD in any dimension

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Proof: this is provided in [Th.1, Bloomfield and Steiger \(1983\)](#). It works “ab absurdum”: then there exist δ s.t. $\langle \delta, x_i \rangle = 0$ for indices with $y_i = \langle x_i, \beta \rangle$ and $\langle \delta, x_i \rangle \neq 0$ for indices with $y_i \neq \langle x_i, \beta \rangle$, then the objective is

$$\sum_{i: y_i \neq \langle x_i, \beta \rangle} |y_i - \langle \beta, x_i \rangle - t \langle \delta, x_i \rangle|$$

for the point $\beta + t\delta$. With the previous lemma, one can create one more point that zeros the residual. This can be repeated except if one reaches $\text{rank}(X)$ indices.

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Regression equivariance

Let T be an estimator of β^* (regression coeff.) based on $Z = (X, \mathbf{y})$

Definition

We say that T is **regression equivariant** when for any dataset (\mathbf{y}, X) and any vector $v \in \mathbb{R}^p$, one has

$$T(X, \mathbf{y} + Xv) = T(X, \mathbf{y}) + v$$

Rem: a simple case is the OLS (full rank case)

$$(X^\top X)^{-1} X^\top (\mathbf{y} + Xv) = (X^\top X)^{-1} X^\top \mathbf{y} + v$$

Scale equivariance

Let T be an estimator of β^* (regression coeff.) based on $Z = (X, \mathbf{y})$

Definition

We say that T is **scale equivariant** when for any dataset (y, X) and any vector $c \in \mathbb{R}$, one has

$$T(X, c \cdot y) = c \cdot T(X, y)$$

Rem: a simple case is the OLS (full rank case)

$$(X^T X)^{-1} X^T (cy) = c(X^T X)^{-1} X^T y$$

Affine equivariance

Let T be an estimator of β^* (regression coeff.) based on $Z = (X, \mathbf{y})$

Definition

We say that T is **affine equivariant** when for any dataset (\mathbf{y}, X) and any non-singular matrix $A \in \mathbb{R}^{p \times p}$, one has

$$T(XA, \mathbf{y}) = A^{-1}T(X, \mathbf{y})$$

Rem: a simple case is the OLS (full rank case)

$$(A^T X^T X A)^{-1} (A^T X^T \mathbf{y}) = A^{-1} (X^T X)^{-1} X^T \mathbf{y}$$

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LTS Definition

Definition

For $h \in [n]$, the **Least Trimmed Squares** (LTS) estimator of order h is defined by

$$\hat{\beta} \in \arg \min_{\beta \in \mathbb{R}^p} \sum_{i=1}^h (r^2(\beta))_{i:n},$$

where the vector $r^2(\beta) = ((y_1 - \langle x_1, \beta \rangle)^2, \dots, (y_n - \langle x_n, \beta \rangle)^2)$ represent the square **residuals** and $(r^2(\beta))_{1:n} \leq \dots \leq (r^2(\beta))_{n:n}$ are the ordered statistics of the squared residuals

Rem: when $h < p$, LTS not uniquely defined

Rem: when $h = n$, LTS reduces to standard OLS

Alternative formulations

Set formulation: For $H \subset [n]$, we write

$$Q(H, \beta) = \|X_H \beta - \mathbf{y}_H\|^2 = \sum_{i \in H} (y_i - \langle \beta, x_i \rangle)^2 \quad \text{then}$$

$$(\hat{\beta}, \hat{H}) \in \underset{\substack{H \subset [n]: \#H=h \\ \beta \in \mathbb{R}^p}}{\arg \min} Q(H, \beta)$$

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Binary variables formulation:

$$(\hat{\beta}, \hat{w}) \in \underset{\substack{\beta \in \mathbb{R}^p \\ w \subset \mathbb{R}^n \\ \forall i \in [n], w_i \in \{0,1\} \\ \text{and } \sum_{i=1}^n w_i = h}}{\arg \min} \sum_{i=1}^n w_i (y_i - \langle \beta, x_i \rangle)^2$$

Rem: the later formulation is called a **Mixed Integer Programming** problem. Convex relaxation can be obtained by substituting $w_i \in [0, 1]$ to $w_i \in \{0, 1\}$, or optimization solver (like mosek, gurobi, etc.) can be considered.

Equivariance

Theorem

The LTS estimator is regression, scale and affine equivariant

Proof: consider the case where the data is $y + Xv$. Fix $H \in [n]$, as the optimal values in the LTS definition:

$$\hat{\beta} \in \arg \min_{\beta} \sum_{i \in H} (y_i + \langle v, x_i \rangle - \langle \beta, x_i \rangle)^2$$

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$$\begin{aligned}\hat{\beta} &\in \arg \min_{\beta} \sum_{i \in H} (y_i + \langle v, x_i \rangle - \langle \beta, x_i \rangle)^2 \\ &\in \arg \min_{\beta} \sum_{i \in H} (y_i - \langle \beta - v, x_i \rangle)^2\end{aligned}$$

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Breakdown point: Donoho's definition

Definition: Breakdown point

For a dataset $Z = (X, \mathbf{y})$ where $X \in \mathbb{R}^{n \times p}$ corresponds to the design matrix and $\mathbf{y} \in \mathbb{R}^n$ to the observation vector, the **breakdown point** of a statistic T is:

$$\varepsilon^* = \varepsilon^*(T, Z) = \frac{m^*}{n + m^*}$$

where

$$m^* = \min \left\{ m : \sup_{\#Z'=m} \|T(Z \cup Z') - T(Z)\| = +\infty \right\}$$

Rem: ε -replacement variants often considered, see proof in Rousseeuw and Leroy (1987)

Breakdown point^{1,2}

For simplicity we assume a classical full rank design assumption (so $p < n$).

Theorem

The breakdown point of any regression and permutation equivariant estimator is less than or equal to $\frac{n-p+1}{2n-p+1}$.

Rem: Asymptotically this is about a 50% breakdown point.

¹P. J. Rousseeuw and A. M. Leroy. *Robust regression and outlier detection*. Wiley Series in Probability and Mathematical Statistics: Applied Probability and Statistics. New York: John Wiley & Sons Inc., 1987, pp. xvi+329.

²D. L. Donoho. "Breakdown properties of multivariate location estimators". PhD thesis. Harvard University, 1982.

Proof

ab absurdum: assume $\exists B$ s.t.

$$\sup_{\#Z'=n-p+1} \|T(Z' \cup Z) - T(Z)\| < B$$

Up to a samples reordering, because $p - 1$ vectors extracted among the row of X are included in a hyperplane, $\exists \mu \in \mathbb{R}^p$, with $\mu \neq 0$, s.t. $\langle \mu, x_1 \rangle = \dots = \langle \mu, x_{p-1} \rangle = 0$.

Proof

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$$Z \cup Z' = \begin{pmatrix} x_1, & y_1 \\ \vdots & \vdots \\ x_{p-1}, & y_{p-1} \\ x_p, & y_p \\ \vdots & \vdots \\ x_n, & y_n \\ x_p, & y_p + \langle \mu, x_p \rangle \\ \vdots & \vdots \\ x_n, & y_n + \langle \mu, x_n \rangle \end{pmatrix}$$

Proof

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Proof (continued)

So by regression equivariance, reminding $Z = (X, \mathbf{y})$

$$T \begin{pmatrix} x_1, & y_1 + \langle \mu, x_1 \rangle \\ \vdots & \vdots \\ x_{p-1}, & y_{p-1} + \langle \mu, x_{p-1} \rangle \\ x_p, & y_p \\ \vdots & \vdots \\ x_n, & y_n \\ x_p, & y_p + \langle \mu, x_p \rangle \\ \vdots & \vdots \\ x_n, & y_n + \langle \mu, x_n \rangle \end{pmatrix} = T \begin{pmatrix} x_1, & y_1 \\ \vdots & \vdots \\ x_{p-1}, & y_{p-1} \\ x_p, & y_p - \langle \mu, x_p \rangle \\ \vdots & \vdots \\ x_n, & y_n - \langle \mu, x_n \rangle \\ x_p, & y_p \\ \vdots & \vdots \\ x_n, & y_n \end{pmatrix} + \mu$$

and then $T(Z \cup Z') = T(Z \cup Z'') + \mu$ for another dataset Z'' of size $n - p + 1$

Proof ending

By hypothesis: $\|T(Z \cup Z') - T(Z)\| \leq B$, but now one has also
$$\|T(Z \cup Z') - T(Z)\| = \|T(Z \cup Z'') + \mu - T(Z)\|$$

But Z'' being of size $n - p + 1$, then one has :
$$\|T(Z \cup Z'') - T(Z)\| \leq B$$

Since $\|\mu\|$ can be made arbitrarily large, leading to a contradiction.

Breakdown point^{3,4}

Theorem

The (ε -contamination) breakdown point of the LTS is $\frac{h}{n+h}$. When $h = n - p + 1$, this reaches the largest bound for regression equivariant estimators, i.e., $\frac{n-p+1}{2n-p+1}$

Rem: when n is large w.r.t. to p this is approximately 50%

³P. J. Rousseeuw and A. M. Leroy. *Robust regression and outlier detection*. Wiley Series in Probability and Mathematical Statistics: Applied Probability and Statistics. New York: John Wiley & Sons Inc., 1987, pp. xvi+329.

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Proof

Let $Z' = Z \cup \tilde{Z}$ the dataset, where one has added the h corrupted elements $(\tilde{x}_1, \tilde{y}_1), \dots, (\tilde{x}_h, \tilde{y}_h)$ (pick $h = n - p + 1$ to reach optimum)

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To simplify the proof, we prove the lower bound for the Ridge version of the LTS estimator only:

$$(\hat{\beta}, \hat{H}) = \arg \min_{\beta \in \mathbb{R}^p, H: \#H=h} Q(H, \beta) + \lambda \|\beta\|^2$$

$$\text{where } Q(H, \beta) = \|X'_H \beta - \mathbf{y}'_H\|^2 = \sum_{i \in H} (y'_i - \langle \beta, x'_i \rangle)^2$$

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$$Q(H^*, 0) = \min_{H: \#H=h} Q(H, 0) = \sum_{i=1}^h y_{i:n}^2 \leq h \|y\|_\infty$$

Proof continued

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$$Q(H^*, 0) = \min_{H: \#H=h} Q(H, 0) = \sum_{i=1}^h y_{i:n}^2 \leq h \|y\|_\infty$$

Assume that $\|\beta\|^2 \geq \frac{1+h\|y\|_\infty}{\lambda}$, then

$$\min_{H: \#H=h} Q(H, \beta) + \lambda \|\beta\|^2 \geq \lambda \|\beta\|^2 \geq \lambda \frac{1+h\|y\|_\infty}{\lambda} > Q(H^*, 0)$$

Proof continued

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$$\min_{H: \#H=h} Q(H, \beta) + \lambda \|\beta\|^2 \geq \lambda \|\beta\|^2 \geq \lambda \frac{1+h\|y\|_\infty}{\lambda} > Q(H^*, 0)$$

Now since $\min_{\beta, H: \#H=h} Q(H, \beta) \leq Q(H^*, 0)$, one needs to have

$\|\hat{\beta}\|^2 \leq \frac{1+h\|y\|_\infty}{\lambda}$, a bound that does not depend on the \tilde{x}_i, \tilde{y}_i \square

Optimization for LTS : Mixed Integer Programming

Generic approach; requires fast solvers like gurobi, mosek, cplex, etc.

Ingredients:

- ▶ Convex relaxation : convexify the binary constraints

$$P = \min_{\substack{\beta \in \mathbb{R}^p \\ w \subset \mathbb{R}^n \\ \forall i \in [n], w_i \in \{0,1\} \\ \text{and } \sum_{i=1}^n w_i = h}} \sum_{i=1}^n w_i (y_i - \langle \beta, x_i \rangle)^2$$

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Rem: $P^{\text{cvx}} \leq P$ (lower bound on the optimal value)

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Branch and bound

Otherwise: “branch and bound”, $\exists i_0 \in [n]$ such that $w_{i_0} \in]0, 1[$ so solve two MIP problems:

$$P_l = \min_{\substack{\beta \in \mathbb{R}^p \\ w \subset \mathbb{R}^n \\ \forall i \in [n], w_i \in \{0, 1\} \\ \sum_{i=1}^n w_i = h \\ w_{i_0} = 0}} \sum_{i=1}^n w_i (y_i - \langle \beta, x_i \rangle)^2 \quad \left| \quad P_r = \min_{\substack{\beta \in \mathbb{R}^p \\ w \subset \mathbb{R}^n \\ \forall i \in [n], w_i \in \{0, 1\} \\ \sum_{i=1}^n w_i = h \\ w_{i_0} = 1}} \sum_{i=1}^n w_i (y_i - \langle \beta, x_i \rangle)^2$$

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Now one has $P = \min(P_l, P_r)$, and one can solve recursively the problems P_r and P_l by proceeding similarly (use a **search tree**, and in general no need to solve the 2^n sub-problems)

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Rem: other useful bounds are $P^{\text{cvx}} \leq \min(P_l^{\text{cvx}}, P_r^{\text{cvx}}) \leq P$

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Rem: other useful bounds are $P^{\text{cvx}} \leq \min(P_l^{\text{cvx}}, P_r^{\text{cvx}}) \leq P$

Rem: upper bounds can be obtained by finding feasible points (e.g., rounding)

Fast LTS

Simple alternative: iterative procedure Rousseeuw and Van Driessen(2006)

Algorithm: FAST LTS

input : h , max. iterations t_{\max} , stopping criterion ε

init : H^0, β^0

for $1 \leq t \leq t_{\max}$ **do**

Break if stopping criterion smaller than ε

$$H^{t+1} \leftarrow \arg \min_{H: \#H=h} \|X_H \beta^t - \mathbf{y}_H\|^2$$

$$\beta^{t+1} \leftarrow \arg \min_{\beta} \|X_{H^{t+1}} \beta - \mathbf{y}_{H^{t+1}}\|^2$$

return β^t, H^t

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Simple alternative: iterative procedure [Rousseeuw and Van Driessen\(2006\)](#)

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return β^t, H^t

Rem: $Q(H^{t+1}, \beta^{t+1}) \leq Q(H^{t+1}, \beta^t) \leq Q(H^t, \beta^t)$

Another simpler alternative : Fast LTS

- ▶ the update

$$H^{t+1} \leftarrow \arg \min_{H: \#H=h} \left\| X_H \beta^t - \mathbf{y}_H \right\|^2$$

can be obtained in a closed form by sorting; cost = $O(n \log(n))$ or less if h is small (use: `np.partition` in `numpy`)

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can be obtained in a closed form by sorting; cost = $O(n \log(n))$ or less if h is small (use: `np.partition` in `numpy`)

- ▶ inner solver needed for the second update:

$$\beta^{t+1} \leftarrow \arg \min_{\beta} \|X_{H^{t+1}} \beta - \mathbf{y}_{H^{t+1}}\|^2$$

A second stopping criteria is then needed; possibly do not solve too precisely the problem at each step

Another simpler alternative : Fast LTS

- ▶ the update

$$H^{t+1} \leftarrow \arg \min_{H:\#H=h} \|X_H \beta^t - \mathbf{y}_H\|^2$$

can be obtained in a closed form by sorting; cost=
 $O(n \log(n))$ or less if h is small (use: `np.partition` in
`numpy`)

- ▶ inner solver needed for the second update:

$$\beta^{t+1} \leftarrow \arg \min_{\beta} \|X_{H^{t+1}} \beta - \mathbf{y}_{H^{t+1}}\|^2$$

A second stopping criteria is then needed; possibly do not
solve too precisely the problem at each step

- ▶ initialization is tricky (e.g., similar to K-means issues), might
use several initialization

Summary on optimizing LTS

2 directions:

- ▶ Mixed Integer Programming
 - ▶ pros: bounds / certificate for optimality
 - ▶ cons: more complex to implement, need of specific solvers
- ▶ Alternate minimization
 - ▶ pros: simple to implement
 - ▶ cons: initialization, no guarantee (only convergence to local minimum)

Rem: hybrid method could be useful, as MIP can benefit from a nicer initialization (through nicer upper bounds)

Rem: “continuation” method can also be proposed, *i.e.*, start by small h (fast to solve) and then increase h progressively

LTS extensions through regularization⁵

Adapt to high dimensional constraints using regularization:

$$(\hat{\beta}, \hat{H}) \in \underset{\substack{H \subset [n]: \#H=h \\ \beta \in \mathbb{R}^p}}{\arg \min} Q(H, \beta) + h\lambda \text{pen}(\beta)$$

where $Q(H, \beta) = \|X_H \beta - \mathbf{y}_H\|^2 = \sum_{i \in H} (y_i - \langle \beta, x_i \rangle)^2$

- ▶ Ridge penalty (as seen earlier): $\text{pen}(\beta) = \|\beta\|^2$
- ▶ Lasso penalty for sparsity enforcing: $\text{pen}(\beta) = \|\beta\|_1$
- ▶ etc.

Rem: such approaches loose regression equivariance by enforcing specific constraints on the targeted solution (e.g., sparsity)

⁵A. Alfons, C. Croux, and S. Gelper. "Sparse least trimmed squares regression for analyzing high-dimensional large data sets". In: *Ann. Appl. Stat.* 7.1 (2013), pp. 226–248.

References and supplementary material

- ▶ For extensions to joint estimation of β and noise level σ cf. Ch. 6, Maronna *et al.* (2006)

Example : consider for $\hat{\beta}$ being the LTS

$$\hat{\sigma} = \frac{1}{h} \sum_{i=1}^h (r^2(\hat{\beta}))_{i:n},$$

- ▶ Heteroscedastic models (case where the noise level differs for each observations) Ch. 6, Maronna *et al.* (2006)
- ▶ branch and bound:
<https://web.stanford.edu/class/ee392o/bb.pdf>

References I

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- ▶ Maronna, R. A., R. D. Martin, and V. J. Yohai. *Robust statistics: Theory and methods*. Chichester: John Wiley & Sons, 2006.
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