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Bachelor's thesis

Probabilistic algorithms for computing the LTS estimate

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THANKS to everybody

Declaration

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Abstrakt

V několika větách shrňte obsah a přínos této práce v českém jazyce.

Klíčová slova LTS odhad, lineÃąrnÃŋ regrese, optimalizace, nejmenÅąÃŋ usekanÃľ ÄŊtvrece, metoda nejmenÅąÃŋch ÄŊtvercÅŕ, outliers

Abstract

The least trimmed squares (LTS) method is a robust version of the classical method of least squares used to find an estimate of coefficients in the linear regression model. Computing the LTS estimate is known to be NP-hard, and hence suboptimal probabilistic algorithms are used in practice.

Keywords LTS, linear regressin, robust estimator, least trimmed squares, ordinary least squares, outliers, outliers detection

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Chapter **3**

Algorithms

3.1 FAST-LTS

In this section we will introduce FAST-LTS algorithm[1]. It is, as well as in other cases, iterative algorithm. We will discuss all main components of the algorithm starting with its core idea called concentration step which authors simply call C-step.

3.1.1 C-step

We will show that from existing LTS estimate $\hat{\boldsymbol{w}}_{\boldsymbol{old}}$ we can construct new LTS estimate $\hat{\boldsymbol{w}}_{\boldsymbol{new}}$ which objective function is less or equal to the old one. Based on this property we will be able to create sequence of LTS estimates which will lead to better results.

Theorem 1. Consider dataset consisting of $\boldsymbol{x_1}, \boldsymbol{x_2} \ldots, \boldsymbol{x_n}$ explanatory variables where $\boldsymbol{x_i} \in \mathbb{R}^p, \forall \boldsymbol{x_i} = (x_1^i, x_2^i, \ldots, x_p^i)$ where $x_1^i = 1$ and its corresponding $y_1, y_2, \ldots, y_n$ response variables. Let's also have $\hat{\boldsymbol{w}}_{\boldsymbol{0}} \in \mathbb{R}^p$ any p-dimensional vector and $H_0 = \{h_i; h_i \in \mathbb{Z}, 1 \leq h_i \leq n\}, |H_0| = h$. Let's now mark $RSS(\hat{\boldsymbol{w}}_{\boldsymbol{0}}) = \sum_{i \in H_0} (r_0(i))^2$ where $r_0(i) = y_i - (w_1^0 x_1^i + w_2^0 x_2^i + \ldots + w_p^0 x_p^i)$. Let's take $\hat{n} = \{1, 2, \ldots, n\}$ and mark $\pi : \hat{n} \to \hat{n}$ permutation of $\hat{n}$ such that $|r_0(\pi(1))| \leq |r_0(\pi(2))| \leq \ldots \leq |r_0(\pi(n))|$ and mark $H_1 = \{\pi(1), \pi(2), \ldots \pi(h)\}$ set of h indexes corresponding to h smallest absolute residuals $r_0(i)$. Finally take $\hat{\boldsymbol{w}}_{\boldsymbol{1}}^{\boldsymbol{OLS(H_1)}}$ ordinary least squares fit on H_1 subset of observations and its corresponding $RSS(\hat{\boldsymbol{w}}_{\boldsymbol{1}}) = \sum_{i \in H_1} (r_1(i))^2$ sum of least squares. Then

$$RSS(\hat{\boldsymbol{w}}_{\boldsymbol{1}}) \leq RSS(\hat{\boldsymbol{w}}_{\boldsymbol{0}}) \tag{3.1}$$

Proof. Because we take h observations with smallest absolute residuals r_0, then for sure $\sum_{i \in H_1} (r_0(i))^2 \leq \sum_{i \in H_0} (r_0(i))^2 = RSS(\hat{\boldsymbol{w}}_{\boldsymbol{0}})$. When we take into account that Ordinary least squares fit OLS_{H_1} minimize objective function of H_1 subset of observations, then for sure $RSS(\hat{\boldsymbol{w}}_{\boldsymbol{1}}) = \sum_{i \in H_1} (r_1(i))^2 \leq$

$\sum_{i \in H_1}(r_0(i))^2$. Together we get

$$RSS(\boldsymbol{\hat{w}_1}) = \sum_{i \in H_1}(r_1(i))^2 \leq \sum_{i \in H_1}(r_0(i))^2 \leq \sum_{i \in H_0}(r_0(i))^2 = RSS(\boldsymbol{\hat{w}_0})$$

$\square$

Corollary 2. Based on previous theorem, using some $\boldsymbol{\hat{w}^{OLS(H_{old})}}$ on H_{old} subset of observations we can construct H_new subset with corresponding $\boldsymbol{\hat{w}^{OLS(H_{new})}}$ such that $RSS(\boldsymbol{\hat{w}^{OLS(H_{new})}}) \leq RSS(\boldsymbol{\hat{w}^{OLS(H_{old})}})$. With this we can apply above theorem again on $\boldsymbol{\hat{w}^{OLS(H_{new})}}$ with H_{new}. This will lead to the iterative sequence of $RSS(\boldsymbol{\hat{w}_{old}}) \leq RSS(\boldsymbol{\hat{w}_{new}}) \leq \ldots$. One step of this process is described by following pseudocode. Note that for C-step we actually need only $\boldsymbol{\hat{w}}$ without need of passing H.

Algorithm 1: C-step

```
Input: dataset consiting of X ∈ ℝ^{n×p} and y ∈ ℝ^{n×1}, ŵ_old ∈ ℝ^{p×1}
Output: ŵ_new, H_new
R ← ∅;
for i ← 1 to n do
 |  R ← R ∪ {|y_i − ŵ_old x_i^T|};
end
H_new ← select set of h smallest absolute residuals from R;
ŵ_new ← OLS(H_new);
return ŵ_new , H_new;
```

Observation 3. Time complexity of algorithm C-step 1 is same as time complexity as OLS. Thus $O(p^2n)$ ***TODO***

Lemma 4. Time complexity of OLS on $\boldsymbol{X}^{n \times p}$ and $\boldsymbol{Y}^{n \times 1}$ is $O(p^2n)$.

Proof. Normal equation of OLS is $\boldsymbol{\hat{w}} = (\boldsymbol{X^T X})^{-1}\boldsymbol{X^T Y}$. Time complexity of matrix multiplication $\boldsymbol{A}^{m \times n}$ and $\boldsymbol{B}^{n \times p}$ is $\sim \mathcal{O}(mnp)$. Time complexity of matrix $\boldsymbol{C}^{m \times m}$ is $\sim \mathcal{O}(m^3)$ So we need to compute $\boldsymbol{A} = \boldsymbol{X^T X} \sim \mathcal{O}(p^2n)$ and $\boldsymbol{B} = \boldsymbol{X^T Y} \sim \mathcal{O}(pn)$ and $\boldsymbol{C} = \boldsymbol{A}^{-1} \sim \mathcal{O}(p^3)$ and finally $\boldsymbol{CB} \sim \mathcal{O}(p^2)$. That give us $\mathcal{O}(p^2n + pn + p^3 + p^2)$. Because $\mathcal{O}(p^2n)$ and $\mathcal{O}(p^3)$ asymptotically dominates over $\mathcal{O}(p^2)$ and $\mathcal{O}(pn)$ we can write $\mathcal{O}(p^2n + p^3)$.

TODO CO zo toho je vic? Neni casove narocnejsi vynasobeni $\boldsymbol{X^T X}$ nez inverze, kdyz bereme v uvahu $n >> p$??? $\square$

Proof. In C-step we must compute n absolute residuals. Computation of one absolute residual consist of matrix multiplication of shapes $\times p$ and $pt \times 1$ that give us $\mathcal{O}(p)$. Rest is in constant time. So time of computation n residuals is $\mathcal{O}(np)$. Next we must select set of h smallest residuals which can be done in $\mathcal{O}(n)$ using modification of algorithm QuickSelect. reference: ***TODO*** Finally we must compute $\hat{w}$ OLS estimate on h subset of data. Because h is linearly dependent on n, we can say that it is $\mathcal{O}(p^2n + p^3)$ which is asymptotically dominant against previous steps which are $\mathcal{O}(np + n)$. $\square$

As ve stated above, repeating algorithm C-step will lead to sequence of $\boldsymbol{\hat{w}_1}, \boldsymbol{\hat{w}_2} \dots$ on subsets $H_1, H_2 \dots$ with corresponding residual sum of squares $RSS(\boldsymbol{\hat{w}_1}) \geq RSS(\boldsymbol{\hat{w}_2}) \geq \dots$. One could ask if this sequence will converge, so that $RSS(\boldsymbol{\hat{w}_i}) == RSS(\boldsymbol{\hat{w}_{i+1}})$. Answer to this question will be answered by the following theorem.

Theorem 5. Sequence of C-step will converge to $\boldsymbol{\hat{w}_m}$ after maximum of $m = \binom{n}{h}$ so that $RSS(\boldsymbol{\hat{w}_m}) == RSS(\boldsymbol{\hat{w}_n}), \forall n \geq m$ where n is number of data samples and h is size of subset H_i.

Proof. Since the $RSS(\boldsymbol{\hat{w}_i})$ is non-negative and $RSS(\boldsymbol{\hat{w}_i}) \leq RSS(\boldsymbol{\hat{w}_{i+i}})$ the sequence will converge. $\boldsymbol{\hat{w}_i}$ is computed out of subset $H_i \subset 1, 2, \dots, n$. When there are finite number of subsets of size h out of n samples, namely $\binom{n}{h}$, the sequence will converge at the latest after this number of steps. $\square$

Above theorem gives us clue to create algorithm described by following pseudocode.

Algorithm 2: Repeat-C-step

Input: dataset consiting of $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ and $\boldsymbol{y} \in \mathbb{R}^{n \times 1}$, $\boldsymbol{\hat{w}_{old}} \in \mathbb{R}^{p \times 1}$, H_0
Output: $\boldsymbol{\hat{w}_{final}}$, H_{final}

$\boldsymbol{\hat{w}_{new}} \leftarrow \emptyset$;
$H_{new} \leftarrow \emptyset$;
$RSS_{new} \leftarrow \infty$;
while $True$ **do**
  $RSS_{old} \leftarrow RSS(\boldsymbol{\hat{w}_{old}})$;
  $\boldsymbol{\hat{w}_{new}}, H_{new} \leftarrow \boldsymbol{X}, \boldsymbol{y}, \boldsymbol{\hat{w}_{old}}$;
  $RSS_{new} \leftarrow RSS(\boldsymbol{\hat{w}_{new}})$;
  if $RSS_{old} == RSS_{new}$ **then**
    break
  end
  $\boldsymbol{\hat{w}_{old}} \leftarrow \boldsymbol{\hat{w}_{new}}$
end
return $\boldsymbol{\hat{w}_{new}}$, H_{new};

It is important to note, that although maximum number of steps of this algorithm is $\binom{n}{h}$ in practice it is very low, most often under 20 steps. ***TODO*** nejaky hezky grafik ktery to ukazuje.... That is not enough for algorithm $Repeat{-}C{-}step$ to converge to global minimum, but it is necessary condition. That gives us, as stated in [1]

$$Chooselotofinitialsubsets H_1 andoneachofthemapplyalgorithmRepeat-C-step.Fromallconvergedsu \tag{3.2}$$

Before we can construct final algorithm we must decide how to choose initial subset H_1 and how many of them means "*lot of*". Let's focus first on how to choose initial subset H_1.

3.1.2 Choosing initial H_1subset

We have couple of different options.

Random

Not random

Input: A finite set $A = \{a_1, a_2, \ldots, a_n\}$ of integers
Output: The largest element in the set

$max \leftarrow a_1$
for $i \leftarrow 2$ ***to*** n **do**
    if $a_i > max$ **then**
        $max \leftarrow a_i$
    end
end
return max

Algorithm 8 is a greedy change-making algorithm (Slide 19 in Class Slides).

Input: A set $C = \{c_1, c_2, \ldots, c_r\}$ of denominations of coins, where $c_i > c_2 > \ldots > c_r$ and a positive number n
Output: A list of coins $d_1, d_2, \ldots, d_k$, such that $\sum_{i=1}^{k} d_i = n$ and k is minimized

$C \leftarrow \emptyset$
for $i \leftarrow 1$ ***to*** r **do**
    while $n \geq c_i$ **do**
        $C \leftarrow C \cup \{c_i\}$
        $n \leftarrow n - c_i$
    end
end
return C

Algorithm 14 and Algorithm 13 will find the first duplicate element in a sequence of integers.

In this section we will describe FAST-LTS algorithm and its main properties. The main idea of this algorithm is based on the fact that from one approximation of the algorithm we can compute another which can have lower

Input: A sequence of integers $\langle a_1, a_2, \ldots, a_n \rangle$
Output: The index of first location witht he same value as in a previous location in the sequence

$location \leftarrow 0$
$i \leftarrow 2$
while $i \leq n$ ***and*** $location = 0$ **do**
    $j \leftarrow 1$
    while $j < i$ ***and*** $location = 0$ **do**
        if $a_i = a_j$ **then**
            $location \leftarrow i$
        else
            $j \leftarrow j + 1$
        end
    end
    $i \leftarrow i + 1$
end
return *location*

Input: A sequence of integers $\langle a_1, a_2, \ldots, a_n \rangle$
Output: The index of first location witht he same value as in a previous location in the sequence

$location \leftarrow 0$
$i \leftarrow 2$
while $i \leq n \wedge location = 0$ **do**
    $j \leftarrow 1$
    while $j < i \wedge location = 0$ **do**
        if $a_i = a_j$ **then** $location \leftarrow i$

        else $j \leftarrow j + 1$

    end
    $i \leftarrow i + 1$
end
return *location*

objective function. TA DAAAAAAAAAAAAAAAAAA Theorem 1: [2] Let w0 ... wp be the LTS estimate. for each data sample we can compute —y-wx—

3.2 Exact algorithm

3.3 Feasible solution

3.4 MMEA

3.5 Branch and bound

3.6 Adding row

Chapter 4

Experiments

4.1 Data

4.2 Results

4.3 Outlier detection

Conclusion

Bibliography

[1] Rousseeuw, P. J.; Driessen, K. V. An Algorithm for Positive-Breakdown Regression Based on Concentration Steps. In *Data Analysis: Scientific Modeling and Practical Application*, edited by M. S. W. Gaul, O. Opitz, Springer-Verlag Berlin Heidelberg, 2000, pp. 335–346.

[2] Rybicka, J. *LaTeX pro začátečníky*. Brno: Konvoj, third edition, ISBN 80-7302-049-1.

Appendix A

Datasets

GUI Graphical user interface

XML Extensible markup language

Appendix B

Contents of enclosed CD

```
readme.txt ....................... the file with CD contents description
exe ................................... the directory with executables
src ....................................the directory of source codes
  wbdcm .................................... implementation sources
  thesis .............the directory of LaTeX source codes of the thesis
text ....................................... the thesis text directory
  thesis.pdf ..........................the thesis text in PDF format
  thesis.ps ............................the thesis text in PS format
```