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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 $H_0 = \{h_i; h_i \in \mathbb{Z}, 1 \le h_i \le n\}, |H_0| = h$. 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 $|r_0(\pi(1))| \le |r_0(\pi(2))| \le \ldots \le |r_0(\pi(n))|$ 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

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

Proof. Because we take h observations with smallest absolute residuals r_0, then for sure $\sum_{i \in H_1} (r_0(i))^2 \le \sum_{i \in H_0} (r_0(i))^2 = RSS(\hat{\boldsymbol{w}}_{\boldsymbol{0}})$. 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 $RSS(\hat{\boldsymbol{w}}_{\boldsymbol{1}}) = \sum_{i \in H_1} (r_1(i))^2 \le$

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

$$RSS(\hat{\boldsymbol{w}}_{\boldsymbol{1}}) = \sum_{i\in H_1}(r_1(i))^2 \leq \sum_{i\in H_1}(r_0(i))^2 \leq \sum_{i\in H_0}(r_0(i))^2 = RSS(\hat{\boldsymbol{w}}_{\boldsymbol{0}})$$

□

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

Algorithm 1: C-step

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

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, time complexity can be stated as follows. $\boldsymbol{A} = \boldsymbol{X^T X} \sim \mathcal{O}(p^2n)$ and $\boldsymbol{B} = \boldsymbol{X^T Y} \sim \mathcal{O}(pn)$ and $\boldsymbol{A}^{-1}\boldsymbol{B} \sim \mathcal{O}(p^3 + p^2)$. That give us $\mathcal{O}p^2n + pn + p^3 + p^2n$ which asymptotically dominates previous steps which time complexity is $\mathcal{O}(np + n)$.
TODO neni tedy casove narocnejsi vynasobeni $\boldsymbol{X^T X}$ nez inverze, kdyz bereme v uvahu $n >> p$??? □

Observation 4.

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

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

```
Input: A finite set A = {a_1, a_2, ..., a_n} of integers
Output: The largest element in the set
max ← a_1
for i ← 2 to n do
    if a_i > max then
        max ← a_i
    end
end
return max
```

```
Input: A set C = {c_1, c_2, ..., c_r} of denominations of coins, where
       c_i > c_2 > ... > c_r and a positive number n
Output: A list of coins d_1, d_2, ..., d_k, such that ∑_{i=1}^{k} d_i = n and k is
        minimized
C ← ∅
for i ← 1 to r do
    while n ≥ c_i do
        C ← C ∪ {c_i}
        n ← n − c_i
    end
end
return C
```

```
Input: A sequence of integers ⟨a_1, a_2, ..., a_n⟩
Output: The index of first location witht he same value as in a
        previous location in the sequence
location ← 0
i ← 2
while i ≤ n and location = 0 do
    j ← 1
    while j < i and location = 0 do
        if a_i = a_j then
            location ← i
        else
            j ← j + 1
        end
    end
    i ← 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 ← 0
i ← 2
while i ≤ n ∧ location = 0 do
    j ← 1
    while j < i ∧ location = 0 do
        if a_i = a_j then  location ← i

        else  j ← j + 1

    end
    i ← i + 1
end
return location
```

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 objective function. TA DAAAAAAAAAAAAAAAAA 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
```